



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:53 am BST

PDB ID : 1M1K  
Title : Co-crystal structure of azithromycin 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 : 2002-06-19  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

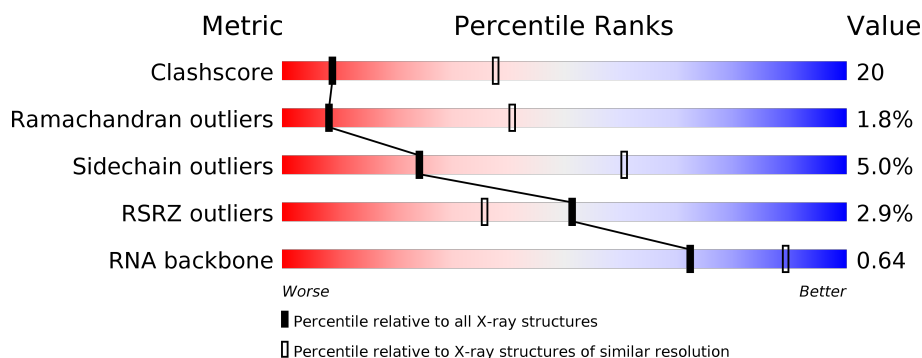
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>51%</span> <span>36%</span> <span>7% • 6%</span> </div> </div>
2	B	122	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>5%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>43%</span> <span>42%</span> <span>9% 6%</span> </div> </div>
3	C	239	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>4%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>52%</span> <span>42%</span> <span>5% •</span> </div> </div>
4	D	337	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>51%</span> <span>43%</span> <span>6%</span> </div> </div>
5	E	246	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>61%</span> <span>34%</span> <span>6%</span> </div> </div>
6	F	176	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>24%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>20%</span> <span>49%</span> <span>9% • 20%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	A	8024	-	-	-	X
32	MG	A	8066	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8329	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8354	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	A	8385	-	-	-	X
34	NA	J	8322	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	A	8513	-	-	X	-
35	CL	A	8515	-	-	-	X
35	CL	K	8502	-	-	X	-
35	CL	N	8518	-	-	X	-
35	CL	O	8507	-	-	X	X
35	CL	R	8511	-	-	-	X

## 2 Entry composition

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	GB 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			

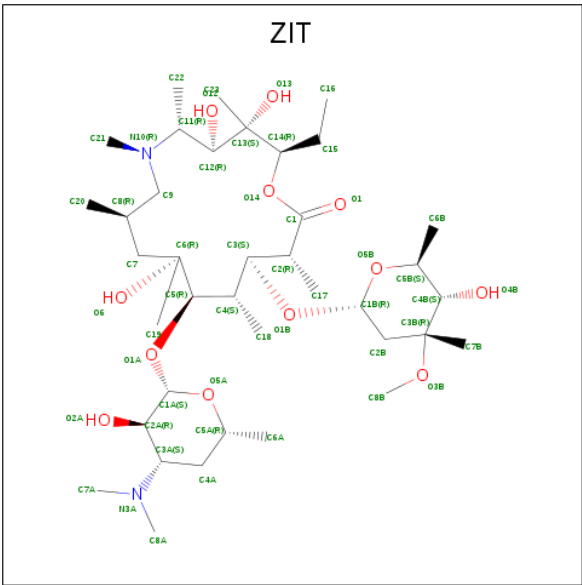
There is a discrepancy between the modelled and reference sequences:

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 AZITHROMYCIN (three-letter code: ZIT) (formula: C<sub>38</sub>H<sub>72</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			52	38	2	12		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	A	9	Total Cl 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	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	5898	Total 5898	O 5898	0	0
37	B	140	Total 140	O 140	0	0
37	C	129	Total 129	O 129	0	0
37	D	152	Total 152	O 152	0	0
37	E	169	Total 169	O 169	0	0
37	F	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	21	Total 21	O 21	0	0
37	J	81	Total 81	O 81	0	0
37	K	56	Total 56	O 56	0	0
37	L	61	Total 61	O 61	0	0
37	M	81	Total 81	O 81	0	0
37	N	129	Total 129	O 129	0	0
37	O	68	Total 68	O 68	0	0
37	P	45	Total 45	O 45	0	0
37	Q	69	Total 69	O 69	0	0
37	R	56	Total 56	O 56	0	0
37	S	89	Total 89	O 89	0	0
37	T	36	Total 36	O 36	0	0
37	U	39	Total 39	O 39	0	0
37	V	27	Total 27	O 27	0	0
37	W	15	Total 15	O 15	0	0
37	X	73	Total 73	O 73	0	0
37	Y	30	Total 30	O 30	0	0
37	Z	93	Total 93	O 93	0	0
37	1	38	Total 38	O 38	0	0

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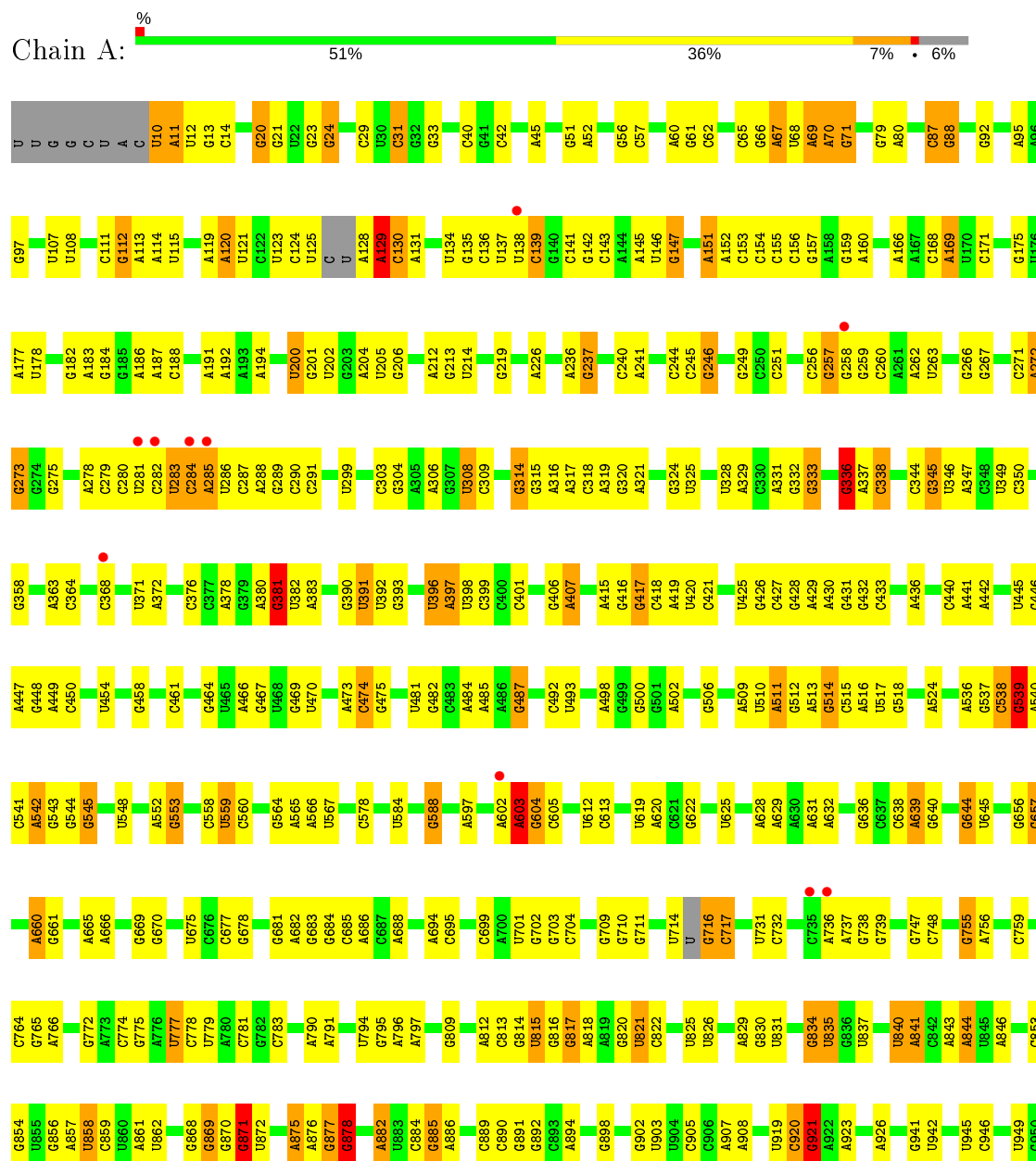
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	57	Total 57	O 57	0	0
37	3	39	Total 39	O 39	0	0
37	4	72	Total 72	O 72	0	0

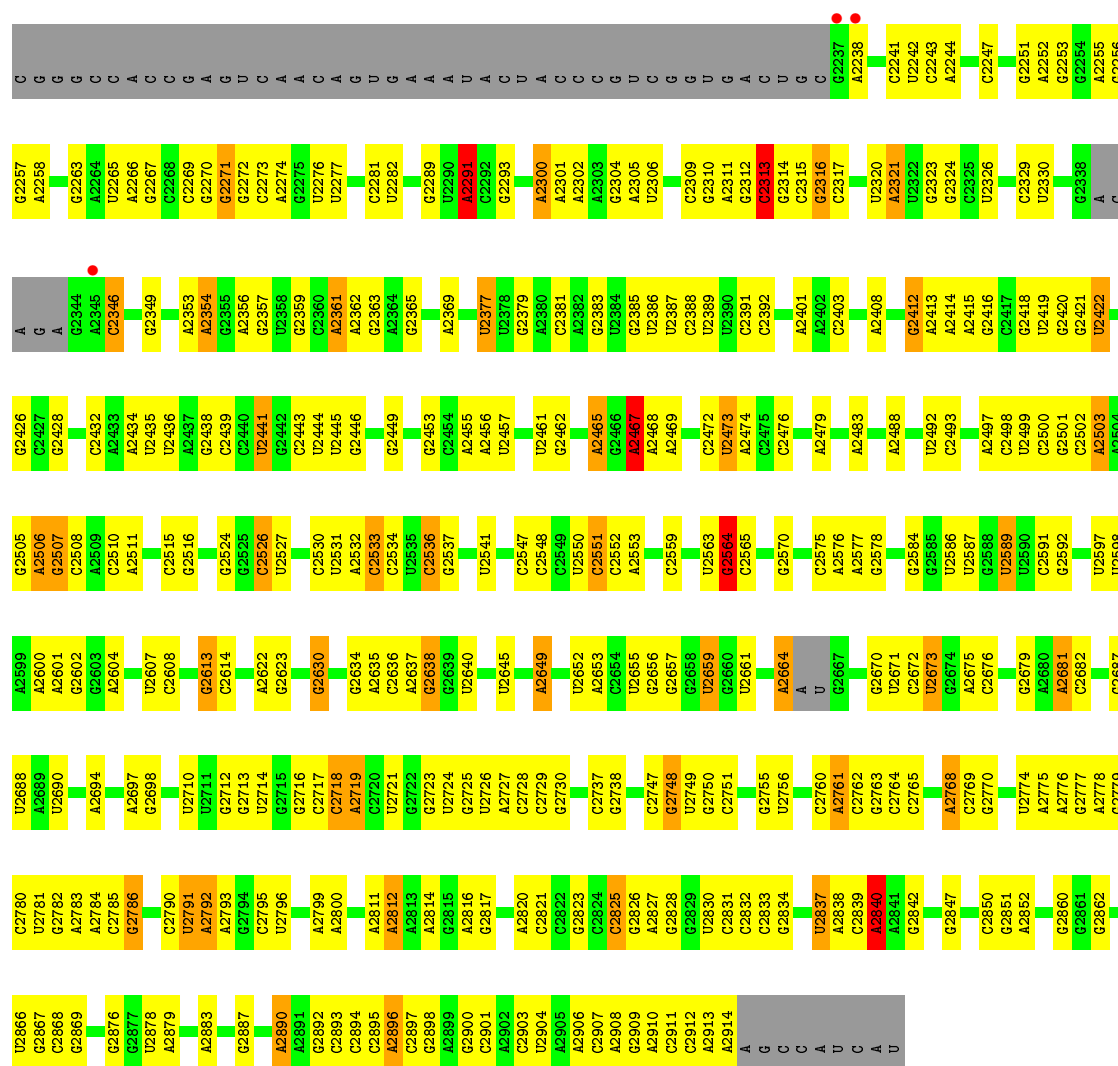
### 3 Residue-property plots

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

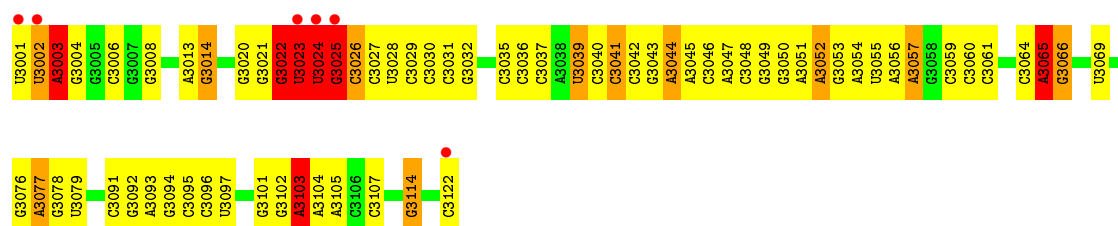
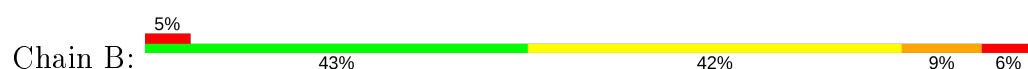
#### • Molecule 1: 23S rRNA



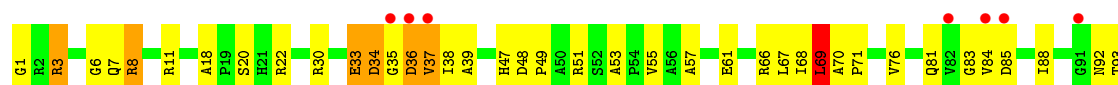
A2039	C1841	U1749	G1670	C1456	C1360	G1265	U1187	G1113	G1024	A951
C2040	A1942	C1750	C1675	U1457	C1361	U1266	A1198	A1114	C1025	G952
G2041	A1843	G1751	G1761	G1752	U1362	C1267	A1199	U1115	G953	G954
U2042	C1762	G1752	C1763	U1676	U1363	C1268	G1190	U1116	U1028	U954
U2043	U1846	C1753	U1677	U1461	U1368	U1269	A1191	A1117	U1029	G958
G2044	A1847	C1758	C1679	A1463	A1369	G1270	A1192	A1118	G1036	C959
C2045	U1759	A1759	G1680	A1463	G1370	A1271	A1193	G1119	G1037	G960
G2046	C1854	U1766	G1681	A1470	U1372	C1272	G1197	U1120	G1038	A961
U2047	G1855	A1767	G1682	C1474	A1375	C1273	A1199	U1122	G1044	C962
G2050	C1856	U1766	C1593	U1478	G1376	U1279	A1200	A1123	G1045	G964
A2054	A1857	G1768	C1594	C1477	C1377	C1289	A1199	G1127	G1046	U970
A2055	C1769	U1770	G1595	U1478	G1378	U1292	A1201	U1128	U1047	G
C	U1860	U1771	U1596	U1478	G1379	U1293	C1204	U1129	G1048	U
C	C1861	G1772	A1597	A1486	A1380	U1299	U1205	U1130	U1051	G
C	C1862	G1773	A1598	U1488	U1380	U1299	U1206	G1131	G1052	U
U	A1865	A1778	A1601	U1488	G1384	G1299	A1207	A1132	C1051	U
G	G1868	A1779	C1602	U1494	G1385	G1300	C1208	A1133	G1055	C
U	A1869	U1783	C1603	C1495	G1389	C1301	G1209	G1134	U1056	G
G	C1870	A1784	G1605	C1496	A1390	U1304	G1210	G1137	U1057	C
C	G1873	U1785	G1605	G1496	G1391	C1305	G1211	G1138	A1058	C
C	U1874	C1786	G1613	G1497	A1392	C1306	G1212	U1139	G1059	U
C	U1874	G1786	C1614	U1500	A1393	U1309	G1213	U1140	C1060	C
A	G1877	C1787	A1615	U1500	C1394	U1310	G1214	U1141	C1061	C
A	G1877	U1788	A1616	U1503	A1407	G1311	A1215	C1142	G1062	G
A	U1878	G1788	C1617	U1504	A1407	G1312	G1216	G1151	U1063	A
C	U1879	C1790	C1617	U1505	A1408	U1312	G1217	G1156	A1067	G
G	U1791	G1791	U1625	U1506	G1409	A1313	U1218	C1157	C1068	G
U	C1792	G1792	A1626	C1507	U1416	G1314	U1219	G1158	G1072	A
U	G1798	C1798	A1626	U1523	G1417	G1315	G1224	G1159	G1076	G
A	A1804	A1804	A1630	G1524	U1418	G1323	C1225	G1160	G1076	U
A	G1805	G1805	A1630	G1525	U1419	G1324	C1229	A1161	C1080	C
C	G1809	G1809	C1633	A1526	C1420	G1325	U1234	G1162	A1081	G
C	C1810	C1810	G1634	A1527	G1421	U1236	G1235	G1163	A1082	C
C	G1814	G1814	U1635	A1528	U1422	A1327	U1237	G1164	C1083	A
C	A1815	U1722	G1636	G1529	C1423	A1328	U1237	A1166	C1084	C
C	C1816	C1723	A1637	U1532	A1424	A1329	G1238	G1167	C1085	A
C	G1823	C1725	A1641	A1533	G1425	A1330	G1239	C1168	A1086	C
C	G1823	C1725	A1642	U1534	A1427	C1332	U1242	G1169	G1087	C
C	G1823	C1725	C1643	C1535	A1434	U1333	A1243	U1170	A1088	A
C	G1823	C1725	U1654	C1536	U1435	C1334	C1243	A1171	U1003	C
C	G1823	C1725	G1655	G1543	C1436	C1335	U1244	G1172	A1005	C
C	G1823	C1725	A1656	G1549	U1440	U1336	C1245	A1173	A1006	C
C	G1823	C1725	A1657	C1549	G1441	C1342	A1247	A1174	A1007	C
C	G1823	C1725	A1658	G1555	A1442	U1348	U1248	G1175	C1008	C
C	G1823	C1725	A1659	G1556	U1446	G1349	U1249	C1176	A1014	C
C	G1823	C1725	A1660	U1559	U1447	U1350	C1251	A1177	C1015	C
C	G1823	C1725	A1661	U1561	U1447	A1351	A1252	G1177	U1016	C
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C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1187		C
C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1188		C
C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1189		C
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C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1246		C
C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1247		C
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C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1253		C
C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1254		C
C	G1823	C1725	C1662	U1561	U1447	C1353	A1262	C1255		C
C	G1823	C1725								

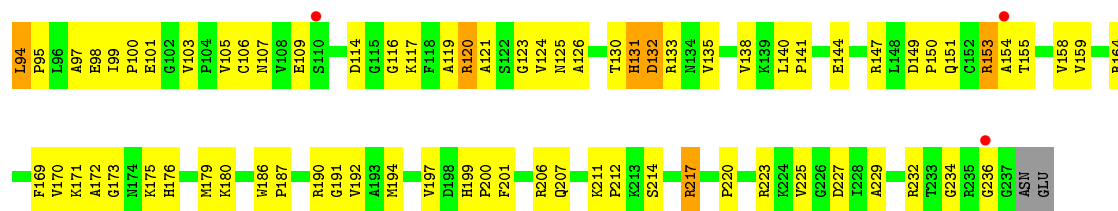


- Molecule 2: 5S rRNA

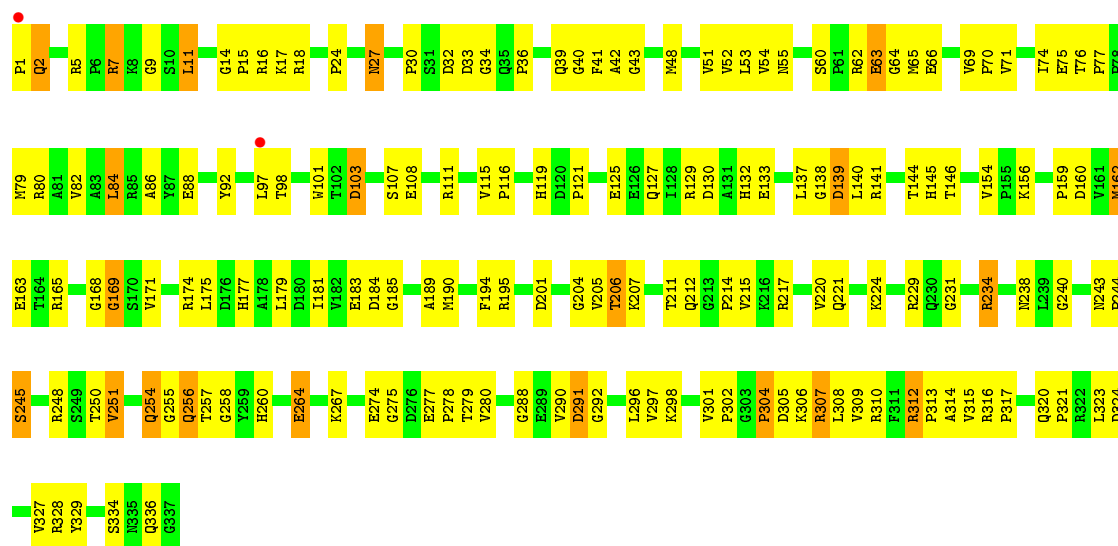


- Molecule 3: RIBOSOMAL PROTEIN L2

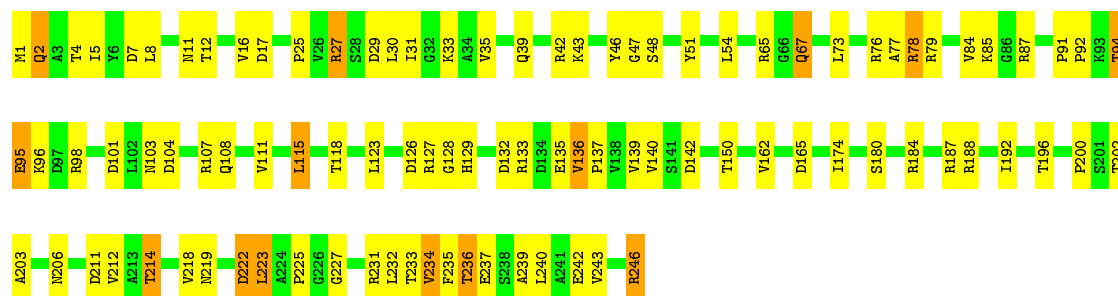




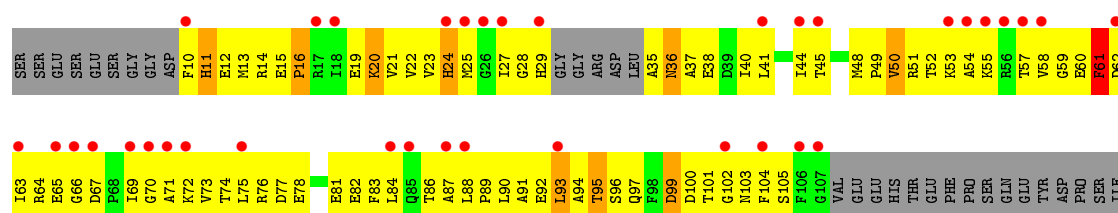
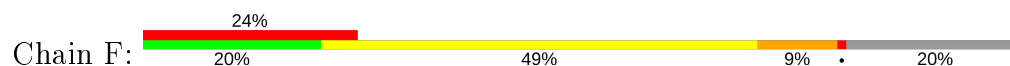
• Molecule 4: RIBOSOMAL PROTEIN L3



• Molecule 5: RIBOSOMAL PROTEIN L4

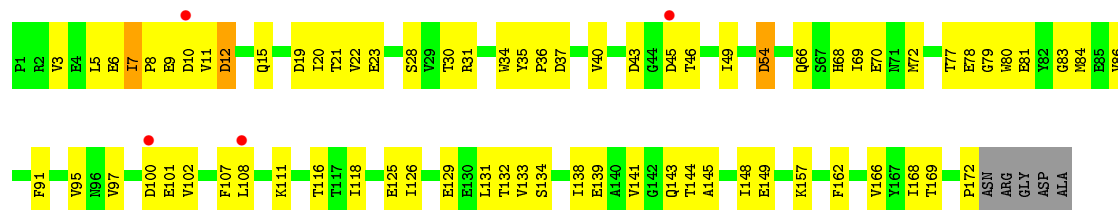


• Molecule 6: RIBOSOMAL PROTEIN L5

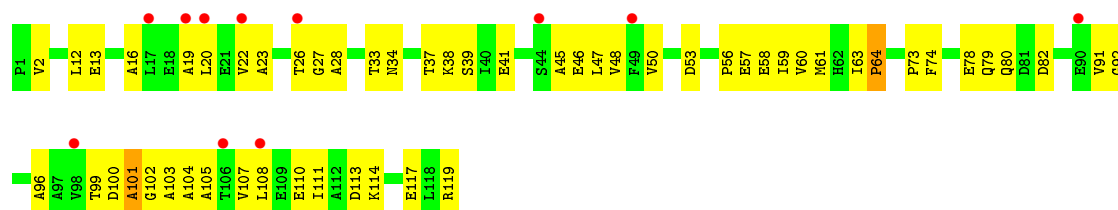




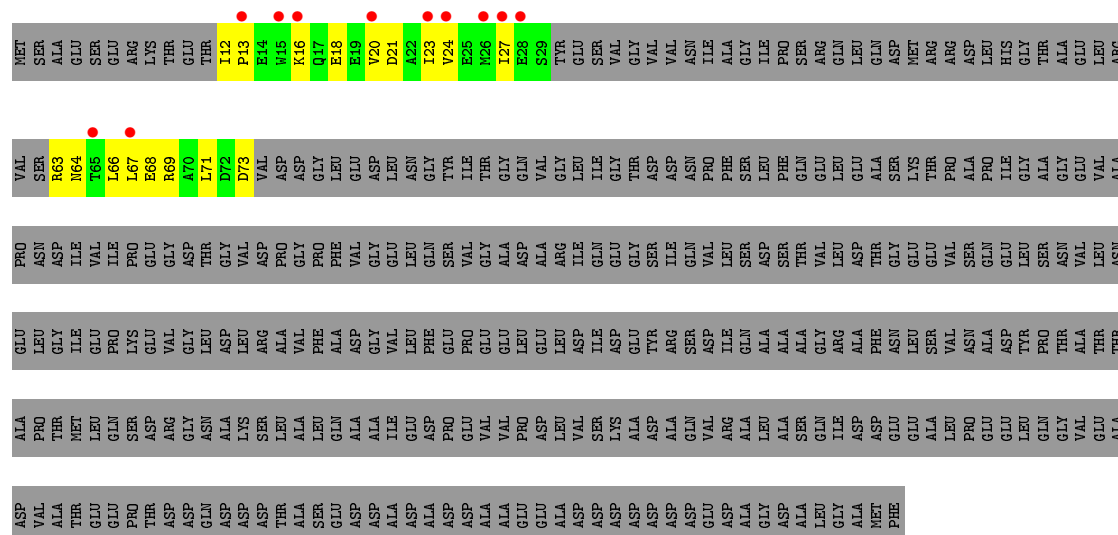
• Molecule 7: RIBOSOMAL PROTEIN L6



• Molecule 8: RIBOSOMAL PROTEIN L7AE

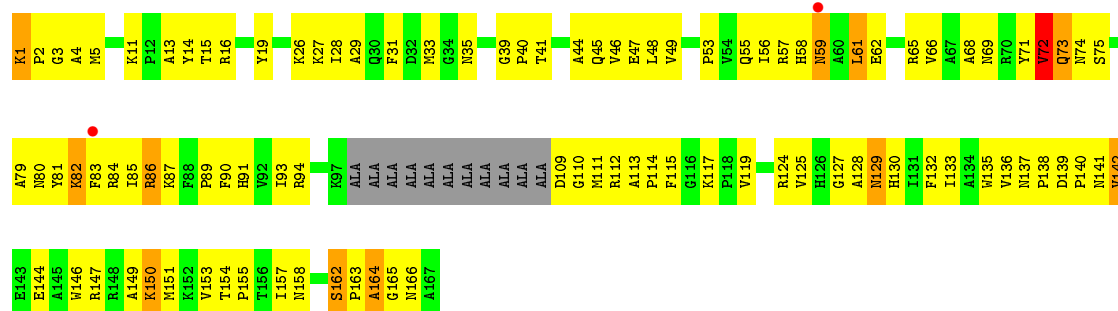


• Molecule 9: RIBOSOMAL PROTEIN L10



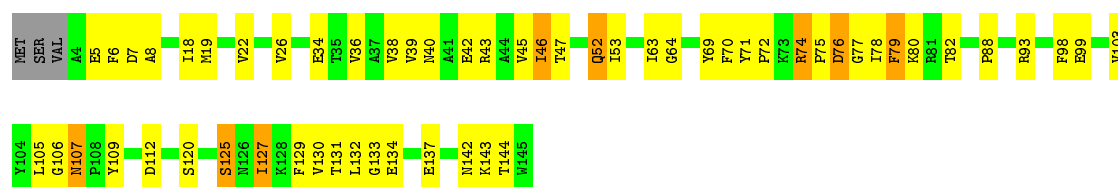
• Molecule 10: RIBOSOMAL PROTEIN L10E





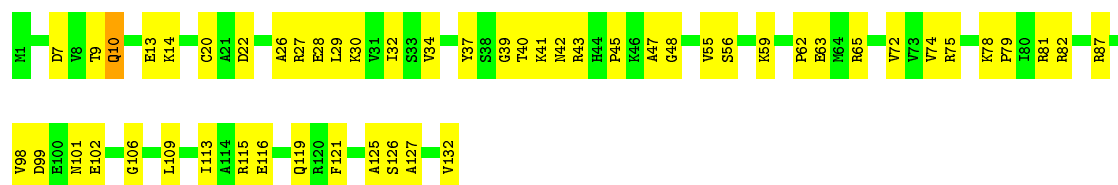
### • Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 59% 34% 6%



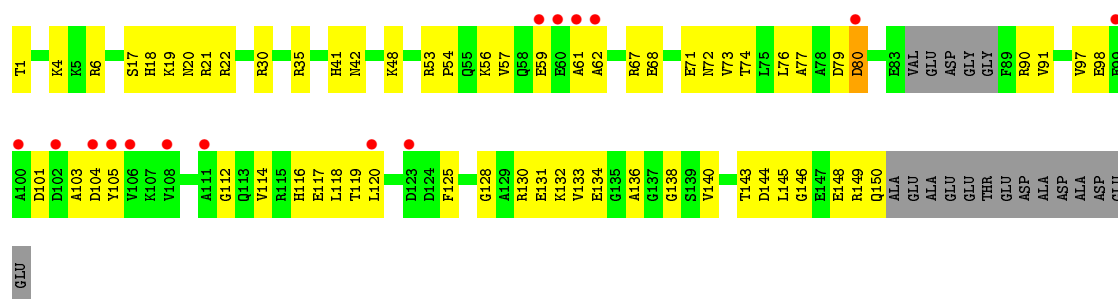
### • Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 61% 39%



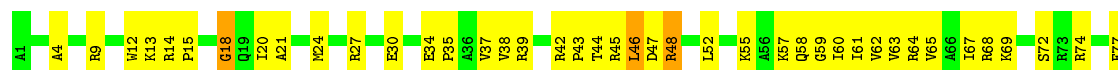
### • Molecule 13: RIBOSOMAL PROTEIN L15

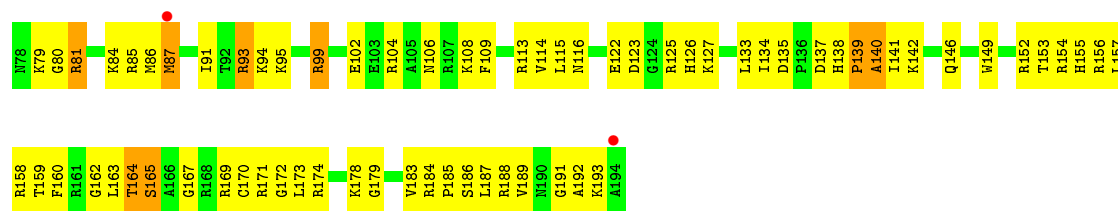
Chain M: 9% 50% 38% 12%



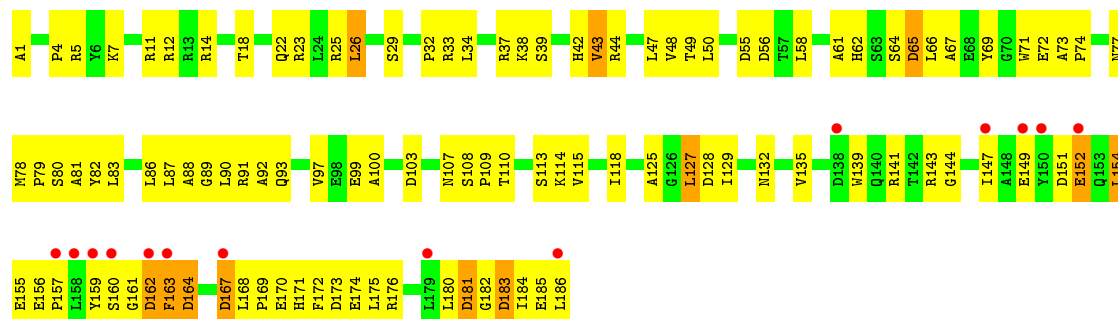
### • Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N: 43% 51% 6%

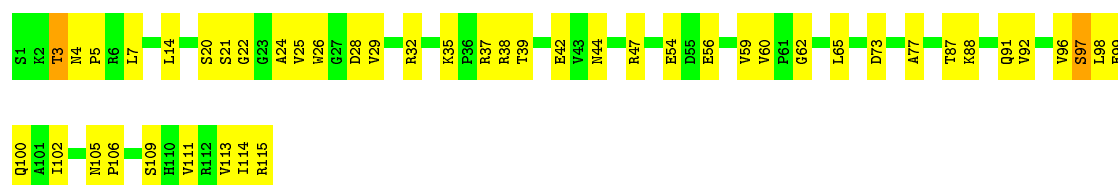




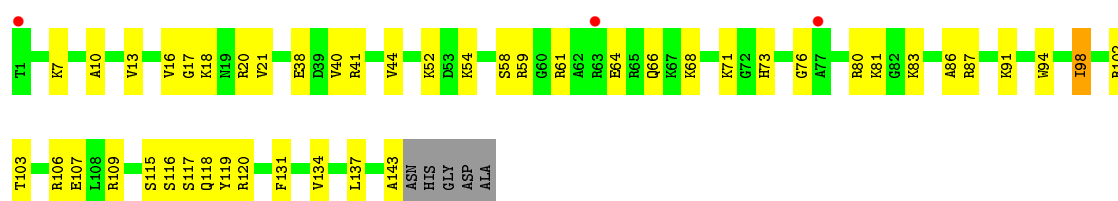
• Molecule 15: RIBOSOMAL PROTEIN L18



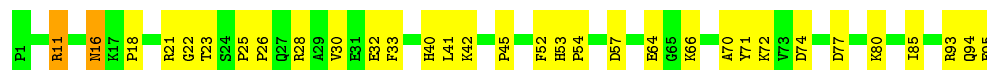
• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E

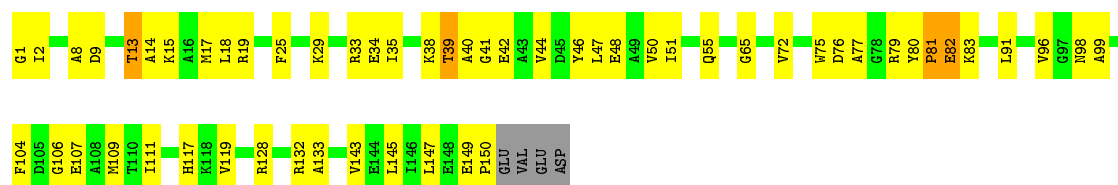


• Molecule 18: RIBOSOMAL PROTEIN L21E




• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S: 



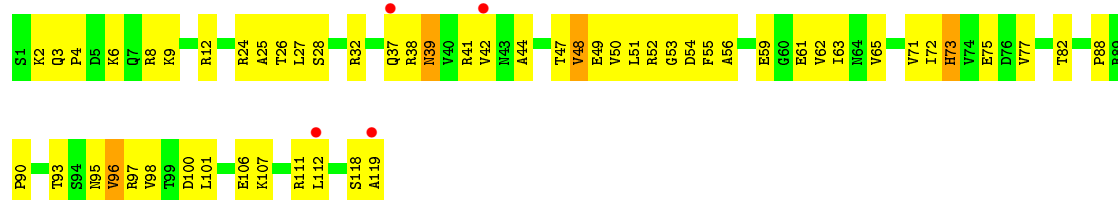
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T: 



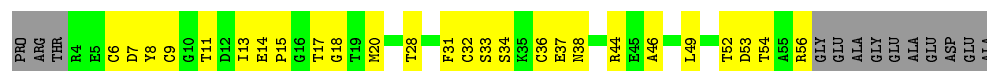
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U: 



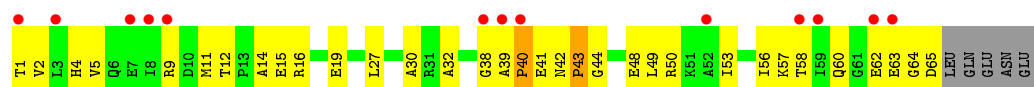
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V: 



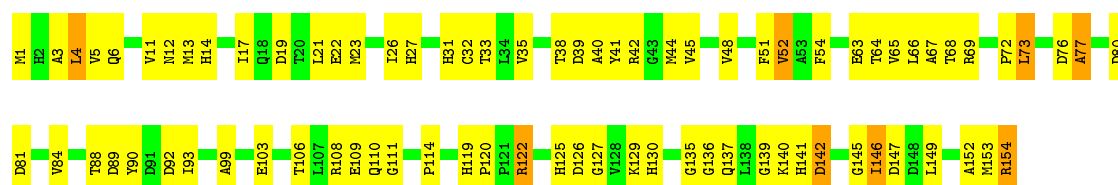
• Molecule 23: RIBOSOMAL PROTEIN L29

Chain W: 

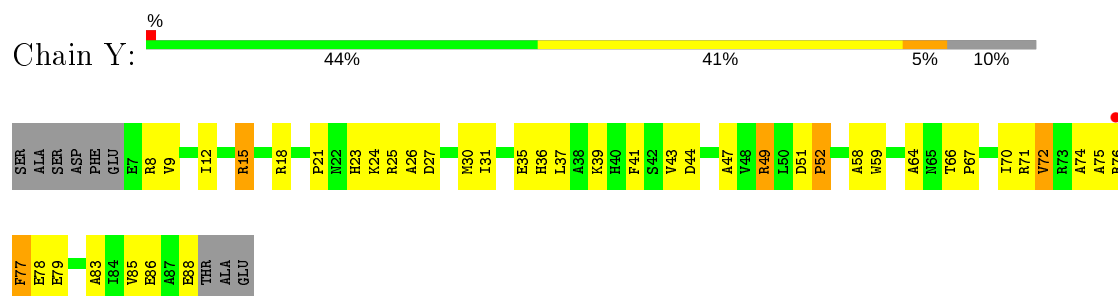


• Molecule 24: RIBOSOMAL PROTEIN L30

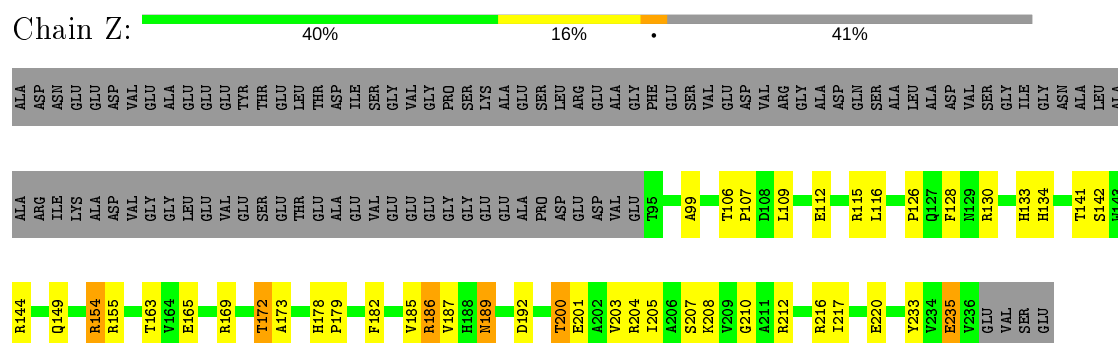
Chain X: 



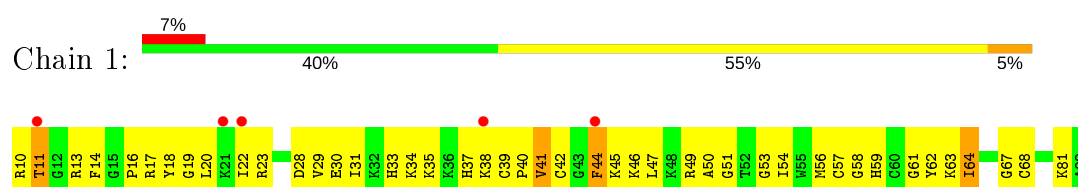
- Molecule 25: RIBOSOMAL PROTEIN L31E



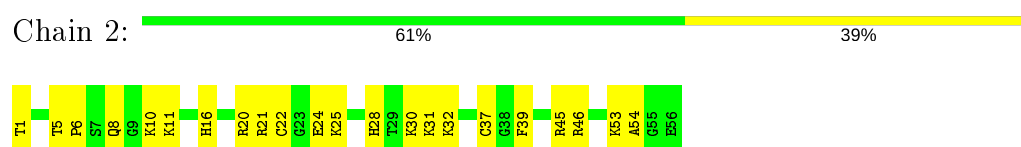
- Molecule 26: RIBOSOMAL PROTEIN L32E



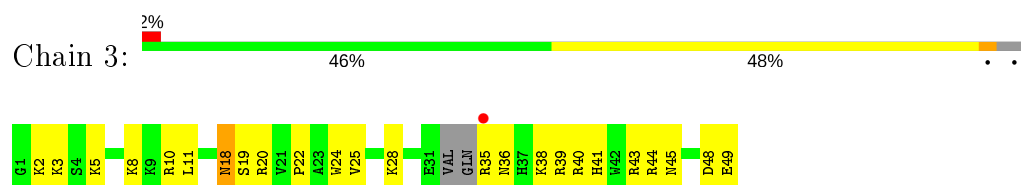
- Molecule 27: RIBOSOMAL PROTEIN L37Ae



- Molecule 28: RIBOSOMAL PROTEIN L37E

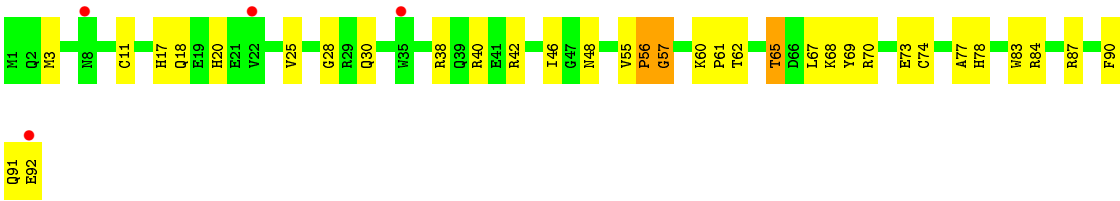


- Molecule 29: RIBOSOMAL PROTEIN L39E



- 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, $\alpha$ , $\beta$ , $\gamma$	213.75Å 301.57Å 574.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-3.20) 87.9 (49.69-3.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.250 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 74.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, ZIT, 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	1/66076 (0.0%)	0.76	33/103052 (0.0%)
2	B	0.92	16/2905 (0.6%)	0.98	20/4528 (0.4%)
3	C	0.47	0/1787	0.75	0/2409
4	D	0.52	0/2689	0.74	0/3652
5	E	0.49	0/1883	0.73	0/2551
6	F	0.43	0/1111	0.68	0/1498
7	G	0.48	0/1382	0.67	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.51	0/241	0.63	0/324
10	J	0.50	0/1246	0.82	2/1686 (0.1%)
11	K	0.53	0/1135	0.69	0/1530
12	L	0.57	1/1003 (0.1%)	0.78	0/1351
13	M	0.47	0/1126	0.76	0/1504
14	N	0.56	0/1633	0.81	1/2180 (0.0%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.49	0/873	0.69	0/1181
17	Q	0.49	0/1143	0.66	0/1521
18	R	0.52	0/748	0.78	0/1005
19	S	0.52	0/1172	0.77	0/1578
20	T	0.48	0/648	0.69	0/875
21	U	0.46	0/957	0.73	0/1289
22	V	0.47	0/417	0.67	0/562
23	W	0.43	0/502	0.63	0/675
24	X	0.52	0/1218	0.72	0/1655
25	Y	0.49	0/664	0.71	0/895
26	Z	0.50	0/1146	0.73	0/1536
27	1	0.52	0/575	0.75	0/763
28	2	0.57	0/437	0.78	0/578
29	3	0.45	0/398	0.63	0/527
30	4	0.57	0/771	0.73	0/1024
All	All	0.57	18/98255 (0.0%)	0.76	56/147027 (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	141
2	B	0	5
All	All	1	146

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3025	G	O3'-P	10.69	1.74	1.61
2	B	3025	G	C4'-O4'	9.77	1.58	1.45
2	B	3023	U	C2'-O2'	9.46	1.53	1.41
2	B	3026	C	P-O5'	-8.76	1.50	1.59
2	B	3003	A	C5'-C4'	8.50	1.61	1.51
2	B	3023	U	O5'-C5'	8.22	1.57	1.44
2	B	3025	G	C2'-C1'	7.80	1.61	1.53
2	B	3025	G	N9-C4	-7.75	1.31	1.38
2	B	3026	C	P-OP2	-7.49	1.36	1.49
2	B	3025	G	O4'-C1'	6.51	1.50	1.41
2	B	3025	G	C2-N3	-6.08	1.27	1.32
2	B	3024	U	O4'-C1'	5.91	1.49	1.41
2	B	3022	G	O3'-P	5.88	1.68	1.61
2	B	3022	G	O5'-C5'	-5.87	1.33	1.42
12	L	63	GLU	CB-CG	5.85	1.63	1.52
2	B	3025	G	C4'-C3'	5.64	1.59	1.53
1	A	1206	U	P-OP2	5.57	1.58	1.49
2	B	3025	G	P-OP2	-5.16	1.40	1.49

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.12	63.13	105.20
1	A	1164	U	OP2-P-O3'	-17.65	66.37	105.20
1	A	1165	G	O5'-P-OP1	-12.66	94.31	105.70
2	B	3024	U	O5'-P-OP2	11.59	124.60	110.70
2	B	3026	C	O5'-P-OP2	-11.13	95.68	105.70
2	B	3023	U	P-O5'-C5'	10.35	137.46	120.90
1	A	1563	G	C2'-C3'-O3'	9.97	131.43	109.50
1	A	1942	A	C5'-C4'-C3'	9.05	130.49	116.00
2	B	3024	U	C5'-C4'-O4'	8.54	119.34	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3025	G	O5'-P-OP2	-8.52	98.04	105.70
1	A	1979	G	C2'-C3'-O3'	7.60	126.21	109.50
2	B	3039	U	N1-C1'-C2'	7.23	123.40	114.00
2	B	3024	U	OP1-P-O3'	6.81	120.18	105.20
1	A	1592	G	N9-C1'-C2'	6.78	122.81	114.00
10	J	74	ASN	N-CA-C	-6.62	93.12	111.00
1	A	1165	G	OP1-P-OP2	6.53	129.40	119.60
1	A	1942	A	C5'-C4'-O4'	6.43	116.82	109.10
1	A	1165	G	O5'-P-OP2	-6.43	99.91	105.70
2	B	3103	A	C5'-C4'-O4'	6.42	116.80	109.10
1	A	1738	C	O4'-C4'-C3'	-6.42	97.58	104.00
2	B	3024	U	P-O5'-C5'	6.24	130.88	120.90
1	A	2467	A	C1'-O4'-C4'	-5.97	105.13	109.90
1	A	1504	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	A	2313	C	C5'-C4'-O4'	5.73	115.98	109.10
2	B	3026	C	C5'-C4'-O4'	5.69	115.93	109.10
2	B	3025	G	N3-C4-N9	-5.67	122.60	126.00
1	A	2312	G	N9-C1'-C2'	-5.65	105.79	112.00
2	B	3023	U	OP2-P-O3'	-5.65	92.78	105.20
14	N	139	PRO	N-CA-C	-5.60	97.54	112.10
1	A	1971	G	O4'-C1'-N9	5.58	112.66	108.20
2	B	3024	U	C4'-C3'-O3'	5.51	124.02	113.00
2	B	3026	C	OP1-P-OP2	5.48	127.82	119.60
1	A	2664	A	N9-C1'-C2'	5.42	121.05	114.00
1	A	314	G	N9-C1'-C2'	-5.40	106.06	112.00
1	A	2291	A	N9-C1'-C2'	5.40	121.02	114.00
1	A	871	G	C5'-C4'-O4'	-5.40	102.62	109.10
2	B	3103	A	C4'-C3'-C2'	-5.36	97.24	102.60
1	A	1342	C	N1-C1'-C2'	-5.33	106.13	112.00
10	J	110	GLY	N-CA-C	-5.33	99.77	113.10
1	A	2311	A	N9-C1'-C2'	-5.33	106.14	112.00
1	A	921	G	N9-C1'-C2'	5.30	120.89	114.00
1	A	1819	G	C5'-C4'-C3'	5.29	124.47	116.00
1	A	1683	G	N9-C1'-C2'	5.26	120.84	114.00
1	A	841	A	C1'-O4'-C4'	-5.25	105.70	109.90
2	B	3022	G	N9-C1'-C2'	5.24	120.82	114.00
1	A	2313	C	C4'-C3'-C2'	-5.22	97.38	102.60
2	B	3025	G	C6-N1-C2	5.20	128.22	125.10
1	A	381	G	N9-C1'-C2'	5.18	120.73	114.00
2	B	3025	G	C2'-C3'-O3'	5.15	121.95	113.70
1	A	206	G	C5'-C4'-C3'	-5.15	107.76	116.00
1	A	129	A	C2'-C3'-O3'	5.14	121.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	A	N9-C1'-C2'	5.10	120.63	114.00
2	B	3023	U	C5'-C4'-C3'	5.08	124.12	116.00
1	A	1829	A	N9-C1'-C2'	-5.06	106.43	112.00
2	B	3003	A	C4'-C3'-C2'	-5.03	97.57	102.60
1	A	1723	G	N9-C1'-C2'	5.02	120.53	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (146) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1005	A	Sidechain
1	A	1036	G	Sidechain
1	A	1038	G	Sidechain
1	A	1118	A	Sidechain
1	A	112	G	Sidechain
1	A	1127	C	Sidechain
1	A	1134	G	Sidechain
1	A	1156	C	Sidechain
1	A	1206	U	Sidechain
1	A	1234	U	Sidechain
1	A	1264	U	Sidechain
1	A	1305	C	Sidechain
1	A	1314	U	Sidechain
1	A	1348	A	Sidechain
1	A	1349	G	Sidechain
1	A	1350	U	Sidechain
1	A	1371	U	Sidechain
1	A	1379	A	Sidechain
1	A	1390	A	Sidechain
1	A	1417	G	Sidechain
1	A	1447	U	Sidechain
1	A	146	U	Sidechain
1	A	147	G	Sidechain
1	A	1470	A	Sidechain
1	A	1635	U	Sidechain
1	A	1677	U	Sidechain
1	A	1685	A	Sidechain
1	A	1688	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1694	G	Sidechain
1	A	1696	U	Sidechain
1	A	171	C	Sidechain
1	A	1720	C	Sidechain
1	A	1736	A	Sidechain
1	A	1737	A	Sidechain
1	A	1758	U	Sidechain
1	A	1809	G	Sidechain
1	A	1819	G	Sidechain
1	A	1823	G	Sidechain
1	A	1828	G	Sidechain
1	A	1829	A	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	1865	A	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1908	G	Sidechain
1	A	1922	A	Sidechain
1	A	194	A	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	20	G	Sidechain
1	A	2023	G	Sidechain
1	A	2035	C	Sidechain
1	A	2047	C	Sidechain
1	A	2088	C	Sidechain
1	A	2110	G	Sidechain
1	A	2115	U	Sidechain
1	A	2117	U	Sidechain
1	A	2123	A	Sidechain
1	A	2263	G	Sidechain
1	A	2293	G	Sidechain
1	A	2300	A	Sidechain
1	A	2306	U	Sidechain
1	A	2313	C	Sidechain
1	A	2316	G	Sidechain
1	A	2377	U	Sidechain
1	A	2381	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	24	G	Sidechain
1	A	2412	G	Sidechain
1	A	2439	C	Sidechain
1	A	2441	U	Sidechain
1	A	2444	U	Sidechain
1	A	246	G	Sidechain
1	A	2465	A	Sidechain
1	A	2473	U	Sidechain
1	A	2479	A	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2530	C	Sidechain
1	A	2551	C	Sidechain
1	A	2564	G	Sidechain
1	A	257	G	Sidechain
1	A	2607	U	Sidechain
1	A	2622	A	Sidechain
1	A	2623	G	Sidechain
1	A	2630	G	Sidechain
1	A	2640	U	Sidechain
1	A	2659	U	Sidechain
1	A	2673	U	Sidechain
1	A	2675	A	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2837	U	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	2887	G	Sidechain
1	A	33	G	Sidechain
1	A	333	G	Sidechain
1	A	336	G	Sidechain
1	A	391	U	Sidechain
1	A	396	U	Sidechain
1	A	397	A	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	474	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	481	U	Sidechain
1	A	482	G	Sidechain
1	A	502	A	Sidechain
1	A	515	C	Sidechain
1	A	517	U	Sidechain
1	A	518	G	Sidechain
1	A	539	G	Sidechain
1	A	548	U	Sidechain
1	A	552	A	Sidechain
1	A	565	A	Sidechain
1	A	619	U	Sidechain
1	A	631	A	Sidechain
1	A	636	G	Sidechain
1	A	639	A	Sidechain
1	A	657	G	Sidechain
1	A	678	G	Sidechain
1	A	755	G	Sidechain
1	A	766	A	Sidechain
1	A	781	C	Sidechain
1	A	815	U	Sidechain
1	A	817	G	Sidechain
1	A	844	A	Sidechain
1	A	871	G	Sidechain
1	A	878	G	Sidechain
1	A	891	G	Sidechain
1	A	898	G	Sidechain
1	A	903	U	Sidechain
1	A	919	U	Sidechain
1	A	954	U	Sidechain
2	B	3022	G	Sidechain
2	B	3024	U	Sidechain
2	B	3052	A	Sidechain
2	B	3065	A	Sidechain
2	B	3094	G	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29803	1165	0
2	B	2600	0	1326	84	0
3	C	1754	0	1763	129	0
4	D	2624	0	2533	180	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	84	0
8	H	885	0	854	66	0
9	I	240	0	231	25	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	56	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	159	0
15	O	1444	0	1401	142	0
16	P	864	0	873	46	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	28	0
19	S	1149	0	1122	64	0
20	T	641	0	605	22	0
21	U	949	0	923	55	0
22	V	410	0	364	36	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	59	0
27	1	563	0	597	51	0
28	2	430	0	426	28	0
29	3	393	0	406	30	0
30	4	755	0	728	41	0
31	A	52	0	72	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	1	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	4	0
35	L	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	2	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	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	38	0	0	8	0
37	2	57	0	0	4	0
37	3	39	0	0	4	0
37	4	72	0	0	12	0
37	A	5898	0	0	232	0
37	B	140	0	0	15	0
37	C	129	0	0	24	0
37	D	152	0	0	27	0
37	E	169	0	0	34	0
37	F	52	0	0	18	0
37	G	42	0	0	13	0
37	H	28	0	0	10	0
37	I	21	0	0	5	0
37	J	81	0	0	17	0
37	K	56	0	0	6	0
37	L	61	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	M	81	0	0	19	0
37	N	129	0	0	22	0
37	O	68	0	0	20	0
37	P	45	0	0	13	0
37	Q	69	0	0	6	0
37	R	56	0	0	3	0
37	S	89	0	0	8	0
37	T	36	0	0	4	0
37	U	39	0	0	5	0
37	V	27	0	0	5	0
37	W	15	0	0	3	0
37	X	73	0	0	7	0
37	Y	30	0	0	8	0
37	Z	93	0	0	14	0
All	All	98587	0	59571	3047	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 (3047) 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'	1.22	1.15
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.26	1.13
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.33	1.11
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.67	1.10
1:A:871:G:H8	1:A:871:G:H5'	1.14	1.07
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.34	1.07
27:1:10:ARG:HA	37:1:8415:HOH:O	1.55	1.07
5:E:236:THR:HG22	5:E:239:ALA:H	1.11	1.06
1:A:156:C:H5''	14:N:171:ARG:HD3	1.35	1.05
1:A:871:G:C8	1:A:871:G:H5'	1.89	1.05
2:B:3023:U:H5''	2:B:3024:U:OP2	1.55	1.04
2:B:3076:G:H3'	2:B:3077:A:H5''	1.38	1.04
1:A:541:C:H2'	1:A:542:A:H5''	1.38	1.03
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.57	1.03
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.41	1.02
1:A:542:A:H8	1:A:542:A:H5'	1.22	1.02
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.40	1.01
6:F:25:MET:HE2	6:F:41:LEU:HG	1.39	1.00
4:D:321:PRO:HA	37:D:8662:HOH:O	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.40	0.99
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.85	0.99
10:J:165:GLY:HA3	37:J:8401:HOH:O	1.61	0.99
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.45	0.98
2:B:3056:A:H2'	2:B:3057:A:H5''	1.44	0.98
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.44	0.98
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.43	0.98
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.42	0.98
14:N:164:THR:HG22	14:N:167:GLY:H	1.24	0.98
1:A:1474:C:H5'	1:A:1474:C:H6	1.28	0.97
1:A:962:C:H1'	15:O:5:ARG:NH1	1.80	0.97
4:D:140:LEU:HA	37:D:8583:HOH:O	1.63	0.97
12:L:10:GLN:NE2	12:L:10:GLN:H	1.63	0.97
1:A:1134:G:H4'	10:J:151:MET:HE1	1.45	0.97
13:M:79:ASP:HB3	37:M:8432:HOH:O	1.65	0.96
1:A:1751:G:H2'	1:A:1752:G:H5''	1.44	0.96
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.45	0.96
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.48	0.95
17:Q:115:SER:H	17:Q:118:GLN:HE21	0.95	0.95
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.48	0.94
14:N:64:ARG:HD2	37:N:8585:HOH:O	1.66	0.94
1:A:1835:U:H5	1:A:1840:A:N7	1.66	0.94
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.32	0.93
1:A:871:G:C5'	1:A:871:G:H8	1.82	0.93
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.69	0.93
10:J:142:VAL:HG13	37:J:8383:HOH:O	1.69	0.92
10:J:4:ALA:HB3	37:J:8367:HOH:O	1.69	0.92
5:E:236:THR:HG21	37:E:8370:HOH:O	1.70	0.92
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.83	0.92
1:A:960:G:H4'	37:A:7000:HOH:O	1.68	0.92
1:A:1667:A:H8	1:A:1667:A:H5'	1.32	0.92
10:J:2:PRO:HB2	37:J:8367:HOH:O	1.69	0.91
12:L:10:GLN:HE21	12:L:10:GLN:H	0.95	0.91
1:A:856:G:H2'	37:A:5003:HOH:O	1.71	0.91
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.51	0.91
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.52	0.90
4:D:62:ARG:HA	4:D:65:MET:HE3	1.53	0.90
24:X:88:THR:HB	37:X:6679:HOH:O	1.72	0.90
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.54	0.90
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.16	0.90
11:K:76:ASP:HA	37:K:5907:HOH:O	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.52	0.90
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.54	0.89
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.37	0.89
1:A:1372:A:H3'	37:A:6759:HOH:O	1.71	0.89
1:A:1119:G:H22	1:A:1246:A:H2	1.20	0.89
37:A:3259:HOH:O	14:N:79:LYS:HD3	1.71	0.89
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.87	0.89
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.54	0.89
37:A:4432:HOH:O	14:N:14:ARG:HG2	1.72	0.89
14:N:94:LYS:HE3	37:N:8581:HOH:O	1.73	0.88
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.56	0.88
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.02	0.88
15:O:144:GLY:O	15:O:147:ILE:HG22	1.72	0.88
12:L:10:GLN:N	12:L:10:GLN:HE21	1.72	0.88
37:A:3362:HOH:O	14:N:189:VAL:HG21	1.74	0.88
29:3:41:HIS:H	29:3:45:ASN:HD22	1.21	0.88
24:X:88:THR:HG22	24:X:89:ASP:H	1.37	0.88
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.73	0.87
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.80	0.87
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.73	0.87
5:E:246:ARG:NH1	5:E:246:ARG:HB3	1.90	0.87
1:A:870:G:H2'	1:A:871:G:H5''	1.53	0.87
1:A:645:U:OP2	13:M:4:LYS:HE2	1.72	0.87
15:O:7:LYS:HE3	18:R:21:ARG:O	1.73	0.87
10:J:150:LYS:HE2	37:J:8385:HOH:O	1.76	0.86
1:A:2717:C:H2'	1:A:2718:C:H5''	1.56	0.86
6:F:105:SER:HB2	6:F:131:THR:HG23	1.56	0.86
13:M:68:GLU:HA	37:M:8417:HOH:O	1.73	0.86
3:C:7:GLN:O	37:C:8515:HOH:O	1.92	0.86
1:A:2506:A:HO2'	1:A:2507:G:H8	0.89	0.86
1:A:1209:C:H4'	37:A:4854:HOH:O	1.76	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
1:A:2586:U:H3	1:A:2592:G:H22	1.23	0.86
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.38	0.86
1:A:506:G:H22	1:A:509:A:C5'	1.89	0.85
6:F:154:LYS:H	6:F:154:LYS:HD2	1.38	0.85
27:1:49:ARG:HD2	37:1:8429:HOH:O	1.75	0.85
1:A:236:A:H4'	1:A:237:G:H5'	1.59	0.85
10:J:26:LYS:HG2	10:J:28:ILE:H	1.39	0.85
37:A:3303:HOH:O	14:N:157:LEU:HD11	1.75	0.85
1:A:541:C:C2'	1:A:542:A:H5''	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:U:H3	1:A:1246:A:H62	1.21	0.85
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.39	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.06	0.85
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.75	0.84
2:B:3023:U:C5'	2:B:3024:U:OP2	2.24	0.84
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.41	0.84
20:T:57:THR:HG22	20:T:59:ASP:H	1.40	0.84
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.42	0.84
10:J:59:ASN:H	10:J:59:ASN:HD22	1.25	0.84
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.77	0.84
37:A:6348:HOH:O	15:O:4:PRO:HD2	1.77	0.84
30:4:60:LYS:HG3	30:4:61:PRO:HD2	1.59	0.84
1:A:545:G:H8	1:A:545:G:H5'	1.43	0.83
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.59	0.83
14:N:164:THR:HG23	14:N:165:SER:N	1.94	0.83
1:A:214:U:H5'	37:A:5719:HOH:O	1.77	0.83
4:D:86:ALA:HA	37:D:8583:HOH:O	1.78	0.83
19:S:44:VAL:O	19:S:48:GLU:HG3	1.78	0.83
14:N:61:ILE:HG13	37:N:8622:HOH:O	1.78	0.83
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.42	0.83
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.41	0.83
10:J:59:ASN:N	10:J:59:ASN:HD22	1.77	0.82
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.94	0.82
1:A:1116:U:HO2'	1:A:1118:A:H2	0.83	0.82
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.61	0.82
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.80	0.82
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.61	0.82
10:J:49:VAL:O	10:J:157:ILE:HG23	1.79	0.82
1:A:962:C:H1'	15:O:5:ARG:HH12	1.45	0.82
5:E:236:THR:HG22	5:E:239:ALA:N	1.95	0.82
13:M:133:VAL:HA	37:M:8445:HOH:O	1.76	0.82
1:A:1603:A:H5'	1:A:1605:G:O4'	1.78	0.82
23:W:1:THR:HG23	23:W:2:VAL:H	1.44	0.82
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.61	0.81
16:P:47:ARG:HG3	16:P:47:ARG:HH11	1.45	0.81
6:F:20:LYS:HA	6:F:75:LEU:O	1.81	0.81
1:A:1666:C:O2'	1:A:1667:A:H5"	1.80	0.81
5:E:236:THR:HA	37:E:8448:HOH:O	1.78	0.81
14:N:80:GLY:O	14:N:81:ARG:HD3	1.81	0.81
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.63	0.81
1:A:1242:A:H5'	11:K:82:THR:HG23	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:G:H22	1:A:509:A:H5''	1.46	0.81
27:1:58:GLY:HA3	37:1:8439:HOH:O	1.81	0.81
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.60	0.81
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.26	0.81
1:A:1184:C:H1'	37:A:7039:HOH:O	1.81	0.80
8:H:46:GLU:O	8:H:73:PRO:HD2	1.81	0.80
1:A:1160:G:H5'	1:A:1161:A:C5'	2.09	0.80
1:A:2426:G:H1'	37:A:5671:HOH:O	1.79	0.80
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.61	0.80
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.78	0.80
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.10	0.80
37:A:7026:HOH:O	4:D:211:THR:HG21	1.81	0.80
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.63	0.80
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.64	0.80
1:A:1205:U:H2'	1:A:1206:U:H5'	1.62	0.80
1:A:1119:G:N2	1:A:1246:A:C2	2.50	0.80
1:A:542:A:C8	1:A:542:A:H5'	2.13	0.80
1:A:1474:C:H5'	1:A:1474:C:C6	2.16	0.80
1:A:1160:G:C5'	1:A:1161:A:H5'	2.08	0.80
3:C:199:HIS:HD2	3:C:201:PHE:H	1.30	0.80
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.63	0.80
1:A:1625:U:H4'	37:A:4242:HOH:O	1.81	0.79
10:J:27:LYS:H	10:J:58:HIS:HD2	1.27	0.79
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.80	0.79
23:W:4:HIS:HB3	37:W:6622:HOH:O	1.83	0.79
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.81	0.79
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.65	0.79
2:B:3056:A:C2'	2:B:3057:A:H5''	2.12	0.79
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.64	0.79
10:J:139:ASP:N	10:J:140:PRO:HD3	1.98	0.79
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.63	0.79
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.47	0.79
19:S:9:ASP:O	19:S:13:THR:HB	1.83	0.79
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.63	0.79
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.65	0.79
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.64	0.78
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.79	0.78
21:U:48:VAL:HG22	21:U:97:ARG:O	1.83	0.78
1:A:282:C:H1'	1:A:368:C:N4	1.98	0.78
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.65	0.78
1:A:1450:C:H4'	1:A:1451:C:OP2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:152:ARG:HG3	37:N:8555:HOH:O	1.84	0.78
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.65	0.78
37:A:6446:HOH:O	14:N:178:LYS:HB2	1.83	0.78
10:J:41:THR:HA	37:J:8398:HOH:O	1.83	0.78
26:Z:220:GLU:HG2	37:Z:8137:HOH:O	1.82	0.78
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.49	0.78
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.30	0.78
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.18	0.78
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.65	0.77
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.65	0.77
1:A:711:G:H1'	37:A:6665:HOH:O	1.84	0.77
2:B:3014:G:H8	2:B:3014:G:H5'	1.49	0.77
7:G:132:THR:HB	37:G:2227:HOH:O	1.84	0.77
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.47	0.77
15:O:113:SER:HB2	37:O:8559:HOH:O	1.83	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.67	0.77
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.50	0.77
1:A:1947:G:OP2	37:A:3246:HOH:O	2.02	0.77
5:E:1:MET:HG2	5:E:2:GLN:H	1.48	0.77
10:J:137:ASN:O	10:J:139:ASP:N	2.18	0.77
3:C:199:HIS:CD2	3:C:201:PHE:H	2.02	0.77
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.65	0.77
1:A:31:C:H4'	37:A:6994:HOH:O	1.84	0.77
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.14	0.77
14:N:87:MET:CG	30:4:46:ILE:HG21	2.14	0.77
10:J:140:PRO:HB3	37:J:8383:HOH:O	1.85	0.77
7:G:37:ASP:OD1	11:K:125:SER:HB3	1.85	0.77
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.66	0.77
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.15	0.77
1:A:1116:U:O2'	1:A:1118:A:H2	1.65	0.76
1:A:1165:G:H4'	1:A:1174:A:O2'	1.85	0.76
13:M:148:GLU:HA	37:M:8444:HOH:O	1.84	0.76
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.66	0.76
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.50	0.76
1:A:288:A:H61	1:A:364:C:H42	1.34	0.76
3:C:35:GLY:O	3:C:36:ASP:HB3	1.84	0.76
24:X:88:THR:HG22	24:X:89:ASP:N	2.00	0.76
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.15	0.76
16:P:32:ARG:O	16:P:32:ARG:HD3	1.85	0.76
1:A:447:A:OP1	21:U:2:LYS:HG2	1.85	0.76
1:A:284:C:H4'	1:A:285:A:O5'	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.66	0.76
11:K:74:ARG:HH11	11:K:74:ARG:HB3	1.49	0.76
1:A:1187:U:H2'	37:A:6468:HOH:O	1.85	0.76
1:A:1191:A:H3'	1:A:1192:A:H5''	1.67	0.76
1:A:2054:A:N3	19:S:128:ARG:NH2	2.33	0.76
1:A:31:C:H2'	37:A:7262:HOH:O	1.85	0.76
1:A:1118:A:C8	1:A:1118:A:H3'	2.21	0.76
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.68	0.76
1:A:2506:A:O2'	1:A:2507:G:H8	1.66	0.76
1:A:544:G:H2'	1:A:545:G:H5''	1.67	0.76
5:E:214:THR:HG21	37:E:8398:HOH:O	1.85	0.76
28:2:10:LYS:HG3	37:2:8433:HOH:O	1.85	0.75
1:A:657:G:OP1	5:E:27:ARG:NH2	2.16	0.75
2:B:3049:G:H5''	37:B:8465:HOH:O	1.85	0.75
5:E:2:GLN:HB3	37:E:8336:HOH:O	1.86	0.75
37:A:4244:HOH:O	20:T:23:LYS:HE2	1.87	0.75
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.67	0.75
14:N:104:ARG:O	14:N:108:LYS:HE2	1.86	0.75
4:D:175:LEU:HD23	4:D:175:LEU:C	2.06	0.75
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.20	0.75
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.49	0.75
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.52	0.75
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.85	0.75
19:S:39:THR:HG23	19:S:107:GLU:O	1.85	0.75
28:2:25:LYS:HG2	28:2:25:LYS:O	1.86	0.75
5:E:214:THR:HG23	37:E:8433:HOH:O	1.86	0.75
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.22	0.75
1:A:2063:U:OP2	37:A:9303:HOH:O	2.04	0.75
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.51	0.75
26:Z:133:HIS:HD2	37:Z:8169:HOH:O	1.70	0.75
4:D:238:ASN:HD22	4:D:240:GLY:H	1.34	0.74
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.17	0.74
22:V:14:GLU:O	22:V:17:THR:HB	1.86	0.74
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.05	0.74
1:A:21:G:H5'	19:S:2:ILE:HA	1.70	0.74
1:A:2533:C:H6	1:A:2533:C:H5'	1.51	0.74
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.87	0.74
1:A:188:C:H5''	14:N:163:LEU:HD21	1.70	0.74
2:B:3023:U:H3'	37:B:8478:HOH:O	1.86	0.74
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.70	0.74
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.86	0.74
1:A:2717:C:C2'	1:A:2718:C:H5''	2.17	0.74
30:4:73:GLU:HB3	37:4:8561:HOH:O	1.87	0.74
1:A:1234:U:N3	4:D:244:PRO:HB3	2.02	0.74
17:Q:143:ALA:HA	37:Q:2178:HOH:O	1.87	0.74
19:S:99:ALA:HB1	19:S:109:MET:CE	2.18	0.74
1:A:560:C:H42	1:A:597:A:H61	1.36	0.74
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.51	0.74
1:A:2637:A:H5'	37:A:8857:HOH:O	1.87	0.73
1:A:871:G:C5'	1:A:871:G:C8	2.62	0.73
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.68	0.73
6:F:27:ILE:HG22	6:F:28:GLY:H	1.52	0.73
1:A:1751:G:C2'	1:A:1752:G:H5''	2.18	0.73
37:A:4797:HOH:O	12:L:39:GLY:HA2	1.88	0.73
14:N:38:VAL:O	14:N:63:VAL:HG13	1.87	0.73
6:F:25:MET:CE	6:F:41:LEU:HG	2.18	0.73
1:A:1667:A:H5'	1:A:1667:A:C8	2.21	0.73
3:C:121:ALA:O	3:C:124:VAL:HG22	1.86	0.73
21:U:47:THR:HB	21:U:100:ASP:HB3	1.69	0.73
1:A:2812:A:H2	1:A:2814:A:H62	1.33	0.73
10:J:141:ASN:HA	37:J:8369:HOH:O	1.88	0.73
1:A:2851:G:O2'	1:A:2852:A:H5'	1.87	0.73
24:X:88:THR:HG23	24:X:110:GLN:NE2	2.03	0.73
1:A:1118:A:H3'	1:A:1118:A:H8	1.53	0.73
7:G:11:VAL:HG12	7:G:12:ASP:N	2.04	0.73
1:A:1164:U:H3	1:A:1192:A:H2	1.36	0.73
1:A:2508:C:H2'	37:A:6330:HOH:O	1.89	0.73
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.71	0.73
13:M:67:ARG:O	13:M:71:GLU:HG3	1.88	0.73
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.53	0.73
1:A:289:G:H22	1:A:363:A:H2	1.37	0.73
11:K:99:GLU:HA	37:K:7377:HOH:O	1.87	0.73
14:N:84:LYS:HE2	37:N:8575:HOH:O	1.89	0.73
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.71	0.73
1:A:2638:G:H1'	37:A:7334:HOH:O	1.87	0.73
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.71	0.73
15:O:164:ASP:CG	15:O:167:ASP:HA	2.09	0.73
4:D:82:VAL:O	4:D:82:VAL:HG12	1.88	0.72
37:A:5369:HOH:O	14:N:170:CYS:SG	2.47	0.72
13:M:143:THR:HG22	13:M:144:ASP:N	2.04	0.72
14:N:104:ARG:O	14:N:108:LYS:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.72	0.72
20:T:57:THR:HG22	20:T:59:ASP:N	2.02	0.72
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.87	0.72
1:A:346:U:H4'	37:A:6416:HOH:O	1.88	0.72
6:F:49:PRO:HG3	37:F:5828:HOH:O	1.88	0.72
6:F:95:THR:O	6:F:97:GLN:N	2.17	0.72
1:A:450:C:OP1	5:E:184:ARG:NH2	2.18	0.72
1:A:559:U:H6	1:A:559:U:H5'	1.53	0.72
5:E:107:ARG:HB3	5:E:107:ARG:NH1	2.04	0.72
37:A:4523:HOH:O	2:B:3103:A:H4'	1.89	0.72
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.71	0.72
24:X:122:ARG:NH2	24:X:154:ARG:HD2	2.03	0.72
14:N:87:MET:CB	30:4:46:ILE:HD13	2.18	0.72
9:I:12:ILE:N	9:I:13:PRO:HD3	2.03	0.72
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.22	0.72
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.72	0.72
6:F:136:ARG:HD2	6:F:155:HIS:O	1.89	0.72
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.53	0.72
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.70	0.72
26:Z:141:THR:HG23	37:Z:8175:HOH:O	1.89	0.72
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.90	0.72
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.18	0.71
11:K:19:MET:CE	11:K:132:LEU:HD11	2.20	0.71
1:A:2716:G:H5''	4:D:206:THR:HG21	1.71	0.71
5:E:132:ASP:HB3	37:E:8360:HOH:O	1.90	0.71
8:H:96:ALA:HA	37:H:3111:HOH:O	1.90	0.71
13:M:114:VAL:HG11	37:M:8445:HOH:O	1.90	0.71
20:T:51:GLN:NE2	20:T:53:ASN:HD21	1.88	0.71
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.55	0.71
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.55	0.71
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.21	0.71
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.71
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.20	0.71
1:A:281:U:H2'	1:A:282:C:O4'	1.90	0.71
5:E:140:VAL:HB	37:E:8448:HOH:O	1.89	0.71
24:X:154:ARG:C	37:X:4276:HOH:O	2.28	0.71
20:T:51:GLN:HE21	20:T:53:ASN:ND2	1.88	0.71
1:A:603:A:H5''	1:A:604:G:OP1	1.90	0.71
4:D:36:PRO:HA	4:D:168:GLY:CA	2.21	0.71
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.89	0.71
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.73	0.71
30:4:70:ARG:HD3	37:4:8539:HOH:O	1.90	0.71
1:A:2779:G:H21	7:G:143:GLN:NE2	1.89	0.71
10:J:162:SER:CB	10:J:163:PRO:HD3	2.19	0.71
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.05	0.71
14:N:164:THR:HG22	14:N:167:GLY:N	2.04	0.71
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.90	0.71
1:A:1185:U:H2'	1:A:1186:C:C6	2.26	0.70
1:A:541:C:H2'	1:A:542:A:C5'	2.18	0.70
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.26	0.70
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.73	0.70
1:A:1187:U:HO2'	1:A:1189:A:H2	1.37	0.70
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.73	0.70
6:F:55:LYS:HA	37:F:6752:HOH:O	1.91	0.70
2:B:3039:U:H1'	2:B:3044:A:H61	1.57	0.70
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.07	0.70
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.39	0.70
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.70
2:B:3026:C:P	37:B:8441:HOH:O	2.48	0.70
6:F:23:VAL:HG23	6:F:23:VAL:O	1.92	0.70
37:A:5870:HOH:O	6:F:99:ASP:HA	1.90	0.70
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.72	0.70
1:A:2768:A:H2'	1:A:2769:C:O4'	1.91	0.69
2:B:3035:C:H5''	37:B:8455:HOH:O	1.91	0.69
1:A:2812:A:N7	37:A:7092:HOH:O	2.24	0.69
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.21	0.69
1:A:2346:C:O2'	6:F:52:THR:HG21	1.92	0.69
8:H:91:VAL:HG12	8:H:92:GLY:H	1.57	0.69
3:C:173:GLY:O	3:C:176:HIS:HB3	1.91	0.69
6:F:35:ALA:N	37:F:5576:HOH:O	2.24	0.69
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.28	0.69
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.56	0.69
1:A:21:G:C5'	19:S:2:ILE:HA	2.22	0.69
1:A:381:G:H5''	37:A:3894:HOH:O	1.92	0.69
35:A:8513:CL:CL	37:A:4259:HOH:O	2.46	0.69
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.92	0.69
1:A:1127:C:H2'	1:A:1128:U:H5'	1.72	0.69
23:W:64:GLY:O	23:W:65:ASP:HB2	1.91	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.92	0.69
1:A:1441:G:O2'	1:A:1442:A:H5'	1.93	0.69
1:A:2301:A:H5''	1:A:2302:A:H5'	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.27	0.69
11:K:107:ASN:ND2	11:K:109:TYR:H	1.90	0.69
14:N:30:GLU:O	14:N:34:GLU:HG3	1.92	0.69
1:A:1328:A:N7	1:A:1329:A:C5	2.61	0.69
16:P:87:THR:O	16:P:91:GLN:HG3	1.93	0.69
12:L:55:VAL:HG12	12:L:56:SER:N	2.08	0.69
14:N:164:THR:CG2	14:N:165:SER:N	2.55	0.69
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.69
1:A:282:C:H1'	1:A:368:C:H42	1.58	0.69
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.58	0.69
1:A:1835:U:C5	1:A:1840:A:N7	2.55	0.68
6:F:95:THR:C	6:F:97:GLN:H	1.96	0.68
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.75	0.68
1:A:1973:A:H8	1:A:1973:A:H5'	1.57	0.68
1:A:1862:C:H1'	37:A:6790:HOH:O	1.92	0.68
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.28	0.68
4:D:297:VAL:HB	37:D:8607:HOH:O	1.93	0.68
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.75	0.68
1:A:1160:G:N3	37:A:5210:HOH:O	2.26	0.68
1:A:820:G:O2'	1:A:856:G:H4'	1.94	0.68
10:J:139:ASP:HA	37:J:8373:HOH:O	1.93	0.68
6:F:69:ILE:O	6:F:69:ILE:HG22	1.93	0.68
11:K:88:PRO:HA	35:K:8502:CL:CL	2.30	0.68
14:N:139:PRO:O	14:N:140:ALA:HB3	1.93	0.68
37:A:3935:HOH:O	16:P:37:ARG:HG3	1.94	0.68
1:A:2420:G:O2'	1:A:2421:G:H5'	1.94	0.68
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.91	0.68
23:W:58:THR:O	23:W:62:GLU:HG3	1.94	0.68
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.58	0.68
1:A:2414:A:H2'	1:A:2415:A:C8	2.28	0.68
2:B:3028:U:H2'	2:B:3029:C:C6	2.29	0.68
22:V:9:CYS:HA	22:V:52:THR:HG23	1.74	0.68
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.74	0.68
1:A:1209:C:H2'	1:A:1210:G:H8	1.59	0.68
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.59	0.68
27:1:19:GLY:O	27:1:23:ARG:HG2	1.93	0.67
15:O:80:SER:HB2	37:O:8536:HOH:O	1.93	0.67
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.57	0.67
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.67
23:W:39:ALA:N	23:W:40:PRO:HD2	2.09	0.67
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2265:U:H2'	1:A:2266:A:C8	2.30	0.67
8:H:110:GLU:HG2	37:H:6926:HOH:O	1.95	0.67
1:A:1119:G:N2	1:A:1246:A:H2	1.91	0.67
1:A:2064:U:OP1	37:A:9929:HOH:O	2.12	0.67
1:A:1003:U:O2	10:J:90:PHE:HZ	1.78	0.67
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.43	0.67
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.77	0.67
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.59	0.67
3:C:131:HIS:O	3:C:132:ASP:HB2	1.93	0.67
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.30	0.67
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.77	0.67
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.94	0.67
1:A:1733:A:H4'	4:D:212:GLN:HA	1.75	0.67
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.93	0.67
24:X:65:VAL:HA	24:X:68:THR:HG22	1.77	0.67
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	1.95	0.67
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.94	0.67
5:E:233:THR:HG22	5:E:234:VAL:N	2.08	0.67
14:N:138:HIS:ND1	14:N:139:PRO:O	2.22	0.67
19:S:39:THR:HB	19:S:42:GLU:HG3	1.76	0.67
1:A:506:G:H22	1:A:509:A:H5'	1.60	0.67
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.77	0.67
8:H:99:THR:HA	37:H:3461:HOH:O	1.95	0.67
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.09	0.67
1:A:1919:A:H4'	37:A:4419:HOH:O	1.95	0.66
1:A:2004:U:H4'	37:A:4881:HOH:O	1.94	0.66
1:A:2578:G:H8	1:A:2578:G:H5'	1.60	0.66
2:B:3023:U:C4'	2:B:3024:U:OP2	2.39	0.66
11:K:133:GLY:O	11:K:137:GLU:HG3	1.95	0.66
20:T:80:ARG:NH1	37:T:8346:HOH:O	2.28	0.66
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.75	0.66
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.26	0.66
37:A:7154:HOH:O	27:1:31:ILE:HG13	1.95	0.66
1:A:69:A:H8	1:A:69:A:H5'	1.60	0.66
1:A:885:G:OP2	37:A:8984:HOH:O	2.14	0.66
3:C:192:VAL:HB	37:C:8596:HOH:O	1.94	0.66
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.76	0.66
14:N:139:PRO:O	14:N:140:ALA:CB	2.43	0.66
1:A:870:G:C2'	1:A:871:G:H5''	2.23	0.66
14:N:38:VAL:C	14:N:63:VAL:HG13	2.15	0.66
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:C:O2'	1:A:1214:G:H5'	1.96	0.66
1:A:2391:C:OP1	37:A:8913:HOH:O	2.14	0.66
1:A:1847:A:OP1	3:C:175:LYS:HG3	1.96	0.66
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.77	0.66
24:X:149:LEU:HG	24:X:153:MET:HE2	1.75	0.66
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.29	0.66
26:Z:212:ARG:HD2	37:Z:8186:HOH:O	1.95	0.66
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.28	0.66
1:A:2361:A:H5''	37:A:8601:HOH:O	1.94	0.66
3:C:200:PRO:O	37:C:8589:HOH:O	2.14	0.66
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.95	0.66
23:W:12:THR:HG22	23:W:15:GLU:CG	2.18	0.66
1:A:2587:U:H2'	1:A:2589:U:H5''	1.78	0.66
10:J:14:TYR:H	10:J:91:HIS:CE1	2.13	0.66
29:3:41:HIS:H	29:3:45:ASN:ND2	1.94	0.66
14:N:87:MET:CB	30:4:46:ILE:HG21	2.25	0.66
1:A:2630:G:O6	3:C:206:ARG:NH2	2.28	0.66
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.77	0.66
37:A:7029:HOH:O	5:E:188:ARG:HD2	1.95	0.66
11:K:93:ARG:HH11	11:K:93:ARG:HB3	1.59	0.66
1:A:1330:A:H5''	1:A:1331:A:OP2	1.95	0.66
1:A:204:A:H2'	1:A:205:U:H5'	1.77	0.66
1:A:2064:U:H5'	1:A:2652:U:O3'	1.96	0.66
2:B:3029:C:H2'	2:B:3030:C:H5'	1.77	0.66
21:U:48:VAL:HG22	21:U:97:ARG:C	2.15	0.66
29:3:41:HIS:N	29:3:45:ASN:HD22	1.92	0.66
1:A:1159:G:P	37:A:3869:HOH:O	2.53	0.66
1:A:428:G:OP1	37:A:5799:HOH:O	2.13	0.66
6:F:97:GLN:O	6:F:97:GLN:HG2	1.96	0.66
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.61	0.66
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.60	0.66
27:1:28:ASP:O	27:1:31:ILE:HG22	1.96	0.65
1:A:2488:A:H61	1:A:2534:C:H42	1.43	0.65
1:A:681:G:N3	1:A:681:G:H5'	2.11	0.65
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.77	0.65
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.31	0.65
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.10	0.65
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.96	0.65
1:A:2719:A:C2	4:D:70:PRO:HG3	2.31	0.65
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.95	0.65
1:A:1119:G:H8	11:K:52:GLN:HE22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:A:N7	37:A:9440:HOH:O	2.30	0.65
6:F:135:VAL:HG22	6:F:136:ARG:H	1.61	0.65
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.11	0.65
1:A:69:A:C8	1:A:69:A:H5'	2.31	0.65
3:C:1:GLY:N	37:C:8611:HOH:O	2.28	0.65
4:D:175:LEU:O	4:D:175:LEU:HD23	1.96	0.65
26:Z:216:ARG:HD3	37:Z:8157:HOH:O	1.95	0.65
1:A:2064:U:H4'	1:A:2653:A:OP1	1.97	0.65
6:F:19:GLU:O	6:F:20:LYS:HG2	1.96	0.65
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.26	0.65
37:B:8473:HOH:O	15:O:23:ARG:HD3	1.96	0.65
23:W:44:GLY:O	23:W:48:GLU:HG2	1.96	0.65
1:A:299:U:H5'	37:A:6908:HOH:O	1.97	0.65
1:A:316:A:H5'	21:U:54:ASP:OD2	1.97	0.65
4:D:145:HIS:HD2	4:D:146:THR:O	1.78	0.65
7:G:6:GLU:HA	7:G:46:THR:HG22	1.77	0.65
8:H:91:VAL:HG12	8:H:92:GLY:N	2.11	0.65
3:C:105:VAL:HG12	3:C:106:CYS:N	2.12	0.65
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.79	0.65
1:A:131:A:OP2	37:A:9746:HOH:O	2.14	0.65
1:A:2502:C:C2'	1:A:2503:A:H5'	2.27	0.65
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.76	0.65
22:V:52:THR:HG22	22:V:54:THR:H	1.62	0.65
1:A:2536:C:OP1	37:A:9702:HOH:O	2.12	0.65
4:D:2:GLN:HA	37:D:8622:HOH:O	1.96	0.65
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.79	0.65
10:J:57:ARG:O	10:J:61:LEU:HD22	1.97	0.65
1:A:545:G:H5'	1:A:545:G:C8	2.30	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.30	0.65
35:K:8501:CL:CL	37:K:4038:HOH:O	2.51	0.65
14:N:60:ILE:C	14:N:61:ILE:HD12	2.17	0.65
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.79	0.65
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.78	0.65
1:A:1130:U:H2'	1:A:1131:G:O4'	1.97	0.64
1:A:1377:C:H5'	1:A:1377:C:H6	1.62	0.64
1:A:2908:A:H2'	1:A:2909:G:O4'	1.97	0.64
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.96	0.64
6:F:37:ALA:O	6:F:40:ILE:HG12	1.97	0.64
20:T:58:MET:SD	29:3:8:LYS:HE3	2.37	0.64
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.64
1:A:272:A:H3'	37:A:7105:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:GLU:O	4:D:129:ARG:HG3	1.96	0.64
11:K:19:MET:HE2	11:K:132:LEU:HD11	1.77	0.64
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.78	0.64
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.63	0.64
27:1:61:GLY:HA3	37:1:8427:HOH:O	1.97	0.64
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.79	0.64
1:A:1329:A:N1	35:A:8513:CL:CL	2.67	0.64
5:E:78:ARG:NH1	5:E:78:ARG:HG3	2.08	0.64
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.12	0.64
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.27	0.64
5:E:236:THR:CG2	5:E:239:ALA:H	2.00	0.64
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.32	0.64
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.33	0.64
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.64
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.12	0.64
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.80	0.64
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.79	0.64
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.10	0.64
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.79	0.64
1:A:558:C:O2'	1:A:559:U:H5"	1.98	0.64
4:D:16:ARG:NE	37:D:8556:HOH:O	2.11	0.64
7:G:7:ILE:HD11	7:G:11:VAL:C	2.18	0.64
13:M:136:ALA:HB3	37:M:8445:HOH:O	1.97	0.64
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.80	0.64
4:D:179:LEU:O	4:D:183:GLU:HG2	1.98	0.64
4:D:258:GLY:H	4:D:260:HIS:CE1	2.14	0.64
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.12	0.64
1:A:182:G:H5'	37:A:4731:HOH:O	1.98	0.64
1:A:2783:A:H3'	37:A:4807:HOH:O	1.98	0.64
11:K:88:PRO:CA	35:K:8502:CL:CL	2.83	0.64
1:A:821:U:O2'	1:A:822:C:H5'	1.98	0.64
15:O:154:LEU:O	15:O:155:GLU:HB3	1.98	0.64
4:D:162:MET:CE	4:D:308:LEU:HD21	2.27	0.64
5:E:180:SER:HB2	37:E:8442:HOH:O	1.97	0.64
5:E:129:HIS:CE1	5:E:232:LEU:H	2.16	0.64
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.80	0.64
14:N:172:GLY:O	14:N:183:VAL:HG11	1.98	0.64
1:A:1741:U:H5'	1:A:1742:A:OP1	1.97	0.63
2:B:3092:G:H2'	2:B:3093:A:C8	2.34	0.63
8:H:58:GLU:HA	8:H:61:MET:HE2	1.80	0.63
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:41:TYR:O	24:X:45:VAL:HG13	1.98	0.63
1:A:2748:G:H2'	37:A:7117:HOH:O	1.97	0.63
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.28	0.63
30:4:65:THR:HG23	30:4:67:LEU:HG	1.80	0.63
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.31	0.63
5:E:219:ASN:O	5:E:222:ASP:OD1	2.16	0.63
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.47	0.63
4:D:75:GLU:C	4:D:77:PRO:HD3	2.19	0.63
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.80	0.63
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.33	0.63
1:A:1441:G:H1'	37:A:7340:HOH:O	1.98	0.63
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.63	0.63
6:F:25:MET:HE1	6:F:37:ALA:O	1.99	0.63
1:A:1015:C:H2'	1:A:1016:U:H6	1.63	0.63
1:A:2502:C:H2'	1:A:2503:A:H5'	1.80	0.63
3:C:94:LEU:HD23	3:C:94:LEU:N	2.13	0.63
4:D:48:MET:N	37:D:8560:HOH:O	2.31	0.63
5:E:242:GLU:HG3	37:E:8378:HOH:O	1.97	0.63
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.81	0.63
1:A:1878:G:H1'	37:A:5700:HOH:O	1.97	0.63
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.32	0.63
1:A:281:U:H3'	37:A:6777:HOH:O	1.99	0.63
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.44	0.63
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.14	0.63
21:U:65:VAL:HG22	21:U:72:ILE:HG22	1.81	0.63
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.20	0.63
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.79	0.63
1:A:1735:C:O2'	1:A:1736:A:H5'	1.99	0.63
1:A:2468:A:H61	30:4:48:ASN:HD21	1.45	0.63
1:A:2419:U:H5''	1:A:2420:G:H5'	1.80	0.63
37:A:6598:HOH:O	3:C:211:LYS:HG2	1.99	0.63
5:E:127:ARG:HH11	5:E:127:ARG:HG2	1.62	0.63
1:A:111:C:O2'	28:2:20:ARG:HG2	1.99	0.62
2:B:3001:U:O3'	2:B:3003:A:H5''	1.99	0.62
10:J:59:ASN:H	10:J:59:ASN:ND2	1.96	0.62
11:K:52:GLN:HG3	11:K:53:ILE:N	2.14	0.62
22:V:52:THR:HG22	22:V:54:THR:N	2.13	0.62
27:1:29:VAL:O	27:1:33:HIS:HB2	1.99	0.62
1:A:1679:C:H5'	37:A:8905:HOH:O	1.98	0.62
1:A:419:A:H1'	1:A:1921:A:C2	2.34	0.62
1:A:2416:G:O2'	37:A:9212:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:THR:HB	37:E:8438:HOH:O	1.98	0.62
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.99	0.62
1:A:1503:U:H2'	1:A:1504:A:O4'	1.98	0.62
1:A:755:G:O2'	1:A:756:A:H5'	1.99	0.62
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.34	0.62
1:A:2099:G:N2	31:A:8600:ZIT:H181	2.14	0.62
1:A:2383:G:N3	37:A:6280:HOH:O	2.31	0.62
5:E:139:VAL:HG13	37:E:8445:HOH:O	1.98	0.62
25:Y:31:ILE:O	25:Y:35:GLU:HG3	2.00	0.62
1:A:960:G:N3	1:A:960:G:H2'	2.15	0.62
4:D:62:ARG:HA	4:D:65:MET:CE	2.28	0.62
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.32	0.62
8:H:19:ALA:O	8:H:22:VAL:HG22	2.00	0.62
14:N:186:SER:OG	14:N:189:VAL:HG12	1.99	0.62
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.82	0.62
1:A:542:A:H8	1:A:542:A:C5'	2.07	0.62
3:C:53:ALA:HB3	37:C:8609:HOH:O	2.00	0.62
12:L:115:ARG:HG3	12:L:116:GLU:N	2.14	0.62
13:M:133:VAL:HB	37:M:8431:HOH:O	1.99	0.62
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.31	0.62
15:O:151:ASP:O	15:O:154:LEU:HB2	2.00	0.62
22:V:37:GLU:HB3	37:V:408:HOH:O	1.98	0.62
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.34	0.62
26:Z:235:GLU:CD	26:Z:235:GLU:H	2.03	0.62
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.00	0.62
11:K:74:ARG:O	11:K:78:ILE:HG12	1.99	0.62
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.80	0.62
1:A:1701:A:H5'	37:A:5859:HOH:O	1.99	0.62
1:A:1701:A:H4'	1:A:1702:U:H5''	1.80	0.62
1:A:1789:G:O6	17:Q:73:HIS:HE1	1.83	0.62
2:B:3013:A:O2'	2:B:3014:G:H5''	2.00	0.62
3:C:109:GLU:HG2	3:C:116:GLY:H	1.65	0.62
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.15	0.62
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.98	0.62
8:H:2:VAL:HG22	8:H:57:GLU:OE1	2.00	0.62
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.00	0.62
1:A:2526:C:O2'	1:A:2527:U:H5'	2.00	0.62
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.35	0.62
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.35	0.62
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	1.81	0.62
27:I:13:ARG:NH1	27:I:14:PHE:CE2	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:U:O2'	1:A:1118:A:C2	2.46	0.61
1:A:396:U:H1'	37:A:7204:HOH:O	1.99	0.61
13:M:57:VAL:HG12	13:M:57:VAL:O	2.00	0.61
15:O:12:ARG:HD3	15:O:18:THR:OG1	2.00	0.61
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.82	0.61
37:A:3767:HOH:O	26:Z:186:ARG:HD2	1.99	0.61
1:A:1306:U:OP1	5:E:184:ARG:HD2	2.00	0.61
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.82	0.61
5:E:236:THR:H	5:E:239:ALA:HB3	1.65	0.61
1:A:1003:U:O2	10:J:90:PHE:CZ	2.53	0.61
4:D:204:GLY:HA3	37:D:8658:HOH:O	1.99	0.61
5:E:118:THR:O	5:E:136:VAL:HG13	2.01	0.61
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.82	0.61
25:Y:41:PHE:O	25:Y:43:VAL:HG23	2.00	0.61
1:A:1329:A:H2	37:A:4259:HOH:O	1.83	0.61
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.35	0.61
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.82	0.61
9:I:12:ILE:N	9:I:13:PRO:CD	2.64	0.61
10:J:53:PRO:HG3	10:J:127:GLY:H	1.64	0.61
11:K:45:VAL:HG23	11:K:130:VAL:O	2.01	0.61
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.82	0.61
20:T:81:ILE:HG23	37:T:8337:HOH:O	2.00	0.61
1:A:1200:A:H4'	37:A:6912:HOH:O	1.99	0.61
1:A:1313:A:H5'	26:Z:208:LYS:O	2.00	0.61
3:C:101:GLU:OE2	3:C:131:HIS:HB2	2.00	0.61
6:F:99:ASP:CB	6:F:103:ASN:H	2.13	0.61
10:J:144:GLU:HA	10:J:144:GLU:OE1	2.00	0.61
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.15	0.61
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.36	0.61
30:4:62:THR:HB	37:4:8551:HOH:O	2.00	0.61
1:A:2827:A:H2'	1:A:2828:G:O4'	1.99	0.61
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.83	0.61
9:I:63:ARG:N	37:I:2569:HOH:O	2.33	0.61
23:W:49:LEU:O	23:W:53:ILE:HG13	1.99	0.61
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.64	0.61
1:A:2501:G:H1'	37:A:4118:HOH:O	2.00	0.61
1:A:2710:U:H1'	37:A:7196:HOH:O	2.00	0.61
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.30	0.61
1:A:1130:U:H5'	37:A:7245:HOH:O	2.00	0.61
1:A:2320:U:H4'	1:A:2321:A:O4'	2.01	0.61
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:237:GLU:HB2	37:E:8426:HOH:O	2.00	0.61
10:J:27:LYS:N	10:J:58:HIS:HD2	1.96	0.61
37:A:4405:HOH:O	11:K:47:THR:HB	1.99	0.61
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.36	0.61
1:A:182:G:H4'	14:N:157:LEU:HD13	1.82	0.61
1:A:184:G:H5''	14:N:153:THR:HG22	1.83	0.61
1:A:558:C:H2'	1:A:559:U:H5'	1.83	0.61
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.47	0.61
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.01	0.61
13:M:104:ASP:O	13:M:105:TYR:HB3	2.00	0.61
1:A:2505:G:O2'	1:A:2506:A:H5'	2.01	0.61
1:A:738:G:H3'	37:A:6619:HOH:O	2.00	0.61
32:A:8036:MG:MG	37:A:7398:HOH:O	1.43	0.61
2:B:3002:U:H4'	2:B:3002:U:OP2	2.00	0.61
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.14	0.61
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.01	0.61
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.81	0.61
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.27	0.61
16:P:42:GLU:HB2	37:P:2176:HOH:O	2.00	0.61
37:A:4040:HOH:O	14:N:146:GLN:HG2	1.99	0.60
1:A:240:C:H4'	14:N:146:GLN:NE2	2.16	0.60
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.35	0.60
1:A:2403:C:H3'	37:A:4787:HOH:O	2.01	0.60
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.83	0.60
5:E:85:LYS:NZ	37:E:8326:HOH:O	2.24	0.60
16:P:26:TRP:N	37:P:3062:HOH:O	2.34	0.60
22:V:52:THR:CG2	22:V:54:THR:HB	2.31	0.60
24:X:130:HIS:O	24:X:136:GLY:HA3	2.01	0.60
30:4:17:HIS:O	30:4:18:GLN:HG3	2.01	0.60
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.65	0.60
1:A:1120:U:H5''	1:A:1120:U:C6	2.36	0.60
1:A:1205:U:H2'	1:A:1206:U:C5'	2.30	0.60
1:A:1636:G:O2'	1:A:1637:A:H5'	2.00	0.60
4:D:305:ASP:O	4:D:306:LYS:HB2	2.02	0.60
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.70	0.60
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.82	0.60
1:A:136:C:H2'	1:A:137:U:O4'	2.00	0.60
1:A:2392:C:N3	37:A:4421:HOH:O	2.31	0.60
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.33	0.60
5:E:84:VAL:O	5:E:85:LYS:HB2	2.00	0.60
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.83	0.60
10:J:139:ASP:H	10:J:140:PRO:HD3	1.66	0.60
1:A:1200:A:C4'	37:A:6912:HOH:O	2.49	0.60
1:A:2346:C:H6	1:A:2346:C:O5'	1.83	0.60
1:A:321:A:H1'	37:A:6605:HOH:O	2.02	0.60
7:G:23:GLU:HG2	7:G:28:SER:CB	2.32	0.60
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.30	0.60
10:J:136:VAL:HG22	10:J:137:ASN:O	2.01	0.60
10:J:26:LYS:HG2	10:J:28:ILE:N	2.15	0.60
10:J:53:PRO:HA	10:J:125:VAL:O	2.02	0.60
10:J:71:TYR:C	10:J:73:GLN:H	2.05	0.60
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.35	0.60
1:A:212:A:O4'	1:A:214:U:C6	2.55	0.60
1:A:2672:C:H1'	37:A:6256:HOH:O	2.01	0.60
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.02	0.60
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.02	0.60
20:T:43:GLU:HB3	37:T:8344:HOH:O	2.01	0.60
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.14	0.60
1:A:1834:C:H2'	1:A:1840:A:N6	2.17	0.60
1:A:2121:G:OP2	37:A:3095:HOH:O	2.17	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.02	0.60
1:A:2756:U:H3	1:A:2896:A:H2	1.46	0.60
11:K:131:THR:HG22	11:K:134:GLU:H	1.65	0.60
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.84	0.60
6:F:101:THR:HG22	37:F:7400:HOH:O	2.01	0.60
4:D:301:VAL:HG13	4:D:302:PRO:HD2	1.83	0.60
7:G:101:GLU:HB2	7:G:116:THR:O	2.02	0.60
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.83	0.60
15:O:37:ARG:NE	37:O:8534:HOH:O	2.34	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.59
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.82	0.59
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.65	0.59
14:N:69:LYS:HG2	14:N:127:LYS:HG3	1.82	0.59
14:N:52:LEU:HD21	37:N:8615:HOH:O	2.02	0.59
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.48	0.59
27:1:53:GLY:HA2	27:1:67:GLY:O	2.01	0.59
1:A:1134:G:H4'	10:J:151:MET:CE	2.27	0.59
3:C:211:LYS:NZ	37:C:8574:HOH:O	2.35	0.59
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.35	0.59
8:H:28:ALA:HB3	8:H:99:THR:O	2.02	0.59
1:A:1766:U:O2	1:A:1778:A:H5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.38	0.59
15:O:169:PRO:O	15:O:172:PHE:HB3	2.02	0.59
24:X:139:GLY:O	24:X:141:HIS:HD2	1.84	0.59
1:A:2256:G:O2'	1:A:2257:G:H5'	2.02	0.59
3:C:191:GLY:HA2	3:C:194:MET:HE3	1.84	0.59
4:D:168:GLY:N	4:D:174:ARG:HD3	2.17	0.59
5:E:104:ASP:O	5:E:108:GLN:HG3	2.03	0.59
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.31	0.59
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.18	0.59
26:Z:185:VAL:HG12	37:Z:8158:HOH:O	2.00	0.59
1:A:1058:A:H2'	1:A:1060:C:H5''	1.83	0.59
1:A:1165:G:OP1	1:A:1165:G:H3'	2.03	0.59
1:A:1159:G:H21	1:A:1189:A:H8	1.49	0.59
1:A:2434:A:O3'	30:4:28:GLY:HA3	2.03	0.59
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.66	0.59
2:B:3107:C:C5	37:B:8437:HOH:O	2.52	0.59
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.84	0.59
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.85	0.59
20:T:53:ASN:ND2	37:T:8323:HOH:O	2.35	0.59
1:A:151:A:C2	1:A:442:A:C8	2.90	0.59
2:B:3039:U:H1'	2:B:3044:A:N6	2.17	0.59
4:D:62:ARG:CA	4:D:65:MET:HE3	2.29	0.59
5:E:16:VAL:HG12	5:E:17:ASP:N	2.17	0.59
10:J:163:PRO:O	10:J:164:ALA:HB2	2.03	0.59
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.03	0.59
1:A:1249:U:H2'	1:A:1250:C:C6	2.37	0.59
1:A:544:G:C2'	1:A:545:G:H5''	2.31	0.59
37:A:6798:HOH:O	14:N:13:LYS:HE2	2.03	0.59
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.83	0.59
1:A:1187:U:O2'	1:A:1189:A:H2	1.85	0.59
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.84	0.59
37:A:8703:HOH:O	5:E:103:ASN:HB3	2.02	0.59
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.14	0.59
28:2:28:HIS:HD2	28:2:31:LYS:H	1.50	0.59
1:A:156:C:H5''	14:N:171:ARG:CD	2.23	0.59
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.59
1:A:263:U:O4'	8:H:59:ILE:HD13	2.02	0.59
3:C:33:GLU:O	3:C:34:ASP:HB2	2.02	0.59
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.85	0.59
10:J:127:GLY:O	10:J:128:ALA:HB3	2.03	0.59
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:61:ILE:HA	37:N:8622:HOH:O	2.03	0.59
1:A:396:U:H5'	30:4:42:ARG:HH12	1.67	0.59
1:A:558:C:H2'	1:A:559:U:C5'	2.33	0.59
2:B:3025:G:N2	37:B:8507:HOH:O	2.36	0.59
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.66	0.59
1:A:449:A:N7	5:E:43:LYS:HG2	2.17	0.59
1:A:1119:G:H8	11:K:52:GLN:NE2	2.01	0.59
13:M:143:THR:HG22	13:M:145:LEU:H	1.66	0.59
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.18	0.59
16:P:25:VAL:HG23	16:P:26:TRP:N	2.18	0.59
28:2:20:ARG:HB2	37:2:8413:HOH:O	2.02	0.58
1:A:2769:C:C2'	1:A:2770:G:H5'	2.33	0.58
1:A:2878:U:H2'	1:A:2879:A:O4'	2.03	0.58
3:C:114:ASP:HB2	3:C:117:LYS:HE2	1.84	0.58
5:E:1:MET:HG2	5:E:2:GLN:N	2.16	0.58
14:N:146:GLN:NE2	37:N:8645:HOH:O	2.36	0.58
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.42	0.58
1:A:157:G:H4'	14:N:95:LYS:HE3	1.85	0.58
3:C:37:VAL:HG22	37:C:8599:HOH:O	2.02	0.58
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.18	0.58
4:D:16:ARG:NH2	37:D:8556:HOH:O	2.34	0.58
23:W:39:ALA:C	23:W:41:GLU:H	2.06	0.58
1:A:1234:U:C4	4:D:244:PRO:HB3	2.39	0.58
1:A:1423:C:O2'	1:A:1424:A:H5'	2.03	0.58
6:F:86:THR:O	6:F:90:LEU:HG	2.03	0.58
37:A:9350:HOH:O	13:M:41:HIS:HE1	1.86	0.58
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.33	0.58
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.85	0.58
1:A:2256:G:C2'	1:A:2257:G:H5'	2.33	0.58
1:A:566:A:H2'	1:A:567:U:O4'	2.03	0.58
14:N:12:TRP:O	14:N:15:PRO:HD3	2.02	0.58
1:A:1192:A:O2'	1:A:1193:A:OP1	2.21	0.58
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.86	0.58
4:D:79:MET:HE1	37:D:8627:HOH:O	2.03	0.58
6:F:50:VAL:O	6:F:71:ALA:HA	2.03	0.58
8:H:28:ALA:CB	8:H:99:THR:HG23	2.32	0.58
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.85	0.58
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.86	0.58
16:P:47:ARG:NH1	16:P:47:ARG:HG3	2.17	0.58
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.33	0.58
1:A:1182:C:H1'	1:A:1192:A:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.34	0.58
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.03	0.58
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.32	0.58
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.01	0.58
1:A:558:C:C2'	1:A:559:U:H5''	2.33	0.58
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.86	0.58
21:U:101:LEU:HD13	21:U:112:LEU:HD11	1.86	0.58
29:3:18:ASN:HD21	29:3:40:ARG:H	1.52	0.58
1:A:1559:A:H1'	37:A:5443:HOH:O	2.04	0.58
9:I:12:ILE:HA	37:I:4499:HOH:O	2.03	0.58
1:A:2094:G:H4'	4:D:245:SER:HB3	1.85	0.58
1:A:241:A:C2	1:A:378:A:H4'	2.39	0.58
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.02	0.58
1:A:656:G:OP2	16:P:37:ARG:HD2	2.03	0.58
1:A:396:U:H5'	30:4:42:ARG:NH1	2.18	0.58
1:A:2276:U:H2'	1:A:2277:U:C6	2.38	0.58
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.18	0.58
5:E:107:ARG:NE	37:E:8454:HOH:O	2.25	0.58
37:A:7282:HOH:O	5:E:94:THR:HG21	2.04	0.58
37:A:5895:HOH:O	6:F:55:LYS:HB2	2.04	0.58
12:L:28:GLU:HB3	12:L:59:LYS:HB2	1.86	0.58
12:L:55:VAL:HG12	12:L:56:SER:H	1.68	0.58
13:M:149:ARG:O	13:M:150:GLN:HB2	2.03	0.58
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
3:C:186:TRP:CG	3:C:187:PRO:HA	2.39	0.57
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.34	0.57
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.86	0.57
19:S:119:VAL:HG12	19:S:119:VAL:O	2.03	0.57
1:A:2265:U:H2'	1:A:2266:A:H8	1.67	0.57
1:A:2472:C:O2'	1:A:2634:G:H4'	2.04	0.57
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.34	0.57
1:A:1086:A:C6	24:X:11:VAL:HG11	2.38	0.57
1:A:281:U:O2'	1:A:282:C:H5'	2.04	0.57
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.86	0.57
24:X:31:HIS:ND1	37:X:2229:HOH:O	2.32	0.57
1:A:20:G:H21	19:S:117:HIS:HD2	1.51	0.57
2:B:3107:C:H5	37:B:8437:HOH:O	1.86	0.57
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.04	0.57
1:A:204:A:C2'	1:A:205:U:H5'	2.33	0.57
1:A:280:C:H2'	1:A:281:U:O4'	2.05	0.57
1:A:336:G:OP1	37:A:3304:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:145:LEU:O	13:M:148:GLU:HG3	2.03	0.57
16:P:39:THR:O	16:P:115:ARG:NH2	2.37	0.57
1:A:1191:A:C3'	1:A:1192:A:H5''	2.35	0.57
4:D:40:GLY:O	37:D:8557:HOH:O	2.17	0.57
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.86	0.57
9:I:64:ASN:HD22	9:I:64:ASN:N	2.02	0.57
15:O:86:LEU:O	15:O:90:LEU:HG	2.05	0.57
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.34	0.57
1:A:1028:U:H1'	37:A:3225:HOH:O	2.05	0.57
1:A:2488:A:H1'	37:A:8685:HOH:O	2.05	0.57
37:A:7029:HOH:O	5:E:188:ARG:CD	2.52	0.57
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.87	0.57
15:O:100:ALA:O	15:O:129:ILE:HG23	2.04	0.57
37:B:8465:HOH:O	15:O:147:ILE:HD12	2.04	0.57
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.04	0.57
1:A:283:U:H5	1:A:284:C:N4	2.02	0.57
1:A:2866:U:C2	37:A:7073:HOH:O	2.53	0.57
3:C:18:ALA:O	3:C:20:SER:N	2.34	0.57
21:U:37:GLN:OE1	21:U:118:SER:HA	2.05	0.57
24:X:38:THR:HG22	24:X:39:ASP:H	1.69	0.57
1:A:1730:G:H5'	1:A:1731:C:C5	2.40	0.57
1:A:629:A:C2	1:A:2074:A:C2	2.93	0.57
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.87	0.57
7:G:69:ILE:HA	7:G:72:MET:CE	2.35	0.57
10:J:65:ARG:CZ	37:J:8387:HOH:O	2.53	0.57
19:S:82:GLU:HG3	19:S:83:LYS:N	2.19	0.57
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.38	0.57
1:A:2415:A:C2	15:O:25:ARG:HB3	2.40	0.57
1:A:2769:C:H2'	1:A:2770:G:O4'	2.05	0.57
4:D:168:GLY:O	4:D:169:GLY:O	2.22	0.57
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.05	0.57
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.87	0.57
1:A:2502:C:H4'	10:J:151:MET:SD	2.45	0.57
37:A:6281:HOH:O	26:Z:165:GLU:HB3	2.04	0.57
1:A:1244:U:OP1	11:K:18:ILE:HD13	2.05	0.56
1:A:2256:G:H2'	1:A:2257:G:H5'	1.87	0.56
1:A:2748:G:H5'	37:A:7117:HOH:O	2.05	0.56
4:D:280:VAL:CG1	4:D:334:SER:HA	2.35	0.56
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.87	0.56
10:J:166:ASN:N	10:J:166:ASN:HD22	2.02	0.56
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:G:H4'	19:S:2:ILE:HG22	1.87	0.56
1:A:1474:C:C5'	1:A:1474:C:H6	2.11	0.56
1:A:2635:A:O2'	1:A:2636:C:H5'	2.05	0.56
2:B:3020:G:O2'	2:B:3021:G:H5'	2.05	0.56
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.70	0.56
1:A:200:U:H2'	37:A:3028:HOH:O	2.04	0.56
37:A:5094:HOH:O	4:D:298:LYS:HD3	2.04	0.56
37:A:4544:HOH:O	10:J:57:ARG:HG3	2.05	0.56
16:P:25:VAL:O	16:P:29:VAL:HG23	2.04	0.56
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.40	0.56
23:W:56:ILE:O	23:W:60:GLN:HG3	2.05	0.56
1:A:1753:C:O2	4:D:229:ARG:NH2	2.38	0.56
1:A:183:A:O2'	1:A:184:G:H5'	2.06	0.56
1:A:371:U:H2'	1:A:372:A:H8	1.70	0.56
4:D:138:GLY:O	4:D:139:ASP:O	2.23	0.56
13:M:143:THR:CG2	13:M:144:ASP:N	2.68	0.56
1:A:2659:U:H4'	19:S:76:ASP:HB3	1.87	0.56
1:A:1333:U:H2'	1:A:1334:C:C6	2.41	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.05	0.56
1:A:1909:A:H2'	1:A:1910:A:C8	2.39	0.56
4:D:254:GLN:HG2	4:D:255:GLY:N	2.19	0.56
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.06	0.56
8:H:110:GLU:O	8:H:114:LYS:HG3	2.05	0.56
10:J:44:ALA:HA	10:J:163:PRO:O	2.06	0.56
13:M:143:THR:HG22	13:M:144:ASP:H	1.71	0.56
15:O:64:SER:C	15:O:66:LEU:H	2.09	0.56
26:Z:144:ARG:NE	37:Z:8197:HOH:O	2.39	0.56
1:A:797:A:C4'	27:I:10:ARG:N	2.69	0.56
1:A:175:G:H2'	14:N:192:ALA:HB3	1.87	0.56
1:A:2713:G:O2'	1:A:2714:U:H5'	2.05	0.56
1:A:328:U:O4'	5:E:202:THR:HG22	2.05	0.56
1:A:775:G:OP1	28:2:16:HIS:HE1	1.89	0.56
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.69	0.56
5:E:79:ARG:O	5:E:87:ARG:HG2	2.06	0.56
6:F:163:VAL:HA	37:F:6326:HOH:O	2.04	0.56
10:J:59:ASN:N	10:J:59:ASN:ND2	2.50	0.56
12:L:34:VAL:HB	37:L:7169:HOH:O	2.06	0.56
15:O:89:GLY:O	15:O:92:ALA:HB3	2.06	0.56
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.20	0.56
1:A:1699:C:H4'	37:A:6017:HOH:O	2.06	0.56
1:A:2011:A:P	37:A:5537:HOH:O	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:C:H4'	5:E:46:TYR:CE1	2.41	0.56
5:E:107:ARG:HB3	5:E:107:ARG:HH11	1.70	0.56
14:N:162:GLY:HA2	37:N:8519:HOH:O	2.04	0.56
26:Z:189:ASN:ND2	26:Z:192:ASP:H	2.04	0.56
1:A:1393:A:H2'	1:A:1394:C:C6	2.41	0.56
1:A:154:C:C2	1:A:155:C:C5	2.93	0.56
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.20	0.56
1:A:2830:U:H3'	37:A:4804:HOH:O	2.05	0.56
5:E:236:THR:C	37:E:8445:HOH:O	2.44	0.56
8:H:99:THR:O	8:H:99:THR:HG23	2.05	0.56
14:N:172:GLY:C	14:N:183:VAL:HG11	2.26	0.56
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.88	0.56
1:A:1137:G:H1'	37:A:3455:HOH:O	2.05	0.56
1:A:661:G:C5	1:A:686:A:C2	2.93	0.56
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.06	0.56
37:A:4628:HOH:O	17:Q:68:LYS:HD3	2.06	0.56
28:2:1:THR:HB	37:2:8457:HOH:O	2.04	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.36	0.56
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.71	0.56
6:F:11:HIS:O	6:F:12:GLU:HB3	2.05	0.56
10:J:27:LYS:H	10:J:58:HIS:CD2	2.17	0.56
14:N:191:GLY:O	14:N:192:ALA:HB3	2.06	0.56
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.88	0.56
16:P:7:LEU:HD22	37:P:5650:HOH:O	2.05	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
1:A:694:A:H2'	1:A:695:C:H5'	1.87	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.18	0.56
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.52	0.56
1:A:135:G:OP1	37:A:6873:HOH:O	2.18	0.55
1:A:2724:U:H2'	1:A:2725:G:O4'	2.05	0.55
1:A:485:A:N3	1:A:487:G:H5"	2.21	0.55
1:A:512:G:O3'	1:A:513:A:H8	1.89	0.55
1:A:952:G:H4'	37:A:3606:HOH:O	2.06	0.55
2:B:3078:G:H22	2:B:3102:G:H2'	1.71	0.55
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.05	0.55
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.71	0.55
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.87	0.55
19:S:39:THR:HB	19:S:42:GLU:CG	2.35	0.55
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.87	0.55
1:A:1015:C:H2'	1:A:1016:U:C6	2.40	0.55
1:A:1362:U:H5'	37:A:9849:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:U:H5''	1:A:284:C:P	2.46	0.55
1:A:558:C:H5'	37:A:4832:HOH:O	2.06	0.55
2:B:3078:G:N2	2:B:3102:G:H2'	2.22	0.55
4:D:146:THR:O	4:D:159:PRO:HB3	2.05	0.55
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.87	0.55
6:F:105:SER:CB	6:F:131:THR:HG23	2.33	0.55
6:F:36:ASN:HA	37:F:7500:HOH:O	2.06	0.55
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.53	0.55
15:O:170:GLU:O	15:O:174:GLU:HG3	2.06	0.55
21:U:4:PRO:O	21:U:8:ARG:HG3	2.05	0.55
1:A:1086:A:N6	24:X:11:VAL:HG11	2.22	0.55
1:A:877:G:H3'	37:A:9699:HOH:O	2.05	0.55
3:C:191:GLY:HA2	3:C:194:MET:CE	2.36	0.55
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.69	0.55
37:A:8978:HOH:O	14:N:94:LYS:HE2	2.07	0.55
2:B:3069:U:OP1	15:O:4:PRO:HG3	2.05	0.55
18:R:32:GLU:HA	18:R:71:TYR:OH	2.06	0.55
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.89	0.55
1:A:1497:G:H4'	1:A:1627:G:O2'	2.07	0.55
1:A:1925:G:O2'	1:A:1926:G:H5'	2.06	0.55
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.36	0.55
6:F:99:ASP:HB3	6:F:103:ASN:H	1.71	0.55
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.87	0.55
1:A:1176:C:H1'	37:A:3506:HOH:O	2.07	0.55
1:A:567:U:H5''	37:A:5977:HOH:O	2.05	0.55
37:A:4444:HOH:O	14:N:174:ARG:HG2	2.07	0.55
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.87	0.55
21:U:48:VAL:HG13	21:U:49:GLU:N	2.21	0.55
1:A:1102:C:H2'	1:A:1103:C:H6	1.72	0.55
1:A:2291:A:C8	1:A:2309:C:H5'	2.42	0.55
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.89	0.55
15:O:154:LEU:HG	15:O:155:GLU:H	1.71	0.55
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.05	0.55
1:A:317:A:H5''	21:U:52:ARG:HD2	1.89	0.55
23:W:39:ALA:N	23:W:40:PRO:CD	2.69	0.55
1:A:470:U:O2'	28:2:16:HIS:HD2	1.89	0.55
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.42	0.55
1:A:814:G:H4'	37:A:9719:HOH:O	2.05	0.55
6:F:135:VAL:HG22	6:F:136:ARG:N	2.21	0.55
7:G:11:VAL:CG1	7:G:12:ASP:N	2.69	0.55
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:77:ALA:HB3	37:M:8402:HOH:O	2.05	0.55
15:O:154:LEU:HG	15:O:155:GLU:N	2.21	0.55
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.87	0.55
24:X:26:ILE:O	24:X:26:ILE:HG13	2.05	0.55
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.06	0.55
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.89	0.55
1:A:2428:G:N7	30:4:60:LYS:NZ	2.50	0.55
1:A:2777:G:O2'	1:A:2778:A:H5'	2.06	0.55
1:A:2816:A:H5''	1:A:2817:G:H5'	1.89	0.55
1:A:324:G:O2'	1:A:325:U:H5'	2.07	0.55
1:A:344:C:H2'	1:A:345:G:O4'	2.07	0.55
2:B:3047:A:C2	2:B:3048:C:C2	2.94	0.55
4:D:214:PRO:HD2	37:D:8522:HOH:O	2.06	0.55
10:J:109:ASP:HB2	37:J:8347:HOH:O	2.05	0.55
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.88	0.55
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.87	0.55
1:A:2247:C:H5''	37:A:6916:HOH:O	2.07	0.55
1:A:2314:G:C2'	1:A:2315:C:H5'	2.37	0.55
1:A:2795:C:O2'	1:A:2796:U:H5'	2.06	0.55
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.88	0.55
5:E:77:ALA:O	5:E:78:ARG:HG3	2.07	0.55
23:W:39:ALA:O	23:W:41:GLU:N	2.40	0.55
24:X:88:THR:CG2	24:X:89:ASP:H	2.15	0.55
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.21	0.55
1:A:1166:A:H61	1:A:1180:U:H3	1.54	0.55
1:A:1391:G:C5	1:A:1435:U:C4	2.95	0.55
1:A:1909:A:N1	1:A:2128:G:H1'	2.22	0.55
1:A:2453:G:H3'	37:A:5499:HOH:O	2.06	0.55
1:A:245:C:H2'	1:A:246:G:H5'	1.89	0.55
1:A:88:G:H8	1:A:88:G:H5'	1.71	0.55
4:D:175:LEU:C	4:D:175:LEU:CD2	2.75	0.55
2:B:3044:A:O4'	6:F:76:ARG:NE	2.40	0.55
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.54	0.55
13:M:73:VAL:HG23	13:M:74:THR:H	1.70	0.55
26:Z:154:ARG:O	26:Z:154:ARG:HG2	2.07	0.55
1:A:1189:A:H1'	1:A:1209:C:O4'	2.07	0.54
1:A:2679:G:H2'	1:A:2681:A:OP2	2.06	0.54
1:A:383:A:H4'	37:A:4903:HOH:O	2.07	0.54
1:A:56:G:H5''	23:W:50:ARG:NH1	2.22	0.54
8:H:58:GLU:HG3	8:H:61:MET:HE1	1.89	0.54
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.89	0.54
15:O:48:VAL:HG12	37:O:8554:HOH:O	2.05	0.54
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.22	0.54
37:A:6994:HOH:O	21:U:9:LYS:HB2	2.06	0.54
1:A:2256:G:H2'	1:A:2257:G:C5'	2.37	0.54
1:A:602:A:O2'	1:A:605:C:H4'	2.07	0.54
1:A:777:U:O2'	28:2:11:LYS:HG2	2.07	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.06	0.54
10:J:39:GLY:O	10:J:41:THR:N	2.40	0.54
10:J:75:SER:O	10:J:79:ALA:HB2	2.07	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
1:A:1995:G:O2'	1:A:1997:A:N7	2.40	0.54
1:A:542:A:H2'	1:A:543:G:O4'	2.06	0.54
3:C:36:ASP:O	3:C:38:ILE:N	2.41	0.54
4:D:238:ASN:ND2	4:D:240:GLY:H	2.05	0.54
4:D:82:VAL:CG1	4:D:82:VAL:O	2.53	0.54
7:G:7:ILE:HD11	7:G:11:VAL:O	2.07	0.54
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.08	0.54
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.54	0.54
22:V:14:GLU:OE1	22:V:15:PRO:CD	2.52	0.54
27:1:58:GLY:CA	37:1:8439:HOH:O	2.50	0.54
1:A:138:U:H5''	1:A:139:C:OP2	2.08	0.54
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.07	0.54
1:A:2241:C:O2'	1:A:2242:U:H5'	2.06	0.54
1:A:894:A:C2	5:E:87:ARG:NH2	2.75	0.54
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.42	0.54
10:J:5:MET:HG3	37:J:8367:HOH:O	2.07	0.54
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.37	0.54
1:A:396:U:OP2	30:4:38:ARG:NH1	2.39	0.54
1:A:1015:C:C2	1:A:1016:U:C5	2.95	0.54
1:A:2070:G:H5''	37:A:3359:HOH:O	2.06	0.54
4:D:51:VAL:HG23	4:D:329:TYR:O	2.08	0.54
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.37	0.54
10:J:69:ASN:O	10:J:72:VAL:HG12	2.07	0.54
15:O:37:ARG:HD3	35:O:8507:CL:CL	2.45	0.54
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.07	0.54
37:A:8936:HOH:O	29:3:3:LYS:HE3	2.07	0.54
30:4:56:PRO:N	37:4:8550:HOH:O	2.39	0.54
1:A:1299:G:H5'	37:A:3648:HOH:O	2.08	0.54
1:A:1505:U:H5'	1:A:1505:U:H6	1.72	0.54
1:A:2324:G:H4'	1:A:2418:G:O2'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:G:H5'	1:A:878:G:OP1	2.07	0.54
3:C:223:ARG:HG3	37:C:8604:HOH:O	2.06	0.54
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.39	0.54
6:F:10:PHE:CE1	6:F:11:HIS:HB3	2.42	0.54
7:G:15:GLN:NE2	7:G:40:VAL:O	2.41	0.54
8:H:100:ASP:O	8:H:101:ALA:O	2.26	0.54
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.36	0.54
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.38	0.54
28:2:28:HIS:CD2	28:2:31:LYS:H	2.26	0.54
1:A:1299:G:O6	13:M:6:ARG:HD3	2.08	0.54
1:A:2761:A:C4	1:A:2763:G:C8	2.95	0.54
1:A:2781:U:C2'	1:A:2782:G:H5'	2.37	0.54
1:A:319:A:H4'	1:A:338:C:C4	2.43	0.54
1:A:902:G:N7	13:M:18:HIS:HD2	2.06	0.54
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.05	0.54
24:X:38:THR:O	24:X:42:ARG:HB2	2.08	0.54
1:A:2359:G:N7	37:A:3279:HOH:O	2.34	0.54
1:A:669:G:O2'	1:A:670:G:H5'	2.07	0.54
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.05	0.54
37:A:6203:HOH:O	10:J:150:LYS:HE2	2.08	0.54
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.43	0.54
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.88	0.54
17:Q:71:LYS:HG3	17:Q:71:LYS:O	2.08	0.54
19:S:106:GLY:HA2	19:S:109:MET:CE	2.38	0.54
24:X:149:LEU:HG	24:X:153:MET:CE	2.38	0.54
1:A:1523:G:H2'	1:A:1524:U:C6	2.43	0.54
1:A:1641:A:H2'	1:A:1642:A:H5'	1.89	0.54
1:A:2270:G:H4'	3:C:223:ARG:NH1	2.21	0.54
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.90	0.54
37:A:9144:HOH:O	4:D:267:LYS:HD3	2.06	0.54
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.37	0.54
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.06	0.54
1:A:714:U:H3'	37:A:6516:HOH:O	2.07	0.54
1:A:812:A:H1'	37:A:3533:HOH:O	2.07	0.54
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.73	0.54
5:E:200:PRO:HB3	5:E:212:VAL:HG23	1.90	0.54
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.90	0.54
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.89	0.54
11:K:88:PRO:C	35:K:8502:CL:CL	2.83	0.54
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.08	0.54
29:3:48:ASP:O	29:3:49:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.73	0.53
37:A:7253:HOH:O	14:N:154:ARG:HB2	2.07	0.53
21:U:32:ARG:NH1	21:U:38:ARG:HH12	2.06	0.53
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.37	0.53
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.90	0.53
27:1:57:CYS:SG	27:1:59:HIS:HB3	2.48	0.53
1:A:1669:A:H2'	1:A:1670:G:C8	2.43	0.53
1:A:2326:U:H4'	1:A:2412:G:H4'	1.91	0.53
1:A:485:A:O2'	1:A:487:G:H5'	2.08	0.53
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.35	0.53
5:E:115:LEU:O	5:E:118:THR:HB	2.07	0.53
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.27	0.53
7:G:79:GLY:HA3	37:G:7046:HOH:O	2.08	0.53
12:L:30:LYS:O	12:L:55:VAL:HG13	2.08	0.53
16:P:21:SER:OG	16:P:106:PRO:HB2	2.08	0.53
22:V:6:CYS:O	22:V:8:TYR:N	2.41	0.53
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.39	0.53
1:A:779:U:H5'	1:A:1836:A:C2	2.42	0.53
1:A:2001:G:O2'	1:A:2002:C:H5'	2.09	0.53
1:A:2251:G:H2'	1:A:2252:A:C8	2.44	0.53
1:A:2359:G:H3'	37:A:5266:HOH:O	2.08	0.53
1:A:2755:G:H1'	37:A:4258:HOH:O	2.08	0.53
1:A:2780:C:H2'	1:A:2781:U:C6	2.44	0.53
7:G:22:VAL:O	7:G:28:SER:HA	2.08	0.53
10:J:75:SER:C	10:J:79:ALA:HB2	2.29	0.53
22:V:8:TYR:OH	37:V:3805:HOH:O	2.18	0.53
24:X:4:LEU:O	24:X:32:CYS:HA	2.09	0.53
1:A:2314:G:H2'	1:A:2315:C:H5'	1.91	0.53
1:A:2656:G:O2'	1:A:2657:G:H5'	2.09	0.53
1:A:316:A:N3	1:A:336:G:O2'	2.40	0.53
4:D:14:GLY:HA2	4:D:15:PRO:C	2.29	0.53
5:E:133:ARG:HD2	37:E:8406:HOH:O	2.08	0.53
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.89	0.53
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.90	0.53
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.89	0.53
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.26	0.53
10:J:46:VAL:O	10:J:146:TRP:HH2	1.91	0.53
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.90	0.53
1:A:1097:A:H5''	24:X:125:HIS:CE1	2.43	0.53
27:1:13:ARG:NH1	27:1:14:PHE:CZ	2.77	0.53
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:G:O2'	1:A:258:G:H5'	2.08	0.53
3:C:109:GLU:HG2	3:C:116:GLY:N	2.23	0.53
6:F:154:LYS:H	6:F:154:LYS:CD	2.15	0.53
7:G:11:VAL:HG13	7:G:23:GLU:O	2.08	0.53
15:O:82:TYR:C	15:O:82:TYR:CD2	2.82	0.53
22:V:6:CYS:C	22:V:8:TYR:H	2.12	0.53
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.12	0.53
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.48	0.53
1:A:1873:G:H2'	1:A:1874:U:H5'	1.90	0.53
1:A:272:A:H5'	1:A:273:G:OP2	2.09	0.53
1:A:315:G:C6	1:A:316:A:C6	2.96	0.53
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.91	0.53
6:F:86:THR:C	6:F:89:PRO:HD2	2.28	0.53
9:I:12:ILE:HG22	9:I:12:ILE:O	2.08	0.53
24:X:122:ARG:NH1	24:X:122:ARG:HG2	2.23	0.53
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.09	0.53
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.08	0.53
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.34	0.53
30:4:55:VAL:HB	30:4:56:PRO:HD2	1.91	0.53
1:A:1495:C:H1'	1:A:1573:A:H1'	1.91	0.53
1:A:1778:A:H2'	1:A:1779:A:H5'	1.91	0.53
1:A:474:C:O3'	5:E:73:LEU:HD21	2.09	0.53
1:A:660:A:H4'	1:A:661:G:O5'	2.09	0.53
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.23	0.53
6:F:25:MET:CE	6:F:37:ALA:HB1	2.36	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.91	0.53
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.43	0.53
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.89	0.53
16:P:25:VAL:HG23	16:P:26:TRP:H	1.74	0.53
37:E:8356:HOH:O	16:P:3:THR:HG21	2.08	0.53
1:A:1168:C:H2'	1:A:1169:U:O4'	2.08	0.53
1:A:1477:C:H5'	1:A:1868:G:C5'	2.39	0.53
1:A:1666:C:C2'	1:A:1667:A:C5'	2.87	0.53
1:A:407:A:H5'	37:A:5603:HOH:O	2.07	0.53
3:C:1:GLY:HA2	3:C:197:VAL:HG23	1.91	0.53
4:D:2:GLN:CD	37:D:8622:HOH:O	2.46	0.53
14:N:67:ILE:CD1	14:N:104:ARG:HD2	2.39	0.53
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.24	0.53
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.38	0.53
37:A:8903:HOH:O	27:1:16:PRO:HG3	2.07	0.53
28:2:25:LYS:HE2	37:3:7213:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:51:TYR:CE2	28:2:53:LYS:HB3	2.44	0.53
1:A:1164:U:C4'	1:A:1165:G:OP1	2.52	0.53
1:A:2064:U:H5'	1:A:2652:U:H4'	1.90	0.53
1:A:628:A:C8	1:A:2071:C:N4	2.77	0.53
1:A:2613:G:O2'	1:A:2614:C:H5'	2.09	0.53
1:A:289:G:N2	1:A:363:A:H2	2.04	0.53
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.90	0.53
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.27	0.53
8:H:22:VAL:HG21	8:H:104:ALA:HB2	1.90	0.53
37:A:3421:HOH:O	10:J:11:LYS:HE2	2.08	0.53
15:O:182:GLY:N	37:O:8571:HOH:O	2.41	0.53
23:W:57:LYS:HA	23:W:60:GLN:HE21	1.73	0.53
1:A:1589:G:N2	1:A:1605:G:H1'	2.24	0.53
1:A:2779:G:H1'	37:A:5684:HOH:O	2.09	0.53
4:D:119:HIS:O	4:D:121:PRO:HD3	2.08	0.53
10:J:139:ASP:N	10:J:140:PRO:CD	2.71	0.53
10:J:81:TYR:C	10:J:81:TYR:CD1	2.81	0.53
19:S:29:LYS:NZ	37:S:8540:HOH:O	2.41	0.53
1:A:1783:A:O2'	1:A:1784:U:H5'	2.09	0.52
1:A:2271:G:N3	1:A:2271:G:H2'	2.24	0.52
1:A:830:G:O2'	1:A:831:U:H5'	2.09	0.52
1:A:92:G:H4'	23:W:44:GLY:HA3	1.90	0.52
37:A:4405:HOH:O	11:K:47:THR:CB	2.55	0.52
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.90	0.52
14:N:149:TRP:O	14:N:152:ARG:HG2	2.09	0.52
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.91	0.52
1:A:1500:U:P	17:Q:41:ARG:HH22	2.31	0.52
24:X:26:ILE:O	24:X:26:ILE:CG1	2.56	0.52
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.17	0.52
27:1:30:GLU:HA	27:1:33:HIS:CB	2.40	0.52
1:A:2435:U:H1'	37:A:5006:HOH:O	2.09	0.52
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.39	0.52
4:D:274:GLU:HA	4:D:292:GLY:O	2.08	0.52
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.92	0.52
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.91	0.52
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.40	0.52
1:A:1527:A:H1'	1:A:1528:A:C8	2.44	0.52
1:A:682:A:H3'	1:A:683:G:H8	1.74	0.52
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.91	0.52
5:E:234:VAL:O	5:E:234:VAL:HG22	2.08	0.52
14:N:164:THR:HB	37:N:8519:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.09	0.52
24:X:38:THR:HG22	24:X:39:ASP:N	2.25	0.52
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.44	0.52
1:A:1268:C:O2'	26:Z:169:ARG:HB2	2.08	0.52
1:A:259:G:H21	14:N:58:GLN:NE2	2.06	0.52
5:E:129:HIS:HD2	5:E:165:ASP:OD2	1.91	0.52
5:E:16:VAL:HG12	5:E:17:ASP:H	1.73	0.52
8:H:46:GLU:N	37:H:3461:HOH:O	2.43	0.52
15:O:167:ASP:O	15:O:168:LEU:HD23	2.10	0.52
15:O:180:LEU:O	15:O:181:ASP:HB3	2.08	0.52
1:A:1847:A:OP1	3:C:175:LYS:NZ	2.42	0.52
1:A:1855:G:H8	3:C:144:GLU:OE2	1.93	0.52
1:A:2082:G:O2'	1:A:2083:A:H5'	2.08	0.52
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.90	0.52
1:A:119:A:H2'	1:A:120:A:H5''	1.91	0.52
1:A:1819:G:H5'	37:A:4285:HOH:O	2.10	0.52
1:A:2769:C:O2'	1:A:2770:G:H5'	2.09	0.52
1:A:51:G:O2'	1:A:52:A:H5'	2.10	0.52
6:F:10:PHE:CG	6:F:11:HIS:N	2.77	0.52
14:N:154:ARG:HD3	37:N:8640:HOH:O	2.10	0.52
1:A:962:C:C1'	15:O:5:ARG:NH1	2.65	0.52
21:U:12:ARG:NH1	37:U:3035:HOH:O	2.42	0.52
37:E:8364:HOH:O	21:U:2:LYS:HE2	2.09	0.52
24:X:125:HIS:HD2	24:X:127:GLY:H	1.57	0.52
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.41	0.52
1:A:1127:C:C2'	1:A:1128:U:H5'	2.40	0.52
1:A:1562:C:O2	1:A:1562:C:H2'	2.10	0.52
1:A:1666:C:H2'	1:A:1667:A:C5'	2.40	0.52
1:A:1934:A:C8	1:A:1935:C:C5	2.97	0.52
1:A:1947:G:N2	1:A:1966:U:C2	2.78	0.52
1:A:2604:A:H5'	37:A:5367:HOH:O	2.09	0.52
1:A:2718:C:H6	1:A:2718:C:H5'	1.75	0.52
1:A:2781:U:H2'	1:A:2782:G:H5'	1.91	0.52
11:K:142:ASN:O	11:K:144:THR:N	2.43	0.52
11:K:77:GLY:O	11:K:78:ILE:C	2.48	0.52
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.40	0.52
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.89	0.52
24:X:122:ARG:HG2	24:X:152:ALA:O	2.09	0.52
1:A:1118:A:H8	1:A:1119:G:H5''	1.75	0.52
1:A:1942:A:O2'	1:A:1943:C:H5'	2.10	0.52
1:A:818:A:O2'	27:1:13:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.33	0.52
3:C:51:ARG:NH2	37:C:8609:HOH:O	2.42	0.52
37:A:3640:HOH:O	4:D:27:ASN:HB2	2.10	0.52
5:E:214:THR:HB	37:E:8325:HOH:O	2.10	0.52
5:E:233:THR:CG2	5:E:234:VAL:N	2.73	0.52
10:J:62:GLU:OE2	10:J:66:VAL:HG23	2.09	0.52
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.10	0.52
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.24	0.52
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.09	0.52
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.44	0.52
1:A:1333:U:H2'	1:A:1334:C:H6	1.75	0.52
1:A:67:A:H5''	1:A:69:A:C8	2.45	0.52
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.91	0.52
4:D:27:ASN:HB3	37:D:8630:HOH:O	2.08	0.52
1:A:2862:G:H4'	4:D:336:GLN:O	2.10	0.52
6:F:58:VAL:HG12	6:F:59:GLY:N	2.25	0.52
8:H:58:GLU:HA	8:H:61:MET:HG3	1.92	0.52
10:J:129:ASN:HD22	10:J:129:ASN:N	2.08	0.52
10:J:28:ILE:HA	10:J:62:GLU:OE1	2.10	0.52
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.91	0.52
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.74	0.52
22:V:34:SER:O	22:V:38:ASN:ND2	2.42	0.52
24:X:142:ASP:HB3	24:X:145:GLY:H	1.73	0.52
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.38	0.52
26:Z:185:VAL:HA	37:Z:8152:HOH:O	2.08	0.52
1:A:1209:C:C2	1:A:1210:G:C8	2.97	0.52
1:A:183:A:H5'	14:N:157:LEU:HD12	1.92	0.52
1:A:2044:G:OP1	25:Y:23:HIS:CE1	2.60	0.52
1:A:2329:C:O2'	1:A:2330:U:H5'	2.10	0.52
1:A:290:C:O2'	1:A:291:C:H5'	2.10	0.52
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.43	0.52
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.58	0.52
19:S:132:ARG:CZ	37:S:8587:HOH:O	2.58	0.52
1:A:1120:U:H6	1:A:1120:U:H5''	1.75	0.51
1:A:1973:A:C8	1:A:1973:A:H5'	2.43	0.51
1:A:245:C:C2'	1:A:246:G:H5'	2.40	0.51
1:A:2779:G:O2'	1:A:2780:C:H5'	2.10	0.51
1:A:329:A:OP2	5:E:206:ASN:HB2	2.09	0.51
1:A:644:G:H5'	1:A:644:G:N3	2.24	0.51
1:A:684:G:H2'	1:A:685:C:C6	2.45	0.51
1:A:920:C:H5'	1:A:921:G:C4	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.39	0.51
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.91	0.51
1:A:431:G:P	14:N:48:ARG:HH12	2.34	0.51
18:R:16:ASN:ND2	18:R:45:PRO:HG2	2.25	0.51
23:W:27:LEU:O	23:W:30:ALA:N	2.43	0.51
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.10	0.51
24:X:88:THR:CG2	24:X:89:ASP:N	2.72	0.51
1:A:1123:A:C6	1:A:1238:C:H5'	2.45	0.51
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.74	0.51
1:A:1717:A:H5''	17:Q:54:LYS:HB2	1.93	0.51
1:A:2894:C:O2'	1:A:2895:C:H5'	2.09	0.51
7:G:11:VAL:HG12	7:G:12:ASP:H	1.75	0.51
14:N:186:SER:O	14:N:189:VAL:HG12	2.10	0.51
22:V:52:THR:HG22	22:V:54:THR:HB	1.93	0.51
24:X:42:ARG:O	24:X:45:VAL:HG22	2.10	0.51
26:Z:144:ARG:CZ	37:Z:8197:HOH:O	2.59	0.51
1:A:331:A:C6	1:A:332:G:C4	2.97	0.51
1:A:319:A:H4'	1:A:338:C:C5	2.46	0.51
1:A:92:G:H5'	37:W:7247:HOH:O	2.10	0.51
4:D:231:GLY:N	37:D:8524:HOH:O	2.35	0.51
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.91	0.51
13:M:104:ASP:HB3	37:M:8437:HOH:O	2.09	0.51
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.92	0.51
26:Z:144:ARG:HH11	26:Z:144:ARG:HG3	1.75	0.51
3:C:170:VAL:HG22	27:I:22:ILE:HG23	1.92	0.51
1:A:1189:A:H1'	1:A:1209:C:H1'	1.93	0.51
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.51
2:B:3049:G:H2'	2:B:3050:G:O4'	2.10	0.51
6:F:23:VAL:CG2	6:F:23:VAL:O	2.58	0.51
14:N:77:PHE:HD2	37:N:8527:HOH:O	1.94	0.51
17:Q:94:TRP:CZ2	17:Q:98:ILE:HG13	2.46	0.51
19:S:39:THR:HG22	19:S:42:GLU:H	1.74	0.51
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.46	0.51
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.45	0.51
1:A:2764:C:H2'	1:A:2765:C:H6	1.74	0.51
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.92	0.51
1:A:1151:G:P	9:I:16:LYS:HZ1	2.30	0.51
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.92	0.51
10:J:14:TYR:N	10:J:91:HIS:CE1	2.79	0.51
14:N:48:ARG:NH2	37:N:8562:HOH:O	2.42	0.51
15:O:152:GLU:C	15:O:154:LEU:H	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:73:ALA:N	37:O:8567:HOH:O	2.44	0.51
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.11	0.51
23:W:64:GLY:O	23:W:65:ASP:CB	2.56	0.51
1:A:907:A:H2'	1:A:908:A:H8	1.76	0.51
4:D:215:VAL:HA	4:D:220:VAL:HG22	1.93	0.51
4:D:76:THR:N	4:D:77:PRO:HD3	2.26	0.51
6:F:10:PHE:CD1	6:F:11:HIS:N	2.78	0.51
12:L:101:ASN:HB3	37:L:6456:HOH:O	2.11	0.51
14:N:106:ASN:ND2	35:N:8518:CL:CL	2.81	0.51
14:N:43:PRO:HG3	14:N:62:VAL:HG21	1.93	0.51
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.92	0.51
1:A:113:A:OP2	1:A:114:A:H2'	2.11	0.51
1:A:1132:A:N6	1:A:1229:C:H2'	2.26	0.51
1:A:2044:G:C6	1:A:2045:G:C5	2.98	0.51
1:A:2392:C:H4'	37:R:2875:HOH:O	2.10	0.51
3:C:105:VAL:CG1	3:C:106:CYS:N	2.74	0.51
8:H:107:VAL:O	8:H:111:ILE:HG13	2.10	0.51
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.11	0.51
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.41	0.51
19:S:33:ARG:NH1	37:S:8544:HOH:O	2.44	0.51
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.25	0.51
27:I:59:HIS:HA	37:I:8441:HOH:O	2.09	0.51
37:A:3804:HOH:O	29:3:38:LYS:HE3	2.11	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.91	0.51
1:A:1804:A:H2'	1:A:1805:G:C8	2.44	0.51
1:A:558:C:C2'	1:A:559:U:C5'	2.89	0.51
2:B:3042:C:H2'	37:B:8500:HOH:O	2.10	0.51
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.46	0.51
37:A:5104:HOH:O	14:N:58:GLN:HG3	2.10	0.51
18:R:66:LYS:HB2	18:R:70:ALA:O	2.11	0.51
19:S:79:ARG:C	19:S:81:PRO:HD3	2.31	0.51
21:U:48:VAL:CG2	21:U:98:VAL:HA	2.40	0.51
22:V:31:PHE:CE2	22:V:37:GLU:HA	2.46	0.51
1:A:1477:C:O2'	1:A:1478:U:H5'	2.11	0.51
1:A:154:C:H2'	1:A:155:C:H6	1.76	0.51
1:A:1940:C:H4'	37:A:6918:HOH:O	2.10	0.51
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.51
4:D:7:ARG:CD	4:D:9:GLY:O	2.59	0.51
9:I:64:ASN:O	9:I:68:GLU:HG3	2.11	0.51
10:J:65:ARG:HB3	37:J:8387:HOH:O	2.10	0.51
10:J:65:ARG:NH1	37:J:8387:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:130:VAL:HG12	11:K:131:THR:N	2.26	0.51
37:B:8519:HOH:O	15:O:107:ASN:HB3	2.10	0.51
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.08	0.51
22:V:9:CYS:CA	22:V:52:THR:HG23	2.40	0.51
24:X:125:HIS:CD2	24:X:127:GLY:H	2.29	0.51
27:1:46:LYS:O	27:1:57:CYS:HA	2.10	0.51
1:A:790:A:H1'	1:A:1710:A:H2'	1.93	0.51
1:A:2832:C:H5	37:A:6784:HOH:O	1.94	0.51
4:D:305:ASP:O	4:D:306:LYS:CB	2.58	0.51
6:F:102:GLY:O	6:F:134:LEU:HD12	2.11	0.51
6:F:57:THR:HG23	6:F:63:ILE:CB	2.41	0.51
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.40	0.51
1:A:2712:G:OP1	12:L:43:ARG:NH1	2.43	0.51
19:S:47:LEU:O	19:S:51:ILE:HG13	2.09	0.51
25:Y:26:ALA:HB1	25:Y:59:TRP:CE2	2.45	0.51
1:A:1174:A:C5	1:A:1201:C:H4'	2.46	0.50
1:A:256:C:H2'	1:A:257:G:O4'	2.11	0.50
4:D:238:ASN:HD22	4:D:240:GLY:N	2.06	0.50
4:D:7:ARG:HD3	4:D:9:GLY:O	2.12	0.50
6:F:53:LYS:HA	6:F:67:ASP:O	2.11	0.50
11:K:131:THR:HG22	11:K:133:GLY:N	2.26	0.50
13:M:143:THR:CG2	13:M:144:ASP:H	2.23	0.50
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.26	0.50
24:X:13:MET:CE	24:X:17:ILE:HG22	2.40	0.50
37:A:5771:HOH:O	29:3:44:ARG:HG2	2.10	0.50
1:A:1060:C:H6	1:A:1060:C:H5'	1.76	0.50
1:A:338:C:H4'	5:E:174:ILE:CD1	2.41	0.50
2:B:3055:U:H4'	2:B:3056:A:C8	2.46	0.50
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.36	0.50
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.11	0.50
7:G:21:THR:HG23	7:G:30:THR:OG1	2.11	0.50
37:A:4118:HOH:O	10:J:151:MET:HE2	2.11	0.50
13:M:73:VAL:HG23	13:M:74:THR:N	2.25	0.50
15:O:163:PHE:HA	37:O:8519:HOH:O	2.10	0.50
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.11	0.50
24:X:122:ARG:CG	24:X:152:ALA:O	2.59	0.50
1:A:1116:U:H3	1:A:1246:A:N6	2.01	0.50
1:A:1139:U:H2'	1:A:1140:C:C6	2.46	0.50
1:A:1162:G:H2'	37:A:6156:HOH:O	2.11	0.50
1:A:639:A:H2'	1:A:640:G:C8	2.45	0.50
1:A:920:C:H4'	1:A:921:G:C2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:107:ARG:CB	5:E:107:ARG:HH11	2.24	0.50
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.11	0.50
1:A:2365:G:H4'	18:R:45:PRO:O	2.11	0.50
1:A:125:U:H2'	37:A:3346:HOH:O	2.11	0.50
4:D:275:GLY:O	4:D:291:ASP:HA	2.11	0.50
4:D:54:VAL:HB	37:D:8614:HOH:O	2.11	0.50
6:F:27:ILE:O	6:F:69:ILE:HG22	2.11	0.50
7:G:84:MET:HE1	7:G:148:ILE:CD1	2.42	0.50
13:M:134:GLU:HA	13:M:138:GLY:O	2.12	0.50
15:O:163:PHE:HE1	15:O:171:HIS:HD1	1.59	0.50
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.41	0.50
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.40	0.50
1:A:710:G:OP1	16:P:24:ALA:HB3	2.12	0.50
1:A:1102:C:H2'	1:A:1103:C:C6	2.46	0.50
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.41	0.50
6:F:140:ARG:O	6:F:144:ARG:HG2	2.11	0.50
7:G:69:ILE:HA	7:G:72:MET:HE3	1.92	0.50
10:J:85:ILE:O	10:J:85:ILE:HG23	2.12	0.50
14:N:186:SER:OG	14:N:189:VAL:CG1	2.59	0.50
15:O:171:HIS:CE1	37:O:8567:HOH:O	2.64	0.50
15:O:182:GLY:O	15:O:183:ASP:O	2.29	0.50
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.76	0.50
1:A:1161:A:H8	1:A:1161:A:O5'	1.95	0.50
1:A:2113:G:C6	1:A:2114:C:C4	3.00	0.50
1:A:951:A:C2'	1:A:952:G:H5'	2.42	0.50
5:E:33:LYS:HE2	37:E:8358:HOH:O	2.12	0.50
7:G:81:GLU:HG2	7:G:134:SER:CB	2.39	0.50
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.45	0.50
16:P:88:LYS:O	37:P:4826:HOH:O	2.20	0.50
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	0.50
1:A:1462:C:H2'	1:A:1463:A:C8	2.47	0.50
1:A:1594:C:C2	1:A:1601:G:C2	3.00	0.50
1:A:2004:U:O2	1:A:2004:U:H2'	2.11	0.50
1:A:2506:A:O2'	1:A:2507:G:O5'	2.30	0.50
1:A:553:G:P	26:Z:204:ARG:HH22	2.34	0.50
1:A:825:U:H5''	1:A:826:U:OP1	2.12	0.50
2:B:3031:C:O2'	2:B:3032:G:H5'	2.11	0.50
11:K:52:GLN:HG3	11:K:53:ILE:H	1.74	0.50
19:S:104:PHE:HB2	19:S:109:MET:HE1	1.93	0.50
1:A:625:U:H5''	1:A:1044:C:N4	2.26	0.50
1:A:1846:U:O2'	3:C:172:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ASP:HB2	37:D:8595:HOH:O	2.11	0.50
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.42	0.50
10:J:166:ASN:ND2	10:J:166:ASN:N	2.60	0.50
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.42	0.50
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.94	0.50
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.47	0.50
19:S:15:LYS:HE3	37:S:8581:HOH:O	2.12	0.50
27:1:11:THR:HG23	27:1:23:ARG:HD2	1.94	0.50
1:A:113:A:OP2	1:A:114:A:H5''	2.12	0.50
1:A:1525:G:H5'	1:A:1526:A:OP2	2.12	0.50
1:A:2274:A:H1'	14:N:86:MET:SD	2.52	0.50
1:A:399:C:H5'	14:N:179:GLY:O	2.12	0.50
1:A:514:G:H2'	1:A:514:G:OP1	2.12	0.50
2:B:3030:C:OP1	6:F:137:PRO:O	2.29	0.50
2:B:3059:C:H2'	2:B:3060:C:C6	2.47	0.50
2:B:3076:G:C3'	2:B:3077:A:H5''	2.23	0.50
4:D:248:ARG:O	4:D:251:VAL:HG13	2.11	0.50
5:E:111:VAL:HB	37:E:8322:HOH:O	2.11	0.50
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.94	0.50
9:I:12:ILE:HD12	37:I:692:HOH:O	2.11	0.50
19:S:39:THR:HG22	19:S:41:GLY:N	2.26	0.50
27:1:51:GLY:HA3	37:1:8417:HOH:O	2.11	0.49
1:A:1840:A:H4'	1:A:1841:C:O5'	2.12	0.49
1:A:2506:A:C1'	37:A:5633:HOH:O	2.60	0.49
1:A:306:A:P	21:U:38:ARG:HH21	2.35	0.49
1:A:275:G:C2	1:A:376:C:N3	2.80	0.49
1:A:638:C:H2'	1:A:639:A:C8	2.47	0.49
2:B:3036:C:C5	2:B:3037:C:C5	3.00	0.49
4:D:162:MET:CE	4:D:310:ARG:HD3	2.42	0.49
7:G:145:ALA:HB1	7:G:168:ILE:CD1	2.42	0.49
14:N:114:VAL:HB	14:N:159:THR:HG23	1.94	0.49
14:N:165:SER:HB3	37:N:8533:HOH:O	2.12	0.49
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.42	0.49
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.47	0.49
1:A:182:G:O3'	14:N:157:LEU:CD1	2.61	0.49
1:A:731:U:O2'	1:A:732:C:H5'	2.12	0.49
1:A:816:G:H5'	1:A:1598:A:H4'	1.93	0.49
1:A:820:G:C5	3:C:171:LYS:HB2	2.48	0.49
6:F:11:HIS:C	6:F:13:MET:H	2.15	0.49
1:A:1003:U:HO2'	10:J:90:PHE:HE1	1.60	0.49
6:F:146:LYS:HZ1	15:O:107:ASN:HD21	1.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.12	0.49
1:A:1120:U:H5'	1:A:1121:G:OP2	2.12	0.49
1:A:1422:U:H2'	1:A:1423:C:C6	2.48	0.49
1:A:2300:A:H4'	1:A:2301:A:O5'	2.13	0.49
1:A:275:G:N2	1:A:376:C:C2	2.80	0.49
1:A:703:G:O2'	1:A:704:C:H5'	2.12	0.49
4:D:205:VAL:O	4:D:307:ARG:NE	2.45	0.49
4:D:41:PHE:HA	4:D:79:MET:HE2	1.93	0.49
6:F:95:THR:C	6:F:97:GLN:N	2.60	0.49
7:G:43:ASP:HA	37:G:5864:HOH:O	2.12	0.49
8:H:105:ALA:HB2	37:H:5522:HOH:O	2.12	0.49
11:K:45:VAL:HG22	11:K:46:ILE:N	2.25	0.49
24:X:139:GLY:O	24:X:141:HIS:CD2	2.64	0.49
30:4:3:MET:O	30:4:90:PHE:HA	2.11	0.49
1:A:152:A:O2'	1:A:153:C:H5'	2.12	0.49
3:C:170:VAL:HG13	27:1:22:ILE:HG21	1.95	0.49
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.94	0.49
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.93	0.49
16:P:105:ASN:HD21	16:P:109:SER:H	1.61	0.49
30:4:74:CYS:N	37:4:8561:HOH:O	2.46	0.49
1:A:2729:C:H2'	1:A:2730:G:H8	1.78	0.49
1:A:665:A:H2'	1:A:666:A:C8	2.47	0.49
2:B:3020:G:P	37:B:8435:HOH:O	2.71	0.49
3:C:194:MET:HE1	3:C:199:HIS:HB2	1.95	0.49
6:F:27:ILE:HG22	6:F:28:GLY:N	2.22	0.49
7:G:77:THR:OG1	7:G:78:GLU:N	2.44	0.49
10:J:154:THR:HB	10:J:155:PRO:HD3	1.95	0.49
16:P:113:VAL:O	16:P:114:ILE:HD13	2.13	0.49
16:P:99:GLU:HA	37:P:7481:HOH:O	2.12	0.49
25:Y:25:ARG:HD3	25:Y:64:ALA:O	2.13	0.49
1:A:1684:A:O2'	1:A:1685:A:H5''	2.13	0.49
1:A:390:G:C5	1:A:391:U:C5	3.00	0.49
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.42	0.49
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.93	0.49
15:O:141:ARG:HB3	37:O:8570:HOH:O	2.13	0.49
17:Q:10:ALA:O	17:Q:13:VAL:HG12	2.13	0.49
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.46	0.49
22:V:20:MET:CG	22:V:28:THR:HG23	2.43	0.49
24:X:51:PHE:N	24:X:51:PHE:CD1	2.79	0.49
26:Z:200:THR:HG22	26:Z:201:GLU:HG2	1.94	0.49
1:A:1189:A:O2'	1:A:1208:C:H2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1682:A:H5''	37:A:9036:HOH:O	2.12	0.49
1:A:716:G:O5'	37:A:5790:HOH:O	2.20	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.12	0.49
4:D:140:LEU:HD23	37:D:8583:HOH:O	2.13	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.13	0.49
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.41	0.49
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.43	0.49
14:N:9:ARG:HG3	37:N:8544:HOH:O	2.12	0.49
15:O:37:ARG:NH2	37:O:8534:HOH:O	2.45	0.49
1:A:1370:G:C4	37:A:9727:HOH:O	2.65	0.49
2:B:3095:C:O2'	2:B:3096:C:H5'	2.13	0.49
5:E:133:ARG:NH2	37:E:8421:HOH:O	2.46	0.49
5:E:236:THR:O	5:E:237:GLU:C	2.50	0.49
6:F:19:GLU:O	6:F:133:ASN:HB3	2.12	0.49
14:N:113:ARG:NH1	14:N:152:ARG:O	2.42	0.49
21:U:38:ARG:NH1	21:U:38:ARG:HG3	2.27	0.49
1:A:797:A:H4'	27:1:10:ARG:N	2.27	0.49
1:A:169:A:H4'	37:N:8534:HOH:O	2.12	0.49
1:A:2420:G:H4'	37:A:3671:HOH:O	2.13	0.49
1:A:2837:U:H2'	37:A:6412:HOH:O	2.13	0.49
1:A:440:C:H2'	1:A:441:A:C8	2.48	0.49
5:E:84:VAL:O	5:E:85:LYS:CB	2.60	0.49
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.42	0.49
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.42	0.49
12:L:132:VAL:C	37:L:3160:HOH:O	2.51	0.49
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.13	0.49
37:A:8974:HOH:O	27:1:34:LYS:HD3	2.13	0.49
1:A:1205:U:C2'	1:A:1206:U:C5'	2.90	0.49
1:A:2896:A:H2'	1:A:2896:A:N3	2.28	0.49
1:A:812:A:H2'	1:A:813:C:C6	2.48	0.49
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.95	0.49
1:A:449:A:C8	5:E:43:LYS:HG2	2.47	0.49
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.13	0.49
6:F:64:ARG:HG2	6:F:66:GLY:O	2.13	0.49
1:A:1119:G:C8	11:K:52:GLN:NE2	2.81	0.49
13:M:72:ASN:HB2	37:M:8453:HOH:O	2.12	0.49
14:N:108:LYS:HD3	14:N:108:LYS:N	2.28	0.49
15:O:132:ASN:O	15:O:135:VAL:HG12	2.12	0.49
19:S:96:VAL:HG13	19:S:106:GLY:HA3	1.94	0.49
24:X:76:ASP:O	24:X:77:ALA:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:40:ARG:HD2	37:4:8549:HOH:O	2.13	0.48
1:A:1166:A:H1'	1:A:1192:A:N1	2.26	0.48
1:A:1236:A:H2'	1:A:1237:U:O4'	2.13	0.48
1:A:2505:G:H8	37:A:5216:HOH:O	1.96	0.48
1:A:907:A:H2'	1:A:908:A:C8	2.47	0.48
2:B:3055:U:H4'	2:B:3056:A:H8	1.78	0.48
4:D:84:LEU:HD13	4:D:84:LEU:O	2.13	0.48
10:J:31:PHE:CD2	10:J:85:ILE:HG23	2.48	0.48
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.78	0.48
19:S:76:ASP:OD1	19:S:77:ALA:N	2.45	0.48
21:U:28:SER:O	21:U:32:ARG:HG3	2.12	0.48
24:X:48:VAL:O	24:X:48:VAL:CG1	2.59	0.48
25:Y:85:VAL:HG12	25:Y:86:GLU:N	2.27	0.48
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.48
1:A:1334:C:H2'	1:A:1335:C:H6	1.77	0.48
1:A:2428:G:C4	1:A:2461:U:C5	3.01	0.48
1:A:2597:U:OP2	37:A:3404:HOH:O	2.20	0.48
1:A:289:G:O2'	1:A:290:C:H5'	2.12	0.48
2:B:3029:C:C2'	2:B:3030:C:H5'	2.43	0.48
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.43	0.48
10:J:44:ALA:HB3	10:J:136:VAL:O	2.13	0.48
12:L:101:ASN:O	12:L:102:GLU:HB2	2.13	0.48
37:A:9381:HOH:O	12:L:39:GLY:HA3	2.12	0.48
12:L:48:GLY:C	37:L:5632:HOH:O	2.50	0.48
37:A:5846:HOH:O	17:Q:59:ARG:HD3	2.13	0.48
19:S:39:THR:HB	19:S:42:GLU:CD	2.33	0.48
21:U:26:THR:HA	21:U:39:ASN:HB3	1.95	0.48
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.27	0.48
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.48	0.48
1:A:1972:U:H2'	1:A:1973:A:C5'	2.43	0.48
1:A:2356:A:H2'	1:A:2357:G:O4'	2.13	0.48
1:A:2421:G:H3'	1:A:2422:U:H5''	1.95	0.48
1:A:2547:C:H2'	1:A:2548:C:H6	1.78	0.48
1:A:2727:A:H2'	1:A:2728:C:H5'	1.94	0.48
1:A:2791:U:H1'	1:A:2792:A:H5''	1.96	0.48
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.78	0.48
11:K:107:ASN:HD22	11:K:109:TYR:H	1.59	0.48
12:L:55:VAL:CG1	12:L:56:SER:N	2.77	0.48
14:N:79:LYS:NZ	37:N:8566:HOH:O	2.46	0.48
37:L:1387:HOH:O	22:V:20:MET:HE3	2.13	0.48
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.13	0.48
1:A:1299:G:N2	37:A:4259:HOH:O	2.46	0.48
1:A:1425:G:O2'	1:A:1426:C:H5'	2.13	0.48
1:A:1701:A:H4'	1:A:1702:U:C5'	2.42	0.48
1:A:1930:A:H2'	1:A:1931:A:C8	2.48	0.48
1:A:837:U:H4'	37:A:9979:HOH:O	2.12	0.48
5:E:107:ARG:NH2	37:E:8454:HOH:O	2.44	0.48
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.45	0.48
8:H:26:THR:HB	8:H:102:GLY:HA3	1.95	0.48
9:I:73:ASP:O	37:I:2218:HOH:O	2.20	0.48
15:O:157:PRO:HA	37:O:8526:HOH:O	2.12	0.48
19:S:132:ARG:HG2	19:S:133:ALA:N	2.27	0.48
1:A:1486:A:C5	29:3:2:LYS:HG3	2.48	0.48
1:A:2445:U:H2'	1:A:2446:G:C8	2.48	0.48
1:A:2727:A:C5	1:A:2756:U:C4	3.01	0.48
1:A:2834:G:C4	1:A:2847:G:N2	2.81	0.48
1:A:390:G:C4	1:A:391:U:C6	3.02	0.48
3:C:123:GLY:HA2	3:C:159:VAL:O	2.14	0.48
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.11	0.48
24:X:110:GLN:HA	24:X:110:GLN:HE21	1.78	0.48
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.28	0.48
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.13	0.48
1:A:1057:A:C6	1:A:1058:A:C6	3.02	0.48
1:A:1117:A:C2	1:A:1244:U:C2	3.01	0.48
1:A:1162:G:H2'	1:A:1162:G:N3	2.28	0.48
1:A:130:C:H5'	37:A:4789:HOH:O	2.13	0.48
1:A:1768:C:H2'	1:A:1769:C:O4'	2.14	0.48
1:A:2401:A:H5'	37:A:9075:HOH:O	2.12	0.48
1:A:2821:C:H4'	4:D:116:PRO:CB	2.41	0.48
5:E:237:GLU:N	37:E:8445:HOH:O	2.46	0.48
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.95	0.48
6:F:23:VAL:HG12	6:F:130:VAL:HG22	1.96	0.48
11:K:107:ASN:HD22	11:K:107:ASN:C	2.17	0.48
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.44	0.48
13:M:61:ALA:HA	37:M:8437:HOH:O	2.14	0.48
16:P:54:GLU:HG2	16:P:73:ASP:O	2.14	0.48
19:S:34:GLU:HG2	19:S:46:TYR:OH	2.14	0.48
19:S:35:ILE:O	19:S:38:LYS:HB2	2.13	0.48
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.14	0.48
1:A:1114:A:H2'	1:A:1115:U:H6	1.77	0.48
1:A:154:C:N3	1:A:155:C:C5	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2559:C:H4'	37:A:6828:HOH:O	2.13	0.48
1:A:29:C:OP2	37:A:9723:HOH:O	2.20	0.48
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.48	0.48
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.44	0.48
18:R:77:ASP:N	18:R:80:LYS:O	2.44	0.48
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.78	0.48
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.96	0.48
20:T:6:LYS:HB2	20:T:27:ALA:O	2.13	0.48
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.43	0.48
37:A:3555:HOH:O	30:4:57:GLY:HA2	2.14	0.48
1:A:1507:C:H4'	37:A:3185:HOH:O	2.13	0.48
1:A:2385:G:H2'	1:A:2386:U:H6	1.78	0.48
1:A:23:G:C6	1:A:24:G:N1	2.81	0.48
1:A:371:U:H2'	1:A:372:A:C8	2.47	0.48
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.95	0.48
4:D:55:ASN:HB3	4:D:64:GLY:H	1.78	0.48
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.44	0.48
8:H:34:ASN:HA	14:N:4:ALA:HB2	1.96	0.48
8:H:37:THR:O	8:H:41:GLU:HG3	2.13	0.48
8:H:59:ILE:O	8:H:59:ILE:HG22	2.14	0.48
15:O:139:TRP:HH2	15:O:176:ARG:HH11	1.62	0.48
17:Q:83:LYS:O	17:Q:86:ALA:HB3	2.14	0.48
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.48	0.48
1:A:1180:U:H2'	1:A:1181:A:O4'	2.14	0.48
1:A:2780:C:H2'	1:A:2781:U:H6	1.78	0.48
1:A:2906:A:H5'	1:A:2907:C:O4'	2.14	0.48
1:A:40:C:O5'	1:A:40:C:H6	1.97	0.48
1:A:484:A:N1	1:A:506:G:H4'	2.29	0.48
1:A:51:G:N2	1:A:111:C:C2	2.81	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
1:A:612:U:H2'	1:A:613:C:C6	2.49	0.48
1:A:920:C:H5''	1:A:921:G:O5'	2.14	0.48
5:E:246:ARG:CB	5:E:246:ARG:HH11	2.19	0.48
7:G:84:MET:HB2	7:G:131:LEU:HB2	1.94	0.48
13:M:1:THR:HA	37:M:8393:HOH:O	2.13	0.48
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.48	0.48
30:4:65:THR:HB	30:4:83:TRP:H	1.78	0.48
1:A:2326:U:H4'	1:A:2412:G:C4'	2.44	0.48
1:A:349:U:O2'	1:A:350:C:H5'	2.14	0.48
1:A:682:A:H2'	1:A:683:G:O4'	2.14	0.48
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:U:O2'	5:E:42:ARG:NH1	2.47	0.48
10:J:117:LYS:O	10:J:119:VAL:HG13	2.13	0.48
10:J:71:TYR:C	10:J:73:GLN:N	2.66	0.48
12:L:125:ALA:C	12:L:127:ALA:H	2.17	0.48
13:M:128:GLY:O	13:M:132:LYS:HG3	2.13	0.48
19:S:39:THR:O	19:S:40:ALA:C	2.51	0.48
20:T:57:THR:CG2	20:T:58:MET:N	2.77	0.48
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.29	0.48
1:A:1462:C:O2'	1:A:1463:A:H5'	2.14	0.47
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.14	0.47
1:A:2507:G:H2'	1:A:2510:C:H42	1.79	0.47
1:A:1741:U:O2'	1:A:2723:G:H4'	2.13	0.47
1:A:797:A:O4'	27:1:10:ARG:N	2.47	0.47
1:A:795:G:N3	1:A:817:G:C2	2.82	0.47
2:B:3026:C:OP2	37:B:8441:HOH:O	2.19	0.47
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.13	0.47
4:D:1:PRO:O	4:D:2:GLN:HB2	2.14	0.47
8:H:58:GLU:HG3	8:H:61:MET:CE	2.44	0.47
11:K:131:THR:HB	11:K:134:GLU:HG3	1.95	0.47
12:L:9:THR:O	12:L:10:GLN:C	2.50	0.47
16:P:77:ALA:HB1	16:P:98:LEU:HD12	1.96	0.47
17:Q:143:ALA:CA	37:Q:5521:HOH:O	2.61	0.47
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.96	0.47
24:X:137:GLN:O	24:X:137:GLN:HG3	2.14	0.47
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.48	0.47
1:A:1167:G:O2'	1:A:1168:C:H5'	2.14	0.47
1:A:128:A:H3'	1:A:128:A:C8	2.49	0.47
1:A:1634:G:H3'	37:A:3471:HOH:O	2.13	0.47
1:A:1947:G:P	37:A:3246:HOH:O	2.69	0.47
1:A:736:A:H2'	1:A:737:A:O4'	2.13	0.47
2:B:3056:A:H1'	6:F:14:ARG:HG2	1.97	0.47
4:D:280:VAL:HG13	4:D:334:SER:HA	1.96	0.47
4:D:52:VAL:O	4:D:53:LEU:HD12	2.14	0.47
7:G:9:GLU:HA	37:G:5240:HOH:O	2.13	0.47
17:Q:61:ARG:NH1	17:Q:61:ARG:HG3	2.28	0.47
19:S:72:VAL:CG1	19:S:75:TRP:HB3	2.44	0.47
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.48	0.47
1:A:56:G:H5''	23:W:50:ARG:HH12	1.78	0.47
1:A:1019:C:O2	18:R:94:GLN:NE2	2.47	0.47
1:A:1440:U:P	37:A:4043:HOH:O	2.72	0.47
1:A:1878:G:C1'	37:A:5700:HOH:O	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2361:A:H2'	1:A:2362:A:C8	2.48	0.47
1:A:2385:G:H2'	1:A:2386:U:C6	2.49	0.47
1:A:401:C:P	37:A:5369:HOH:O	2.72	0.47
1:A:447:A:O2'	1:A:448:G:H5'	2.15	0.47
1:A:514:G:O5'	1:A:514:G:H8	1.97	0.47
1:A:603:A:H4'	1:A:604:G:O5'	2.14	0.47
1:A:737:A:H2'	1:A:738:G:O4'	2.14	0.47
2:B:3049:G:O2'	2:B:3050:G:H5'	2.14	0.47
3:C:153:ARG:NH1	3:C:153:ARG:HB2	2.23	0.47
3:C:171:LYS:NZ	37:C:8527:HOH:O	2.41	0.47
4:D:177:HIS:O	4:D:181:ILE:HG13	2.14	0.47
6:F:99:ASP:HB2	6:F:103:ASN:H	1.79	0.47
12:L:20:CYS:HB3	12:L:26:ALA:O	2.15	0.47
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.95	0.47
14:N:154:ARG:HG3	37:N:8612:HOH:O	2.15	0.47
14:N:57:LYS:HB3	14:N:60:ILE:HD12	1.96	0.47
24:X:90:TYR:CD1	24:X:90:TYR:N	2.81	0.47
24:X:63:GLU:HG2	24:X:93:ILE:HG22	1.96	0.47
1:A:1114:A:H2'	1:A:1115:U:C6	2.49	0.47
1:A:2377:U:O5'	1:A:2377:U:H6	1.97	0.47
4:D:189:ALA:HB1	37:D:8567:HOH:O	2.14	0.47
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.30	0.47
6:F:169:THR:O	6:F:170:TYR:HB2	2.15	0.47
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.27	0.47
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.95	0.47
14:N:27:ARG:O	14:N:30:GLU:N	2.45	0.47
1:A:2274:A:C4'	14:N:77:PHE:HE1	2.27	0.47
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.15	0.47
17:Q:131:PHE:CE1	17:Q:137:LEU:HD13	2.49	0.47
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.44	0.47
22:V:52:THR:HG21	22:V:54:THR:HB	1.96	0.47
23:W:11:MET:HB3	23:W:15:GLU:HB2	1.95	0.47
24:X:122:ARG:HH22	24:X:154:ARG:C	2.18	0.47
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.14	0.47
1:A:107:U:H2'	1:A:108:U:H5'	1.96	0.47
1:A:2389:U:H4'	18:R:53:HIS:HD2	1.80	0.47
1:A:2769:C:H2'	1:A:2770:G:H5'	1.97	0.47
1:A:516:A:OP2	37:A:5223:HOH:O	2.20	0.47
1:A:542:A:C8	1:A:542:A:C5'	2.91	0.47
1:A:95:A:H5''	1:A:97:G:O4'	2.14	0.47
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:54:LEU:HD23	5:E:79:ARG:HG3	1.96	0.47
6:F:84:LEU:C	6:F:86:THR:H	2.18	0.47
7:G:34:TRP:HA	37:G:4572:HOH:O	2.14	0.47
1:A:2415:A:O2'	15:O:29:SER:HB3	2.13	0.47
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.68	0.47
30:4:60:LYS:CG	30:4:61:PRO:HD2	2.40	0.47
1:A:1370:G:N3	37:A:9727:HOH:O	2.35	0.47
1:A:2524:G:H21	1:A:2526:C:N4	2.12	0.47
1:A:319:A:H2'	1:A:320:G:C8	2.49	0.47
1:A:536:A:H3'	37:A:4623:HOH:O	2.13	0.47
4:D:36:PRO:HA	4:D:168:GLY:HA2	1.93	0.47
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.45	0.47
11:K:103:VAL:HG12	37:K:5907:HOH:O	2.14	0.47
15:O:141:ARG:N	37:O:8570:HOH:O	2.47	0.47
19:S:29:LYS:HD3	37:S:8533:HOH:O	2.15	0.47
21:U:24:ARG:O	21:U:93:THR:OG1	2.23	0.47
22:V:33:SER:O	22:V:37:GLU:HG3	2.14	0.47
1:A:2456:A:H2'	1:A:2457:U:C6	2.50	0.47
1:A:2769:C:H2'	1:A:2770:G:C5'	2.44	0.47
1:A:2775:A:C6	1:A:2799:A:C8	3.02	0.47
1:A:844:A:C6	1:A:882:A:C5	3.02	0.47
1:A:960:G:N3	1:A:960:G:C2'	2.77	0.47
3:C:211:LYS:NZ	37:C:8625:HOH:O	2.46	0.47
10:J:26:LYS:CG	10:J:28:ILE:H	2.17	0.47
37:A:9350:HOH:O	13:M:41:HIS:CE1	2.62	0.47
2:B:3008:G:O6	15:O:11:ARG:NH1	2.47	0.47
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.13	0.47
19:S:132:ARG:NH1	37:S:8587:HOH:O	2.48	0.47
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.45	0.47
28:2:21:ARG:HD2	28:2:39:PHE:HB2	1.96	0.47
1:A:1209:C:H2'	1:A:1210:G:C8	2.46	0.47
1:A:1218:U:H2'	1:A:1219:U:C6	2.50	0.47
1:A:1385:G:O3'	25:Y:49:ARG:NH1	2.48	0.47
1:A:1543:G:N1	1:A:1641:A:OP2	2.34	0.47
1:A:584:U:H3'	37:A:5674:HOH:O	2.13	0.47
3:C:194:MET:CE	3:C:199:HIS:HB2	2.45	0.47
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.47
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.96	0.47
14:N:69:LYS:HD3	14:N:125:ARG:HA	1.96	0.47
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.50	0.47
24:X:66:LEU:HA	24:X:66:LEU:HD23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:C:H1'	37:A:6844:HOH:O	2.14	0.47
1:A:1453:G:N2	1:A:1675:C:C2	2.83	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.67	0.47
1:A:694:A:C2'	1:A:695:C:H5'	2.45	0.47
1:A:889:C:H2'	1:A:890:C:C6	2.50	0.47
2:B:3076:G:C8	2:B:3077:A:H2'	2.50	0.47
7:G:162:PHE:CD1	7:G:162:PHE:N	2.82	0.47
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.26	0.47
13:M:112:GLY:O	13:M:132:LYS:NZ	2.33	0.47
19:S:25:PHE:CE2	19:S:29:LYS:CE	2.98	0.47
19:S:33:ARG:NH2	37:S:8533:HOH:O	2.39	0.47
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.96	0.47
1:A:10:U:H5'	37:A:5616:HOH:O	2.13	0.47
1:A:1161:A:O5'	1:A:1161:A:C8	2.68	0.47
1:A:1304:U:H2'	1:A:1305:C:C6	2.50	0.47
1:A:142:G:O2'	1:A:143:C:H5'	2.14	0.47
1:A:2474:A:N3	37:A:4234:HOH:O	2.36	0.47
1:A:677:C:H4'	5:E:246:ARG:NH2	2.30	0.47
1:A:739:G:N7	37:A:7119:HOH:O	2.46	0.47
1:A:926:A:O2'	13:M:41:HIS:CD2	2.68	0.47
9:I:67:LEU:O	9:I:71:LEU:HG	2.15	0.47
13:M:17:SER:C	13:M:19:LYS:H	2.18	0.47
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.50	0.47
24:X:76:ASP:O	24:X:77:ALA:O	2.33	0.47
1:A:1477:C:H5'	1:A:1868:G:H5''	1.96	0.47
1:A:2531:U:O2'	1:A:2532:A:H5'	2.14	0.47
1:A:2785:C:H4'	1:A:2786:G:OP2	2.15	0.47
1:A:308:U:H5'	21:U:97:ARG:NH2	2.30	0.47
3:C:11:ARG:HD3	37:C:8519:HOH:O	2.15	0.47
3:C:169:PHE:O	3:C:170:VAL:HB	2.15	0.47
5:E:196:THR:HG23	37:E:8395:HOH:O	2.14	0.47
6:F:64:ARG:O	6:F:67:ASP:OD2	2.32	0.47
9:I:16:LYS:O	9:I:20:VAL:HG23	2.15	0.47
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.30	0.47
1:A:1616:A:H5''	1:A:1617:C:OP1	2.14	0.46
1:A:329:A:H5'	1:A:347:A:C1'	2.45	0.46
1:A:564:G:H1'	37:A:5885:HOH:O	2.15	0.46
3:C:100:PRO:O	3:C:103:VAL:HG23	2.14	0.46
3:C:175:LYS:HE2	37:C:8577:HOH:O	2.15	0.46
1:A:474:C:O3'	5:E:73:LEU:CD2	2.63	0.46
1:A:1151:G:P	9:I:16:LYS:NZ	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:101:ASN:O	12:L:102:GLU:CB	2.63	0.46
13:M:101:ASP:C	13:M:103:ALA:H	2.17	0.46
13:M:59:GLU:HG2	13:M:104:ASP:OD2	2.14	0.46
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.14	0.46
37:L:7438:HOH:O	22:V:20:MET:HE1	2.15	0.46
24:X:65:VAL:CA	24:X:68:THR:HG22	2.45	0.46
1:A:2445:U:H2'	1:A:2446:G:H8	1.80	0.46
1:A:2737:C:H2'	37:A:5721:HOH:O	2.14	0.46
1:A:2783:A:O2'	1:A:2784:A:H5'	2.15	0.46
1:A:2897:C:H2'	1:A:2898:G:H8	1.78	0.46
1:A:2900:G:H2'	1:A:2901:C:O4'	2.15	0.46
1:A:622:G:H5'	1:A:1357:A:H61	1.79	0.46
1:A:962:C:H5''	37:A:4487:HOH:O	2.14	0.46
3:C:69:LEU:HD12	3:C:69:LEU:C	2.34	0.46
5:E:246:ARG:NE	37:E:8419:HOH:O	2.48	0.46
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.50	0.46
15:O:175:LEU:HD11	37:O:8539:HOH:O	2.15	0.46
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.96	0.46
20:T:11:THR:H	20:T:14:ALA:HB3	1.80	0.46
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.46
24:X:80:ASP:O	24:X:84:VAL:HG23	2.15	0.46
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.96	0.46
28:2:5:THR:N	28:2:6:PRO:HD2	2.29	0.46
1:A:2415:A:N3	15:O:26:LEU:HD13	2.30	0.46
1:A:2656:G:C2'	1:A:2657:G:H5'	2.45	0.46
5:E:150:THR:HA	5:E:203:ALA:O	2.16	0.46
8:H:117:GLU:C	8:H:119:ARG:H	2.19	0.46
10:J:57:ARG:HG3	10:J:57:ARG:HH11	1.81	0.46
15:O:184:ILE:HG22	15:O:185:GLU:N	2.30	0.46
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.14	0.46
1:A:21:G:H5''	19:S:1:GLY:O	2.16	0.46
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.50	0.46
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.15	0.46
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.97	0.46
27:1:50:ALA:HB3	27:1:54:ILE:HG22	1.97	0.46
1:A:1250:C:O2'	1:A:1251:C:H5'	2.16	0.46
1:A:1594:C:C2	1:A:1601:G:N2	2.83	0.46
1:A:506:G:N2	1:A:509:A:H5''	2.22	0.46
9:I:12:ILE:HB	37:I:4714:HOH:O	2.15	0.46
10:J:157:ILE:CG2	10:J:158:ASN:N	2.79	0.46
12:L:99:ASP:OD1	12:L:101:ASN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:O3'	14:N:157:LEU:HD13	2.16	0.46
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.98	0.46
14:N:87:MET:HG3	14:N:87:MET:H	1.29	0.46
1:A:380:A:OP2	14:N:9:ARG:HD2	2.16	0.46
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.71	0.46
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.45	0.46
1:A:841:A:OP2	19:S:128:ARG:HD2	2.15	0.46
20:T:57:THR:C	20:T:59:ASP:H	2.19	0.46
22:V:44:ARG:CB	37:V:3805:HOH:O	2.63	0.46
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.79	0.46
24:X:13:MET:HA	37:X:4944:HOH:O	2.16	0.46
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.97	0.46
24:X:65:VAL:HA	24:X:68:THR:CG2	2.45	0.46
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.51	0.46
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.96	0.46
1:A:1902:G:N2	1:A:1936:C:C2	2.83	0.46
1:A:2443:C:H3'	37:A:3056:HOH:O	2.15	0.46
1:A:275:G:C2	1:A:376:C:C2	3.04	0.46
1:A:283:U:H5''	1:A:284:C:OP2	2.16	0.46
1:A:426:G:H2'	1:A:427:C:O4'	2.15	0.46
1:A:382:U:O2'	1:A:430:A:H1'	2.15	0.46
3:C:232:ARG:NH2	3:C:236:GLY:O	2.40	0.46
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.74	0.46
4:D:243:ASN:HA	4:D:244:PRO:C	2.36	0.46
6:F:94:ALA:O	6:F:95:THR:O	2.33	0.46
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.31	0.46
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.33	0.46
37:B:8465:HOH:O	15:O:147:ILE:HB	2.15	0.46
27:1:34:LYS:HE2	37:1:8426:HOH:O	2.15	0.46
1:A:121:U:OP2	29:3:10:ARG:NH2	2.36	0.46
1:A:1335:C:H2'	1:A:1336:U:C6	2.51	0.46
1:A:2673:U:C2	1:A:2817:G:N2	2.84	0.46
1:A:2909:G:O2'	1:A:2910:A:H5'	2.16	0.46
1:A:417:G:P	37:A:6989:HOH:O	2.72	0.46
1:A:51:G:C2	1:A:111:C:C2	3.04	0.46
1:A:816:G:C6	1:A:817:G:N1	2.83	0.46
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.45	0.46
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.45	0.46
7:G:5:LEU:HD21	7:G:66:GLN:HG3	1.98	0.46
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.15	0.46
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:164:THR:HG23	14:N:165:SER:OG	2.15	0.46
15:O:32:PRO:HD2	15:O:99:GLU:O	2.16	0.46
15:O:71:TRP:N	37:O:8539:HOH:O	2.48	0.46
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.48	0.46
17:Q:64:GLU:HG2	37:Q:2495:HOH:O	2.14	0.46
1:A:1185:U:H5'	37:A:7039:HOH:O	2.16	0.46
1:A:2266:A:H2'	1:A:2267:G:C8	2.51	0.46
1:A:2500:C:O2'	1:A:2501:G:H5'	2.16	0.46
1:A:2533:C:C6	1:A:2533:C:H5'	2.41	0.46
1:A:425:U:O2'	1:A:426:G:H5'	2.16	0.46
5:E:218:VAL:HG12	37:E:8419:HOH:O	2.15	0.46
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.46
14:N:164:THR:HG23	14:N:165:SER:H	1.76	0.46
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.98	0.46
1:A:1377:C:C6	1:A:1377:C:H5'	2.47	0.46
1:A:177:A:H2'	1:A:178:U:O4'	2.16	0.46
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.15	0.46
1:A:80:A:H5''	21:U:41:ARG:CZ	2.46	0.46
2:B:3041:C:H4'	6:F:48:MET:HB2	1.98	0.46
3:C:85:ASP:HA	37:C:8620:HOH:O	2.14	0.46
4:D:211:THR:HA	4:D:255:GLY:O	2.16	0.46
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.45	0.46
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.16	0.46
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.31	0.46
14:N:184:ARG:HG3	14:N:185:PRO:HA	1.98	0.46
18:R:28:ARG:HG2	37:R:4350:HOH:O	2.16	0.46
19:S:8:ALA:CB	19:S:13:THR:HG21	2.37	0.46
1:A:1301:C:O2'	1:A:1331:A:H4'	2.16	0.46
1:A:1419:U:O2	1:A:1419:U:H3'	2.16	0.46
1:A:1461:U:H2'	1:A:1462:C:C6	2.51	0.46
1:A:2432:C:OP1	13:M:48:LYS:NZ	2.38	0.46
1:A:2502:C:C4'	10:J:151:MET:HG2	2.46	0.46
1:A:2712:G:O2'	1:A:2713:G:H5'	2.16	0.46
1:A:396:U:O2'	1:A:418:C:H4'	2.16	0.46
1:A:429:A:C6	1:A:430:A:C6	3.04	0.46
1:A:559:U:C6	1:A:559:U:H5'	2.42	0.46
4:D:43:GLY:O	4:D:308:LEU:HD12	2.15	0.46
5:E:27:ARG:O	5:E:31:ILE:HG13	2.16	0.46
6:F:21:VAL:HG13	6:F:131:THR:O	2.16	0.46
7:G:68:HIS:O	7:G:72:MET:HG3	2.16	0.46
8:H:60:VAL:O	8:H:60:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:123:ASP:OD1	14:N:123:ASP:C	2.54	0.46
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.51	0.46
1:A:2072:G:C6	1:A:2533:C:H1'	2.51	0.46
1:A:2251:G:H4'	37:A:6980:HOH:O	2.16	0.46
1:A:716:G:C2'	1:A:717:C:O5'	2.64	0.46
3:C:66:ARG:HH11	3:C:66:ARG:HB2	1.80	0.46
3:C:36:ASP:HB2	3:C:84:VAL:N	2.31	0.46
4:D:132:HIS:HB2	4:D:137:LEU:HD22	1.97	0.46
10:J:132:PHE:O	10:J:133:ILE:HD13	2.16	0.46
10:J:35:ASN:ND2	10:J:79:ALA:O	2.49	0.46
14:N:35:PRO:CG	14:N:38:VAL:CG2	2.87	0.46
1:A:1368:U:H6	1:A:1368:U:O5'	1.99	0.45
1:A:2346:C:O3'	6:F:52:THR:HG23	2.16	0.45
1:A:2361:A:H5'	1:A:2361:A:H8	1.81	0.45
1:A:2645:U:H4'	31:A:8600:ZIT:H172	1.98	0.45
1:A:702:G:O2'	1:A:703:G:H5'	2.16	0.45
1:A:861:A:H2'	1:A:862:U:C6	2.51	0.45
1:A:941:G:O2'	1:A:942:U:H5'	2.16	0.45
10:J:26:LYS:CD	10:J:28:ILE:HB	2.46	0.45
1:A:2413:A:N7	15:O:109:PRO:HB3	2.32	0.45
1:A:380:A:H5''	14:N:48:ARG:NH2	2.31	0.45
1:A:790:A:H2'	1:A:791:A:O4'	2.16	0.45
4:D:144:THR:HG22	4:D:145:HIS:N	2.31	0.45
7:G:95:VAL:O	7:G:126:ILE:HD13	2.16	0.45
7:G:11:VAL:CG1	7:G:12:ASP:H	2.29	0.45
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.43	0.45
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.52	0.45
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.47	0.45
15:O:154:LEU:CG	15:O:155:GLU:H	2.27	0.45
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.16	0.45
21:U:6:LYS:NZ	37:U:644:HOH:O	2.42	0.45
21:U:96:VAL:HG13	21:U:97:ARG:N	2.31	0.45
30:4:87:ARG:HG3	37:4:8572:HOH:O	2.16	0.45
1:A:1060:C:O2'	1:A:1061:C:H5'	2.16	0.45
1:A:1129:C:H5''	1:A:1130:U:OP2	2.16	0.45
1:A:1450:C:C4'	1:A:1451:C:OP2	2.59	0.45
1:A:1617:C:C4	1:A:1643:C:H4'	2.51	0.45
1:A:1669:A:H2'	1:A:1670:G:H8	1.81	0.45
1:A:314:G:N2	1:A:316:A:H3'	2.31	0.45
1:A:492:C:C2'	1:A:493:U:H5'	2.46	0.45
1:A:57:C:H5''	37:A:6335:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:PRO:HD3	37:C:8523:HOH:O	2.15	0.45
3:C:93:THR:C	3:C:94:LEU:HD23	2.36	0.45
4:D:88:GLU:O	4:D:88:GLU:HG3	2.15	0.45
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.46	0.45
7:G:133:VAL:HG12	7:G:141:VAL:HG13	1.98	0.45
1:A:1972:U:H2'	1:A:1973:A:H5'	1.99	0.45
1:A:2661:U:H3	1:A:2812:A:H62	1.64	0.45
1:A:278:A:H2'	1:A:279:C:O4'	2.17	0.45
1:A:2814:A:OP2	37:A:4646:HOH:O	2.21	0.45
1:A:2852:A:H5''	37:A:4808:HOH:O	2.16	0.45
1:A:45:A:N6	1:A:147:G:C4	2.84	0.45
3:C:153:ARG:HD3	37:C:8533:HOH:O	2.15	0.45
4:D:248:ARG:HG2	37:K:3517:HOH:O	2.15	0.45
5:E:211:ASP:HB2	5:E:231:ARG:HH12	1.81	0.45
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.98	0.45
6:F:92:GLU:O	6:F:93:LEU:O	2.33	0.45
10:J:84:ARG:CZ	10:J:135:TRP:CH2	3.00	0.45
13:M:20:ASN:O	13:M:22:ARG:N	2.50	0.45
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.99	0.45
15:O:37:ARG:HA	15:O:37:ARG:HD3	1.82	0.45
15:O:37:ARG:HA	35:O:8507:CL:CL	2.53	0.45
16:P:77:ALA:HA	16:P:96:VAL:O	2.16	0.45
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.56	0.45
1:A:236:A:H4'	1:A:237:G:OP1	2.16	0.45
1:A:1815:A:H4'	1:A:2751:C:O4'	2.16	0.45
1:A:303:C:H2'	1:A:304:G:O4'	2.16	0.45
3:C:192:VAL:O	3:C:192:VAL:HG12	2.16	0.45
4:D:36:PRO:CA	4:D:168:GLY:HA3	2.43	0.45
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.46	0.45
5:E:246:ARG:NH2	37:E:8419:HOH:O	2.50	0.45
6:F:59:GLY:O	6:F:61:PHE:N	2.38	0.45
7:G:132:THR:O	7:G:132:THR:HG23	2.16	0.45
7:G:97:VAL:C	37:G:4191:HOH:O	2.54	0.45
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.52	0.45
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.52	0.45
12:L:87:ARG:CZ	37:L:4854:HOH:O	2.63	0.45
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.80	0.45
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.51	0.45
1:A:1750:C:N4	1:A:1751:G:C6	2.85	0.45
1:A:2316:G:H4'	37:A:5671:HOH:O	2.16	0.45
1:A:236:A:C4'	1:A:237:G:H5'	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:C:O2	1:A:240:C:H2'	2.17	0.45
1:A:2860:G:H1'	37:A:6376:HOH:O	2.16	0.45
3:C:132:ASP:OD1	3:C:133:ARG:N	2.48	0.45
3:C:39:ALA:HB3	3:C:61:GLU:OE2	2.16	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.46	0.45
14:N:37:VAL:HG22	14:N:65:VAL:HG22	1.99	0.45
16:P:73:ASP:HA	16:P:92:VAL:O	2.17	0.45
37:A:3563:HOH:O	21:U:82:THR:HA	2.17	0.45
22:V:6:CYS:C	22:V:8:TYR:N	2.70	0.45
24:X:67:ALA:HB2	24:X:93:ILE:HD13	1.98	0.45
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.97	0.45
29:3:18:ASN:HA	29:3:18:ASN:HD22	1.58	0.45
1:A:1118:A:C8	1:A:1119:G:H5''	2.52	0.45
1:A:1197:G:N2	37:A:5811:HOH:O	2.49	0.45
1:A:1209:C:O2	1:A:1210:G:C8	2.69	0.45
1:A:123:U:H2'	1:A:124:C:C6	2.52	0.45
1:A:1730:G:H5'	1:A:1731:C:C6	2.52	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.17	0.45
1:A:2781:U:H2'	1:A:2782:G:C5'	2.46	0.45
1:A:625:U:H5'	37:A:9771:HOH:O	2.15	0.45
1:A:885:G:H5''	1:A:886:A:H5'	1.99	0.45
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.56	0.45
6:F:159:PRO:O	6:F:162:ALA:HB3	2.16	0.45
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.47	0.45
15:O:37:ARG:CZ	37:O:8534:HOH:O	2.64	0.45
15:O:38:LYS:HB2	15:O:38:LYS:HE3	1.64	0.45
22:V:17:THR:HG22	22:V:18:GLY:N	2.31	0.45
25:Y:43:VAL:HG22	25:Y:76:ARG:NH1	2.32	0.45
1:A:1335:C:OP2	26:Z:207:SER:CB	2.65	0.45
30:4:91:GLN:O	30:4:92:GLU:HB2	2.17	0.45
1:A:1205:U:C2'	1:A:1206:U:H5'	2.41	0.45
1:A:2106:C:H2'	1:A:2107:U:C6	2.51	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.45
1:A:2851:G:C2'	1:A:2852:A:H5'	2.47	0.45
1:A:716:G:H2'	1:A:717:C:O5'	2.17	0.45
2:B:3042:C:O2	6:F:76:ARG:NH1	2.50	0.45
2:B:3064:C:C2'	2:B:3065:A:H5'	2.47	0.45
2:B:3096:C:H2'	2:B:3097:U:C6	2.52	0.45
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.46	0.45
7:G:107:PHE:CZ	7:G:108:LEU:HD13	2.52	0.45
13:M:130:ARG:NH2	37:M:8418:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:97:VAL:HG12	13:M:98:GLU:O	2.17	0.45
18:R:72:LYS:HG2	18:R:85:ILE:HD13	1.99	0.45
26:Z:187:VAL:HB	37:Z:8158:HOH:O	2.17	0.45
27:1:56:MET:HA	27:1:62:TYR:O	2.17	0.45
30:4:70:ARG:HG2	30:4:70:ARG:NH1	2.32	0.45
1:A:1252:A:H2'	1:A:1253:C:O4'	2.17	0.45
1:A:1574:C:O5'	1:A:1574:C:H6	1.99	0.45
1:A:1593:C:OP1	17:Q:117:SER:CB	2.65	0.45
1:A:1635:U:O2'	1:A:1636:G:H5'	2.17	0.45
1:A:2050:G:H5''	19:S:80:TYR:O	2.17	0.45
1:A:2729:C:O2'	1:A:2730:G:H5'	2.17	0.45
1:A:949:U:O2'	18:R:40:HIS:HE1	2.00	0.45
6:F:65:GLU:HA	37:F:6752:HOH:O	2.16	0.45
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.46	0.45
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.50	0.45
15:O:67:ALA:HA	15:O:71:TRP:H	1.82	0.45
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.17	0.45
19:S:119:VAL:CG1	19:S:119:VAL:O	2.63	0.45
19:S:82:GLU:HG3	19:S:83:LYS:H	1.81	0.45
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.16	0.45
27:1:10:ARG:HG3	27:1:11:THR:N	2.32	0.45
37:A:8939:HOH:O	28:2:1:THR:HA	2.17	0.45
28:2:22:CYS:SG	28:2:24:GLU:HB2	2.57	0.45
1:A:1535:G:H2'	1:A:1536:C:C6	2.52	0.45
1:A:1634:G:H2'	1:A:1635:U:C6	2.51	0.45
1:A:1810:C:OP1	22:V:44:ARG:NE	2.28	0.45
1:A:2039:A:H4'	1:A:2760:C:O2'	2.17	0.45
1:A:2273:C:OP1	37:A:9184:HOH:O	2.21	0.45
1:A:830:G:H2'	1:A:831:U:C6	2.51	0.45
5:E:214:THR:CG2	37:E:8433:HOH:O	2.55	0.45
6:F:15:GLU:HA	6:F:16:PRO:HD3	1.89	0.45
10:J:71:TYR:O	10:J:73:GLN:N	2.50	0.45
14:N:20:ILE:O	14:N:24:MET:HG2	2.17	0.45
14:N:47:ASP:CG	14:N:48:ARG:N	2.71	0.45
15:O:163:PHE:O	15:O:164:ASP:O	2.35	0.45
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.32	0.45
15:O:58:LEU:N	15:O:58:LEU:HD12	2.32	0.45
16:P:96:VAL:HG13	16:P:100:GLN:HB2	1.99	0.45
23:W:12:THR:HG23	23:W:14:ALA:N	2.32	0.45
24:X:3:ALA:O	24:X:54:PHE:HA	2.17	0.45
1:A:1008:C:OP1	10:J:16:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:U:O4'	1:A:1165:G:OP1	2.34	0.44
1:A:1549:C:N3	1:A:1637:A:C2	2.84	0.44
1:A:1666:C:O2'	1:A:1667:A:C5'	2.60	0.44
1:A:2387:U:H2'	1:A:2388:C:C6	2.51	0.44
1:A:2898:G:H4'	4:D:288:GLY:HA2	1.98	0.44
1:A:2911:C:H2'	1:A:2912:C:C6	2.53	0.44
1:A:542:A:H1'	37:A:4253:HOH:O	2.17	0.44
2:B:3078:G:O2'	2:B:3079:U:P	2.75	0.44
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.80	0.44
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.17	0.44
10:J:82:LYS:NZ	10:J:82:LYS:CB	2.80	0.44
1:A:251:C:H1'	14:N:58:GLN:HE22	1.81	0.44
1:A:869:G:OP1	14:N:79:LYS:HE2	2.16	0.44
17:Q:16:VAL:CG1	17:Q:20:ARG:HB2	2.48	0.44
37:A:9534:HOH:O	25:Y:23:HIS:HD2	1.99	0.44
1:A:88:G:N7	29:3:28:LYS:HD2	2.31	0.44
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.32	0.44
30:4:56:PRO:HA	37:4:8550:HOH:O	2.17	0.44
1:A:1532:G:C6	1:A:1533:A:C6	3.05	0.44
1:A:764:C:C2'	1:A:765:G:H5'	2.46	0.44
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.32	0.44
10:J:58:HIS:CE1	10:J:59:ASN:ND2	2.85	0.44
15:O:143:ARG:HH12	15:O:173:ASP:CG	2.18	0.44
1:A:1095:U:O2	24:X:120:PRO:HG2	2.17	0.44
1:A:120:A:H2'	1:A:120:A:N3	2.32	0.44
1:A:1746:A:N3	1:A:1748:U:C4	2.85	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.17	0.44
1:A:963:C:H2'	1:A:964:G:C8	2.52	0.44
2:B:3039:U:H3'	2:B:3040:C:H5"	1.98	0.44
3:C:220:PRO:HD2	3:C:223:ARG:HD3	1.99	0.44
3:C:51:ARG:HB2	37:C:8609:HOH:O	2.16	0.44
7:G:118:ILE:HG23	7:G:144:THR:HG21	1.99	0.44
9:I:63:ARG:HB2	9:I:66:LEU:HG	1.99	0.44
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.98	0.44
1:A:2274:A:H4'	14:N:77:PHE:HE1	1.82	0.44
15:O:48:VAL:HG13	15:O:55:ASP:HB3	1.95	0.44
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.48	0.44
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.52	0.44
26:Z:144:ARG:CG	26:Z:144:ARG:HH11	2.29	0.44
30:4:70:ARG:HG2	30:4:70:ARG:HH11	1.81	0.44
1:A:1157:C:C2	1:A:1158:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:G:H2'	1:A:1927:A:C8	2.53	0.44
1:A:201:G:N2	1:A:202:U:C2	2.86	0.44
1:A:2243:C:HO2'	1:A:2244:A:H8	1.66	0.44
1:A:2791:U:H4'	1:A:2792:A:OP1	2.17	0.44
1:A:492:C:O2'	1:A:493:U:H5'	2.18	0.44
1:A:853:C:H2'	1:A:854:G:O4'	2.17	0.44
2:B:3027:C:OP1	15:O:39:SER:OG	2.33	0.44
2:B:3031:C:H2'	2:B:3032:G:O4'	2.17	0.44
1:A:244:C:OP2	8:H:38:LYS:HE3	2.18	0.44
11:K:19:MET:HE1	11:K:79:PHE:HA	1.99	0.44
13:M:143:THR:HG21	37:M:8412:HOH:O	2.16	0.44
13:M:72:ASN:O	13:M:76:LEU:HG	2.18	0.44
14:N:74:ARG:HD3	14:N:91:ILE:HD12	2.00	0.44
15:O:139:TRP:CH2	15:O:176:ARG:NH1	2.85	0.44
1:A:1747:A:O3'	1:A:2584:G:H5'	2.17	0.44
1:A:266:G:C2	1:A:267:G:C8	3.06	0.44
1:A:2781:U:O2'	1:A:2782:G:H5'	2.18	0.44
1:A:61:G:C2	1:A:62:C:C2	3.05	0.44
2:B:3104:A:O2'	2:B:3105:A:H5'	2.18	0.44
4:D:248:ARG:O	4:D:251:VAL:CG1	2.66	0.44
1:A:2719:A:N1	4:D:70:PRO:HG3	2.32	0.44
5:E:246:ARG:CZ	37:E:8419:HOH:O	2.65	0.44
37:A:4797:HOH:O	12:L:37:TYR:CE1	2.70	0.44
1:A:1299:G:N7	13:M:6:ARG:NH1	2.65	0.44
15:O:154:LEU:O	15:O:155:GLU:CB	2.63	0.44
5:E:27:ARG:HD2	16:P:5:PRO:HD2	2.00	0.44
19:S:39:THR:HG22	19:S:41:GLY:H	1.82	0.44
21:U:49:GLU:OE2	21:U:97:ARG:NH1	2.43	0.44
26:Z:133:HIS:CD2	37:Z:8169:HOH:O	2.57	0.44
27:1:30:GLU:O	27:1:33:HIS:HB3	2.17	0.44
1:A:1072:G:OP2	26:Z:154:ARG:NH2	2.51	0.44
1:A:1730:G:H4'	1:A:1731:C:O5'	2.17	0.44
1:A:1854:C:O2'	1:A:1858:A:N3	2.45	0.44
1:A:2505:G:C2'	1:A:2506:A:H5'	2.47	0.44
1:A:2723:G:H1'	37:A:4410:HOH:O	2.16	0.44
1:A:686:A:O2'	1:A:747:G:H4'	2.18	0.44
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.48	0.44
3:C:48:ASP:HB3	37:C:8609:HOH:O	2.17	0.44
37:A:9281:HOH:O	4:D:254:GLN:HG3	2.16	0.44
4:D:27:ASN:HD22	4:D:27:ASN:H	1.66	0.44
7:G:11:VAL:HG11	7:G:22:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:99:THR:O	8:H:100:ASP:HB2	2.18	0.44
10:J:141:ASN:CA	37:J:8369:HOH:O	2.56	0.44
37:A:5139:HOH:O	12:L:41:LYS:HE3	2.17	0.44
13:M:41:HIS:O	13:M:42:ASN:HB2	2.18	0.44
22:V:36:CYS:O	22:V:37:GLU:C	2.56	0.44
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.44
28:2:45:ARG:NH1	37:2:8435:HOH:O	2.50	0.44
1:A:1380:U:O4	1:A:2043:U:H4'	2.17	0.44
1:A:2727:A:N6	1:A:2756:U:C6	2.86	0.44
2:B:3020:G:H3'	37:B:8435:HOH:O	2.17	0.44
2:B:3054:A:O2'	2:B:3055:U:H5'	2.18	0.44
14:N:46:LEU:HB2	37:N:8606:HOH:O	2.17	0.44
15:O:108:SER:HA	15:O:109:PRO:HD3	1.84	0.44
15:O:143:ARG:NH1	15:O:173:ASP:OD1	2.51	0.44
15:O:161:GLY:O	15:O:162:ASP:C	2.55	0.44
1:A:2659:U:C4'	19:S:76:ASP:HB3	2.48	0.44
24:X:40:ALA:O	24:X:44:MET:HG3	2.18	0.44
37:A:5709:HOH:O	29:3:20:ARG:HB3	2.17	0.44
1:A:10:U:HO2'	1:A:11:A:P	2.41	0.44
1:A:134:U:C2	1:A:145:A:C2	3.06	0.44
1:A:2673:U:C2	1:A:2817:G:C2	3.06	0.44
1:A:382:U:C5	1:A:406:G:N2	2.86	0.44
1:A:941:G:C5	1:A:942:U:C4	3.06	0.44
4:D:129:ARG:O	4:D:133:GLU:HG3	2.18	0.44
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.18	0.44
1:A:2274:A:N3	14:N:86:MET:CE	2.81	0.44
17:Q:134:VAL:O	17:Q:137:LEU:HB3	2.17	0.44
1:A:1021:G:O2'	1:A:1022:A:H5'	2.18	0.44
1:A:1085:C:H2'	1:A:1086:A:O4'	2.18	0.44
1:A:2467:A:H2'	37:A:5033:HOH:O	2.18	0.44
1:A:2563:U:H2'	1:A:2565:C:O5'	2.17	0.44
1:A:2831:C:H2'	1:A:2832:C:H5'	2.00	0.44
1:A:316:A:H1'	1:A:336:G:N3	2.32	0.44
1:A:241:A:N1	1:A:378:A:H4'	2.33	0.44
1:A:511:A:H1'	37:A:7229:HOH:O	2.18	0.44
1:A:945:U:H2'	1:A:946:C:C6	2.53	0.44
3:C:57:ALA:HA	3:C:67:LEU:HD23	2.00	0.44
6:F:99:ASP:HB2	6:F:103:ASN:CB	2.47	0.44
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.17	0.44
10:J:140:PRO:HA	10:J:142:VAL:HG12	1.99	0.44
11:K:19:MET:HE3	11:K:132:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:18:GLY:O	14:N:21:ALA:HB3	2.18	0.44
14:N:67:ILE:HD11	14:N:104:ARG:HD2	1.98	0.44
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.47	0.44
15:O:73:ALA:HB1	15:O:74:PRO:HD2	1.99	0.44
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.24	0.44
28:2:5:THR:HB	28:2:6:PRO:CD	2.48	0.43
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.17	0.43
1:A:1434:A:H2'	1:A:1436:C:C5	2.53	0.43
1:A:1656:A:H2'	1:A:1657:A:O4'	2.18	0.43
1:A:204:A:H2'	1:A:205:U:C5'	2.46	0.43
1:A:213:G:O2'	1:A:214:U:OP2	2.36	0.43
1:A:2251:G:H2'	1:A:2252:A:H8	1.83	0.43
1:A:2421:G:H3'	1:A:2422:U:C5'	2.48	0.43
1:A:2649:A:H8	1:A:2649:A:H5'	1.82	0.43
1:A:469:G:C6	1:A:473:A:N6	2.86	0.43
1:A:926:A:O2'	13:M:41:HIS:HD2	2.00	0.43
2:B:3041:C:C6	6:F:50:VAL:HG21	2.52	0.43
2:B:3056:A:C3'	2:B:3057:A:H5''	2.48	0.43
4:D:16:ARG:NH1	37:D:8618:HOH:O	2.51	0.43
11:K:6:PHE:O	11:K:8:ALA:N	2.51	0.43
1:A:159:G:H5''	14:N:74:ARG:HH22	1.82	0.43
17:Q:109:ARG:NH1	17:Q:119:TYR:CE2	2.86	0.43
24:X:126:ASP:HB3	24:X:135:GLY:O	2.18	0.43
25:Y:85:VAL:HG12	25:Y:86:GLU:H	1.83	0.43
1:A:1311:G:C2	1:A:1312:G:C8	3.06	0.43
1:A:1555:G:O2'	1:A:1556:G:H5'	2.18	0.43
1:A:1667:A:H2'	1:A:1668:U:C6	2.53	0.43
1:A:1902:G:H2'	1:A:1903:U:O4'	2.19	0.43
1:A:2289:G:H21	1:A:2291:A:H2	1.60	0.43
1:A:259:G:O2'	1:A:260:C:H5'	2.18	0.43
1:A:2697:A:H2'	1:A:2698:G:O4'	2.18	0.43
1:A:416:G:OP1	1:A:417:G:H5'	2.18	0.43
1:A:426:G:C2	1:A:427:C:C2	3.06	0.43
1:A:821:U:H2'	1:A:822:C:H6	1.82	0.43
4:D:279:THR:OG1	4:D:290:VAL:HB	2.18	0.43
4:D:316:ARG:N	4:D:317:PRO:HD3	2.34	0.43
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.88	0.43
7:G:80:TRP:O	7:G:134:SER:HA	2.17	0.43
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.18	0.43
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.53	0.43
13:M:17:SER:C	13:M:19:LYS:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:157:LEU:HA	35:N:8518:CL:CL	2.55	0.43
24:X:146:ILE:HG22	24:X:147:ASP:N	2.33	0.43
1:A:1056:U:H2'	1:A:1057:A:O4'	2.18	0.43
1:A:135:G:H1'	14:N:135:ASP:OD2	2.18	0.43
1:A:1420:C:C2	1:A:1445:G:N2	2.86	0.43
1:A:283:U:H5	1:A:284:C:H42	1.66	0.43
1:A:812:A:C6	1:A:813:C:C4	3.06	0.43
1:A:843:A:C2	1:A:846:A:C8	3.06	0.43
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.53	0.43
1:A:1352:A:N1	5:E:48:SER:HB3	2.33	0.43
7:G:9:GLU:HG3	7:G:10:ASP:N	2.33	0.43
7:G:7:ILE:HG22	7:G:45:ASP:O	2.19	0.43
9:I:20:VAL:O	9:I:24:VAL:HG23	2.18	0.43
10:J:112:ARG:O	10:J:113:ALA:C	2.56	0.43
21:U:25:ALA:O	21:U:39:ASN:CB	2.67	0.43
1:A:1313:A:H5''	26:Z:210:GLY:N	2.32	0.43
27:1:41:VAL:HG12	27:1:42:CYS:N	2.32	0.43
1:A:1047:U:H2'	1:A:1048:G:H8	1.84	0.43
1:A:1076:G:C2	1:A:1084:C:C2	3.06	0.43
1:A:1098:A:H2'	1:A:1099:G:O4'	2.18	0.43
1:A:2379:G:N7	1:A:2408:A:N1	2.65	0.43
1:A:2497:A:H2'	1:A:2498:C:C6	2.52	0.43
1:A:2776:A:H2'	1:A:2777:G:O4'	2.17	0.43
1:A:2840:A:OP1	4:D:211:THR:HG23	2.18	0.43
1:A:2909:G:H2'	1:A:2910:A:H8	1.83	0.43
1:A:470:U:O2'	28:2:16:HIS:CD2	2.69	0.43
1:A:920:C:H4'	1:A:921:G:N2	2.33	0.43
3:C:192:VAL:CG1	3:C:192:VAL:O	2.66	0.43
5:E:25:PRO:HD2	37:E:8424:HOH:O	2.17	0.43
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.86	0.43
10:J:165:GLY:C	10:J:166:ASN:HD22	2.22	0.43
23:W:5:VAL:CG1	23:W:9:ARG:NH1	2.81	0.43
1:A:1309:U:C2'	1:A:1310:U:H5'	2.49	0.43
1:A:1323:G:C2	1:A:1324:G:C8	3.07	0.43
1:A:1407:A:O2'	1:A:1408:U:H3'	2.19	0.43
1:A:1815:A:H3'	1:A:1816:C:C6	2.53	0.43
1:A:1878:G:O2'	1:A:1879:U:P	2.76	0.43
1:A:1562:C:H42	1:A:2738:G:H1	1.65	0.43
1:A:2868:C:H2'	1:A:2869:G:O4'	2.19	0.43
1:A:396:U:H4'	37:4:8531:HOH:O	2.18	0.43
1:A:68:U:O2'	1:A:69:A:H5''	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:U:H5	37:A:3763:HOH:O	2.01	0.43
1:A:814:G:H2'	1:A:815:U:O4'	2.18	0.43
3:C:150:PRO:HG3	37:C:8598:HOH:O	2.18	0.43
3:C:51:ARG:CZ	37:C:8609:HOH:O	2.66	0.43
4:D:139:ASP:HB2	4:D:165:ARG:HE	1.84	0.43
4:D:63:GLU:HG3	4:D:63:GLU:O	2.18	0.43
8:H:26:THR:HB	8:H:102:GLY:C	2.39	0.43
14:N:137:ASP:HA	14:N:142:LYS:HE3	2.01	0.43
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.43	0.43
23:W:42:ASN:O	23:W:44:GLY:N	2.51	0.43
24:X:73:LEU:HA	24:X:73:LEU:HD12	1.81	0.43
1:A:1603:A:H5''	1:A:1604:G:H3'	1.99	0.43
1:A:2833:C:O2	1:A:2906:A:O2'	2.36	0.43
1:A:604:G:H2'	37:A:7331:HOH:O	2.18	0.43
1:A:783:C:OP1	3:C:180:LYS:HE3	2.19	0.43
1:A:876:A:H2'	1:A:876:A:N3	2.34	0.43
4:D:11:LEU:HA	37:D:8618:HOH:O	2.19	0.43
7:G:54:ASP:OD1	7:G:54:ASP:N	2.52	0.43
7:G:69:ILE:HA	7:G:72:MET:HE2	2.00	0.43
8:H:22:VAL:CG2	8:H:104:ALA:HB2	2.49	0.43
8:H:91:VAL:CG1	8:H:92:GLY:H	2.28	0.43
1:A:2502:C:C4'	10:J:151:MET:SD	3.06	0.43
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.37	0.43
14:N:115:LEU:HD13	14:N:116:ASN:HB2	2.01	0.43
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.49	0.43
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.85	0.43
21:U:50:VAL:HG12	21:U:56:ALA:HA	2.00	0.43
1:A:1164:U:C1'	1:A:1165:G:OP1	2.66	0.43
1:A:1301:C:O4'	1:A:1330:A:C2	2.71	0.43
1:A:1314:U:H5''	1:A:1316:G:O4'	2.19	0.43
1:A:1327:G:C6	1:A:1331:A:C6	3.07	0.43
1:A:1375:A:C2'	1:A:1376:G:H5'	2.49	0.43
1:A:2255:A:C6	1:A:2256:G:C5	3.06	0.43
1:A:2506:A:H1'	37:A:3327:HOH:O	2.19	0.43
1:A:661:G:C4	1:A:686:A:C2	3.07	0.43
3:C:214:SER:HA	3:C:227:ASP:O	2.18	0.43
4:D:156:LYS:HE3	37:D:8635:HOH:O	2.18	0.43
7:G:11:VAL:HG11	7:G:22:VAL:CG1	2.49	0.43
7:G:23:GLU:HG2	7:G:28:SER:HB2	2.01	0.43
9:I:66:LEU:O	9:I:69:ARG:HB3	2.18	0.43
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:22:VAL:O	11:K:26:VAL:HG23	2.19	0.43
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.99	0.43
11:K:38:VAL:HB	11:K:103:VAL:HG13	2.00	0.43
1:A:392:U:C5'	14:N:193:LYS:HB3	2.49	0.43
14:N:39:ARG:NH2	37:N:8622:HOH:O	2.52	0.43
16:P:56:GLU:HB2	37:P:6111:HOH:O	2.17	0.43
18:R:93:ARG:HG3	18:R:93:ARG:NH1	2.34	0.43
28:2:28:HIS:O	28:2:32:LYS:N	2.43	0.43
1:A:13:G:H2'	1:A:14:C:C6	2.54	0.43
1:A:1659:A:H2'	1:A:1660:G:O4'	2.19	0.43
1:A:1783:A:C2'	1:A:1784:U:H5'	2.49	0.43
1:A:1787:C:H4'	1:A:2883:A:O4'	2.18	0.43
1:A:2269:C:C2'	1:A:2270:G:H5'	2.48	0.43
1:A:137:U:OP1	1:A:259:G:O2'	2.36	0.43
1:A:1269:G:H5''	35:A:8520:CL:CL	2.55	0.43
1:A:958:G:O2'	1:A:959:C:H5'	2.19	0.43
3:C:135:VAL:N	37:C:8598:HOH:O	2.50	0.43
4:D:168:GLY:H	4:D:174:ARG:HD3	1.82	0.43
4:D:41:PHE:HB3	4:D:190:MET:CE	2.48	0.43
6:F:11:HIS:O	6:F:12:GLU:CB	2.66	0.43
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.49	0.43
6:F:35:ALA:O	6:F:37:ALA:N	2.52	0.43
10:J:31:PHE:HD2	10:J:85:ILE:O	2.01	0.43
15:O:100:ALA:O	15:O:129:ILE:HG12	2.17	0.43
37:A:7470:HOH:O	15:O:1:ALA:CB	2.67	0.43
18:R:33:PHE:N	18:R:71:TYR:OH	2.46	0.43
23:W:19:GLU:HA	23:W:19:GLU:OE1	2.19	0.43
25:Y:78:GLU:CG	25:Y:79:GLU:N	2.80	0.43
26:Z:109:LEU:HA	37:Z:8159:HOH:O	2.18	0.43
1:A:892:G:H5''	28:2:54:ALA:HB2	2.01	0.43
2:B:3050:G:C6	2:B:3051:A:C6	3.06	0.43
1:A:1861:C:H4'	3:C:6:GLY:O	2.19	0.43
5:E:233:THR:HG22	5:E:234:VAL:H	1.82	0.43
6:F:77:ASP:HB3	6:F:78:GLU:H	1.56	0.43
7:G:84:MET:CE	7:G:148:ILE:CD1	2.97	0.43
8:H:101:ALA:HA	37:H:5413:HOH:O	2.19	0.43
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.48	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.79	0.43
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.19	0.43
17:Q:143:ALA:HB2	37:Q:5521:HOH:O	2.18	0.43
19:S:65:GLY:C	37:S:8517:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:29:ASP:OD2	20:T:31:ARG:NH1	2.51	0.43
24:X:64:THR:O	24:X:68:THR:HG22	2.18	0.43
29:3:19:SER:O	29:3:36:ASN:ND2	2.52	0.43
1:A:1450:C:O2'	1:A:1494:A:H5'	2.19	0.43
1:A:1828:G:H2'	1:A:1829:A:H5'	2.00	0.43
1:A:2010:A:H2'	37:A:5537:HOH:O	2.19	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.01	0.43
1:A:829:A:C6	1:A:830:G:N7	2.87	0.43
2:B:3065:A:O2'	2:B:3066:G:P	2.76	0.43
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.33	0.43
3:C:22:ARG:NH1	37:C:8567:HOH:O	2.52	0.43
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.78	0.43
6:F:29:HIS:C	37:F:5858:HOH:O	2.57	0.43
6:F:49:PRO:CG	37:F:5828:HOH:O	2.57	0.43
6:F:49:PRO:HA	6:F:73:VAL:HG22	2.01	0.43
8:H:104:ALA:HA	37:H:6617:HOH:O	2.19	0.43
9:I:18:GLU:O	9:I:21:ASP:HB2	2.18	0.43
9:I:71:LEU:C	9:I:73:ASP:H	2.21	0.43
11:K:71:TYR:CG	11:K:72:PRO:HD2	2.54	0.43
21:U:71:VAL:CG1	21:U:90:PRO:HB3	2.24	0.43
24:X:19:ASP:O	24:X:23:MET:HG3	2.18	0.43
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	2.00	0.43
1:A:1269:G:H2'	1:A:1270:U:C6	2.54	0.42
1:A:2269:C:H2'	1:A:2270:G:H5'	1.99	0.42
1:A:2281:C:C2'	1:A:2282:U:H5'	2.48	0.42
1:A:2820:A:H2'	1:A:2821:C:O4'	2.19	0.42
1:A:539:G:H2'	1:A:540:A:C8	2.54	0.42
1:A:820:G:H5'	1:A:821:U:H5'	2.00	0.42
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.49	0.42
4:D:248:ARG:NH2	37:D:8526:HOH:O	2.51	0.42
6:F:60:GLU:O	6:F:62:ASP:N	2.52	0.42
14:N:38:VAL:O	14:N:63:VAL:CG1	2.62	0.42
15:O:22:GLN:HG2	15:O:26:LEU:HD22	2.00	0.42
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.49	0.42
1:A:1114:A:O2'	1:A:1115:U:H5'	2.19	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:1335:C:H2'	1:A:1336:U:H6	1.83	0.42
1:A:1375:A:H2'	1:A:1376:G:H5'	2.01	0.42
1:A:1657:A:H2'	1:A:1658:A:C8	2.54	0.42
1:A:1947:G:H2'	1:A:1948:G:C8	2.53	0.42
1:A:2760:C:H5''	37:A:4902:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:C:H2'	1:A:291:C:O4'	2.19	0.42
1:A:420:U:H2'	1:A:421:C:C6	2.54	0.42
1:A:42:C:H1'	37:A:4252:HOH:O	2.18	0.42
2:B:3051:A:H5'	15:O:160:SER:HB3	2.01	0.42
2:B:3060:C:O2'	2:B:3061:C:H5'	2.19	0.42
6:F:173:GLU:O	6:F:174:VAL:C	2.58	0.42
13:M:130:ARG:HA	37:M:8431:HOH:O	2.19	0.42
15:O:80:SER:CB	37:O:8536:HOH:O	2.62	0.42
24:X:108:ARG:O	24:X:111:GLY:N	2.49	0.42
24:X:38:THR:HG22	37:X:3580:HOH:O	2.18	0.42
24:X:48:VAL:O	24:X:48:VAL:HG12	2.18	0.42
25:Y:70:ILE:HG23	25:Y:70:ILE:O	2.19	0.42
1:A:1014:A:H5''	2:B:3101:G:O2'	2.19	0.42
1:A:1044:C:H5	37:A:6177:HOH:O	2.01	0.42
1:A:1127:C:C5	1:A:1128:U:C4	3.07	0.42
1:A:111:C:H2'	1:A:112:G:O4'	2.19	0.42
1:A:2092:G:H2'	1:A:2613:G:OP1	2.20	0.42
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.40	0.42
3:C:211:LYS:HB2	37:C:8624:HOH:O	2.17	0.42
3:C:211:LYS:CB	3:C:212:PRO:HD2	2.35	0.42
5:E:76:ARG:HD2	37:E:8429:HOH:O	2.19	0.42
6:F:48:MET:HA	6:F:49:PRO:HD3	1.84	0.42
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.34	0.42
11:K:34:GLU:HA	11:K:34:GLU:OE1	2.19	0.42
12:L:22:ASP:OD1	12:L:22:ASP:C	2.57	0.42
13:M:148:GLU:HG2	37:M:8425:HOH:O	2.20	0.42
8:H:56:PRO:CG	14:N:44:THR:HA	2.49	0.42
14:N:80:GLY:O	14:N:81:ARG:CD	2.61	0.42
21:U:55:PHE:CG	21:U:77:VAL:HG13	2.54	0.42
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.80	0.42
1:A:1014:A:H2'	1:A:1015:C:H5'	2.01	0.42
1:A:1029:U:O2'	1:A:1273:C:OP1	2.34	0.42
1:A:128:A:O2'	1:A:129:A:H5'	2.19	0.42
1:A:1380:U:H5'	37:A:8803:HOH:O	2.19	0.42
1:A:1869:A:H2'	1:A:1870:C:O4'	2.20	0.42
1:A:1940:C:H5''	3:C:234:GLY:HA3	2.02	0.42
4:D:312:ARG:HG2	4:D:313:PRO:N	2.34	0.42
6:F:52:THR:HB	6:F:70:GLY:O	2.19	0.42
20:T:8:PRO:HD2	23:W:32:ALA:HA	2.02	0.42
21:U:96:VAL:CG1	21:U:97:ARG:N	2.83	0.42
22:V:44:ARG:HB2	37:V:3805:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:11:THR:HG21	27:1:23:ARG:HB2	2.01	0.42
1:A:2436:U:H5'	30:4:68:LYS:HE2	1.99	0.42
1:A:1559:A:C1'	37:A:5443:HOH:O	2.66	0.42
1:A:1920:C:O2'	1:A:1921:A:H5'	2.19	0.42
1:A:2079:G:H2'	1:A:2080:G:O4'	2.20	0.42
1:A:1857:A:N6	1:A:2247:C:H1'	2.34	0.42
1:A:2756:U:N3	1:A:2896:A:H2	2.14	0.42
1:A:775:G:H3'	37:A:4010:HOH:O	2.20	0.42
1:A:844:A:C6	1:A:882:A:C6	3.08	0.42
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.49	0.42
4:D:279:THR:CG2	4:D:280:VAL:N	2.82	0.42
11:K:39:VAL:HG13	11:K:106:GLY:O	2.19	0.42
13:M:42:ASN:HB2	37:M:8421:HOH:O	2.18	0.42
13:M:91:VAL:O	13:M:91:VAL:HG13	2.19	0.42
14:N:133:LEU:O	14:N:134:ILE:HD13	2.19	0.42
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.20	0.42
15:O:113:SER:CB	37:O:8559:HOH:O	2.55	0.42
16:P:60:VAL:C	16:P:62:GLY:H	2.23	0.42
23:W:5:VAL:HG11	23:W:9:ARG:NH1	2.34	0.42
1:A:1052:G:C5	1:A:1063:G:C6	3.08	0.42
1:A:1183:C:N4	37:A:3977:HOH:O	2.46	0.42
1:A:1389:G:N2	1:A:1391:G:H3'	2.35	0.42
1:A:1785:G:OP1	17:Q:76:GLY:HA3	2.20	0.42
1:A:1820:G:C6	1:A:2030:A:C2	3.08	0.42
1:A:2040:C:H2'	1:A:2041:G:O4'	2.20	0.42
1:A:2408:A:H2	37:4:8516:HOH:O	2.01	0.42
1:A:500:G:H21	19:S:98:ASN:HD21	1.66	0.42
1:A:682:A:H3'	1:A:683:G:C8	2.55	0.42
3:C:47:HIS:O	3:C:49:PRO:HD3	2.19	0.42
10:J:31:PHE:HE2	10:J:87:LYS:O	2.03	0.42
10:J:15:THR:HG22	10:J:91:HIS:HA	2.01	0.42
11:K:63:ILE:HG22	11:K:64:GLY:N	2.33	0.42
15:O:93:GLN:HG2	37:O:8557:HOH:O	2.19	0.42
21:U:51:LEU:HD11	21:U:97:ARG:HB2	2.02	0.42
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.55	0.42
1:A:1206:U:H2'	1:A:1207:A:O4'	2.19	0.42
1:A:1555:G:H4'	1:A:1630:A:H2	1.85	0.42
1:A:2892:G:C6	1:A:2893:C:C4	3.08	0.42
1:A:553:G:O4'	1:A:1325:G:H5'	2.19	0.42
3:C:199:HIS:HD2	3:C:201:PHE:N	2.07	0.42
4:D:115:VAL:HA	4:D:116:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:LEU:HG	37:F:3862:HOH:O	2.19	0.42
14:N:61:ILE:N	14:N:61:ILE:HD12	2.34	0.42
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.19	0.42
37:A:9118:HOH:O	17:Q:81:LYS:HG2	2.20	0.42
19:S:50:VAL:HG22	19:S:55:GLN:O	2.20	0.42
1:A:1094:G:H21	24:X:119:HIS:CE1	2.38	0.42
26:Z:155:ARG:NH1	37:Z:8147:HOH:O	2.52	0.42
1:A:1165:G:O2'	1:A:1166:A:OP1	2.25	0.42
1:A:1189:A:N3	37:A:7254:HOH:O	2.52	0.42
1:A:1270:U:H2'	1:A:1271:A:C8	2.55	0.42
1:A:187:A:H3'	1:A:188:C:H6	1.83	0.42
1:A:2015:A:H2'	1:A:2016:U:O4'	2.19	0.42
1:A:2575:C:H2'	1:A:2576:A:O4'	2.19	0.42
1:A:2687:G:O2'	1:A:2688:U:H5'	2.19	0.42
1:A:2764:C:H2'	1:A:2765:C:C6	2.54	0.42
1:A:524:A:H5''	19:S:29:LYS:HE2	2.01	0.42
1:A:65:C:O2'	1:A:66:G:H5'	2.19	0.42
1:A:834:G:H4'	1:A:835:U:OP2	2.19	0.42
1:A:772:G:N2	1:A:890:C:O2	2.53	0.42
2:B:3078:G:O2'	2:B:3079:U:OP2	2.37	0.42
3:C:3:ARG:HB2	3:C:8:ARG:NE	2.35	0.42
4:D:127:GLN:HG3	37:D:8646:HOH:O	2.19	0.42
5:E:200:PRO:HB3	5:E:212:VAL:CG2	2.50	0.42
5:E:4:THR:HB	5:E:135:GLU:OE1	2.19	0.42
5:E:95:GLU:H	5:E:95:GLU:CD	2.14	0.42
6:F:104:PHE:CE2	6:F:166:ILE:CD1	3.02	0.42
6:F:60:GLU:C	6:F:62:ASP:N	2.73	0.42
7:G:15:GLN:HG2	7:G:19:ASP:O	2.20	0.42
7:G:7:ILE:HA	7:G:8:PRO:HD3	1.88	0.42
13:M:130:ARG:O	13:M:131:GLU:C	2.57	0.42
14:N:72:SER:HB2	14:N:93:ARG:HG2	2.01	0.42
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.42
16:P:59:VAL:CG2	16:P:111:VAL:HG23	2.49	0.42
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.19	0.42
18:R:41:LEU:HD12	18:R:41:LEU:N	2.34	0.42
1:A:1331:A:OP2	26:Z:142:SER:OG	2.37	0.42
27:1:39:CYS:HA	27:1:40:PRO:HD3	1.95	0.42
1:A:578:C:O2	1:A:1112:G:H4'	2.20	0.42
1:A:622:G:H5'	1:A:1357:A:N6	2.34	0.42
1:A:1523:G:C6	1:A:1524:U:O4	2.73	0.42
1:A:1979:G:O2'	1:A:1980:U:OP1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:C:H6	1:A:287:C:O5'	2.02	0.42
2:B:3114:G:O6	15:O:11:ARG:HD3	2.20	0.42
4:D:277:GLU:N	4:D:278:PRO:HD2	2.35	0.42
5:E:218:VAL:CG1	37:E:8419:HOH:O	2.67	0.42
5:E:7:ASP:OD1	5:E:11:ASN:O	2.37	0.42
8:H:33:THR:HG21	8:H:59:ILE:O	2.20	0.42
9:I:64:ASN:N	9:I:64:ASN:ND2	2.68	0.42
15:O:110:THR:HB	15:O:113:SER:OG	2.19	0.42
15:O:43:VAL:HG13	15:O:118:ILE:HD11	2.02	0.42
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.85	0.42
18:R:30:VAL:HG12	18:R:30:VAL:O	2.20	0.42
21:U:27:LEU:HD23	21:U:98:VAL:HB	2.02	0.42
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.55	0.42
29:3:40:ARG:HG3	29:3:45:ASN:CB	2.50	0.42
29:3:41:HIS:O	29:3:45:ASN:HB2	2.20	0.42
1:A:1391:G:C6	1:A:1435:U:C5	3.08	0.42
1:A:1772:C:H5'	1:A:1773:G:C5	2.55	0.42
1:A:2012:U:H2'	1:A:2013:G:OP1	2.19	0.42
1:A:201:G:N1	1:A:202:U:C4	2.88	0.42
1:A:2247:C:C5'	37:A:6916:HOH:O	2.67	0.42
1:A:2591:C:H2'	1:A:2592:G:O4'	2.20	0.42
1:A:2791:U:C1'	1:A:2792:A:H5''	2.50	0.42
1:A:332:G:O2'	1:A:333:G:H5'	2.20	0.42
1:A:441:A:H1'	1:A:442:A:N7	2.35	0.42
1:A:731:U:H2'	1:A:732:C:C6	2.55	0.42
1:A:858:U:H2'	1:A:859:C:C6	2.54	0.42
2:B:3057:A:H5'	2:B:3057:A:N3	2.35	0.42
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.55	0.42
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.20	0.42
9:I:63:ARG:O	9:I:67:LEU:HG	2.20	0.42
11:K:42:GLU:O	11:K:131:THR:HG23	2.19	0.42
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.19	0.42
1:A:1191:A:N1	1:A:1206:U:O4	2.53	0.41
1:A:1496:G:H5'	1:A:1572:A:H1'	2.02	0.41
1:A:154:C:C2	1:A:155:C:C6	3.08	0.41
1:A:1862:C:N4	1:A:1868:G:C6	2.88	0.41
1:A:2362:A:H2'	1:A:2363:G:C8	2.55	0.41
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.48	0.41
1:A:2570:G:H5''	37:A:4485:HOH:O	2.20	0.41
1:A:2912:C:H2'	1:A:2913:A:O4'	2.20	0.41
4:D:130:ASP:HB2	37:D:8599:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:ASP:HA	37:D:8575:HOH:O	2.19	0.41
1:A:902:G:N7	13:M:18:HIS:CD2	2.85	0.41
14:N:95:LYS:HG2	14:N:99:ARG:HB3	2.02	0.41
16:P:96:VAL:CG1	16:P:97:SER:N	2.82	0.41
1:A:1164:U:O5'	1:A:1164:U:H6	2.03	0.41
1:A:1182:C:H1'	1:A:1192:A:C8	2.52	0.41
1:A:1292:G:HO2'	1:A:1293:U:H6	1.65	0.41
1:A:1829:A:H2'	1:A:1830:C:H5'	2.02	0.41
1:A:2120:U:H2'	1:A:2121:G:O4'	2.19	0.41
1:A:2438:G:H5'	37:4:8552:HOH:O	2.21	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.19	0.41
1:A:2498:C:O2'	1:A:2499:U:H5'	2.20	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
1:A:2896:A:OP1	37:A:3447:HOH:O	2.22	0.41
1:A:464:G:N2	1:A:475:G:H2'	2.34	0.41
1:A:79:G:N2	1:A:80:A:N6	2.68	0.41
1:A:834:G:H3'	1:A:835:U:H4'	2.03	0.41
3:C:105:VAL:HG13	3:C:155:THR:O	2.20	0.41
4:D:80:ARG:HD3	37:D:8608:HOH:O	2.20	0.41
5:E:27:ARG:CG	5:E:29:ASP:OD1	2.66	0.41
6:F:174:VAL:CG1	37:F:6555:HOH:O	2.64	0.41
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.50	0.41
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.50	0.41
15:O:154:LEU:CG	15:O:155:GLU:N	2.81	0.41
15:O:42:HIS:CG	15:O:62:HIS:HE1	2.38	0.41
26:Z:106:THR:HG22	26:Z:107:PRO:O	2.20	0.41
29:3:19:SER:HB3	37:3:4479:HOH:O	2.19	0.41
1:A:160:A:C4	1:A:177:A:C2	3.09	0.41
1:A:1707:G:N2	1:A:1709:G:H3'	2.36	0.41
1:A:1565:C:O4'	1:A:2738:G:H1'	2.21	0.41
1:A:226:A:H1'	1:A:393:G:C5	2.55	0.41
1:A:398:U:H2'	1:A:399:C:C6	2.55	0.41
1:A:415:A:O2'	1:A:416:G:H5'	2.20	0.41
4:D:313:PRO:O	4:D:314:ALA:C	2.59	0.41
4:D:54:VAL:O	4:D:55:ASN:C	2.58	0.41
6:F:170:TYR:N	6:F:170:TYR:CD1	2.89	0.41
6:F:59:GLY:C	6:F:61:PHE:H	2.20	0.41
11:K:46:ILE:HA	37:K:1123:HOH:O	2.19	0.41
14:N:122:GLU:HB2	14:N:126:HIS:O	2.20	0.41
15:O:175:LEU:CD1	37:O:8539:HOH:O	2.68	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:13:VAL:HG11	17:Q:40:VAL:HG11	2.02	0.41
1:A:588:G:O6	24:X:154:ARG:NH1	2.53	0.41
1:A:1603:A:H5'	1:A:1605:G:C4'	2.49	0.41
1:A:1758:U:H2'	1:A:1759:A:O4'	2.21	0.41
1:A:1477:C:C5'	1:A:1868:G:H5''	2.50	0.41
1:A:2506:A:H1'	37:A:5633:HOH:O	2.20	0.41
1:A:2838:A:H2'	1:A:2839:C:O4'	2.20	0.41
2:B:3053:G:O2'	2:B:3054:A:H5'	2.20	0.41
6:F:23:VAL:HG23	6:F:41:LEU:HD22	2.01	0.41
6:F:81:GLU:O	6:F:83:PHE:N	2.54	0.41
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.21	0.41
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.93	0.41
10:J:83:PHE:CE1	10:J:146:TRP:NE1	2.88	0.41
7:G:34:TRP:O	11:K:127:ILE:HD11	2.19	0.41
12:L:13:GLU:O	12:L:14:LYS:C	2.59	0.41
37:A:4923:HOH:O	21:U:3:GLN:HG2	2.19	0.41
37:A:5825:HOH:O	22:V:56:ARG:HD3	2.19	0.41
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.50	0.41
30:4:30:GLN:HB3	30:4:30:GLN:HE21	1.69	0.41
1:A:1614:G:H2'	37:A:4202:HOH:O	2.21	0.41
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.48	0.41
1:A:1843:A:O5'	1:A:1843:A:C8	2.73	0.41
1:A:2252:A:C5	1:A:2253:G:H1'	2.55	0.41
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.04	0.41
5:E:126:ASP:C	5:E:128:GLY:N	2.72	0.41
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.51	0.41
7:G:125:GLU:O	7:G:132:THR:HG22	2.20	0.41
9:I:23:ILE:O	9:I:27:ILE:HG13	2.20	0.41
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.35	0.41
16:P:97:SER:HB3	16:P:100:GLN:HE21	1.85	0.41
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.56	0.41
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.99	0.41
1:A:1327:G:N1	1:A:1331:A:C6	2.88	0.41
1:A:1683:G:H1'	1:A:1723:G:HO2'	1.86	0.41
1:A:1690:C:C5	1:A:1692:C:C4	3.09	0.41
1:A:2321:A:C4	1:A:2323:G:N7	2.89	0.41
1:A:419:A:C2	1:A:2449:G:C2	3.08	0.41
1:A:249:G:O2'	1:A:266:G:H5'	2.20	0.41
1:A:820:G:C6	3:C:171:LYS:HB2	2.56	0.41
4:D:101:TRP:HB2	4:D:119:HIS:CD2	2.56	0.41
4:D:177:HIS:NE2	4:D:181:ILE:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:5:ILE:HD13	37:E:8426:HOH:O	2.20	0.41
7:G:66:GLN:O	7:G:70:GLU:HG3	2.21	0.41
8:H:20:LEU:O	8:H:23:ALA:HB3	2.20	0.41
13:M:125:PHE:CE1	13:M:140:VAL:HG13	2.56	0.41
13:M:146:GLY:C	13:M:148:GLU:H	2.24	0.41
17:Q:103:THR:O	17:Q:106:ARG:HB3	2.21	0.41
25:Y:30:MET:HE3	25:Y:59:TRP:HE1	1.85	0.41
1:A:1051:C:H2'	1:A:1052:G:O4'	2.21	0.41
1:A:1268:C:H2'	1:A:1269:G:H8	1.86	0.41
1:A:1409:G:H5'	37:A:3305:HOH:O	2.21	0.41
1:A:1626:A:H2'	1:A:1627:G:H5'	2.02	0.41
1:A:1661:A:O2'	1:A:1662:C:H5'	2.21	0.41
1:A:1706:G:C5	1:A:1707:G:C6	3.09	0.41
1:A:1791:U:H2'	1:A:1792:C:C6	2.56	0.41
1:A:1943:C:O4'	3:C:212:PRO:HA	2.20	0.41
1:A:2779:G:H21	7:G:143:GLN:HE22	1.64	0.41
1:A:2890:A:H1'	22:V:56:ARG:HH21	1.82	0.41
1:A:329:A:H5'	1:A:347:A:H1'	2.03	0.41
1:A:876:A:N3	1:A:876:A:C2'	2.83	0.41
10:J:111:MET:O	10:J:114:PRO:HD3	2.21	0.41
10:J:149:ALA:C	10:J:151:MET:H	2.24	0.41
10:J:84:ARG:NH2	10:J:135:TRP:CH2	2.81	0.41
17:Q:38:GLU:CA	17:Q:41:ARG:NH1	2.82	0.41
1:A:97:G:C2	21:U:107:LYS:HD2	2.55	0.41
21:U:111:ARG:HB3	21:U:119:ALA:HB2	2.02	0.41
1:A:1246:A:C4	1:A:1248:A:C8	3.09	0.41
1:A:2281:C:H2'	1:A:2282:U:H5'	2.03	0.41
1:A:2304:G:C6	1:A:2305:A:C6	3.08	0.41
1:A:2323:G:H5'	37:A:6592:HOH:O	2.20	0.41
1:A:2515:C:H2'	1:A:2516:G:O4'	2.20	0.41
10:J:114:PRO:O	10:J:115:PHE:C	2.58	0.41
7:G:35:TYR:HA	11:K:127:ILE:HD12	2.03	0.41
14:N:187:LEU:HD23	14:N:187:LEU:HA	1.91	0.41
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.44	0.41
24:X:14:HIS:HB2	24:X:17:ILE:HG13	2.02	0.41
1:A:1456:C:H2'	1:A:1457:U:C6	2.56	0.41
1:A:1588:G:C6	1:A:1589:G:C6	3.09	0.41
1:A:303:C:O2'	1:A:304:G:H5'	2.21	0.41
1:A:383:A:C2	1:A:407:A:C4	3.08	0.41
1:A:445:U:H2'	1:A:446:G:H8	1.85	0.41
1:A:524:A:C5'	19:S:29:LYS:HE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:C:H5'	28:2:46:ARG:HH21	1.86	0.41
1:A:795:G:HO2'	1:A:796:A:P	2.44	0.41
1:A:963:C:H6	1:A:963:C:O5'	2.04	0.41
2:B:3057:A:O2'	6:F:152:PRO:HD2	2.21	0.41
3:C:211:LYS:HD3	37:C:8614:HOH:O	2.19	0.41
4:D:60:SER:C	4:D:62:ARG:H	2.23	0.41
5:E:27:ARG:HD2	5:E:29:ASP:OD1	2.21	0.41
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.21	0.41
8:H:60:VAL:O	8:H:60:VAL:CG1	2.69	0.41
8:H:91:VAL:CG1	8:H:92:GLY:N	2.80	0.41
11:K:42:GLU:HG2	11:K:43:ARG:HG3	2.02	0.41
15:O:159:TYR:CE2	15:O:163:PHE:HE2	2.37	0.41
23:W:38:GLY:C	23:W:40:PRO:HD2	2.41	0.41
1:A:1067:A:O2'	24:X:12:ASN:OD1	2.36	0.41
26:Z:112:GLU:O	26:Z:116:LEU:HG	2.21	0.41
26:Z:149:GLN:HB3	26:Z:149:GLN:HE21	1.73	0.41
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.86	0.41
1:A:1675:C:H5''	29:3:5:LYS:HD2	2.03	0.41
1:A:1218:U:H2'	1:A:1219:U:H6	1.86	0.41
1:A:1695:G:C6	1:A:1696:U:C4	3.09	0.41
1:A:1947:G:N2	1:A:1966:U:O2	2.53	0.41
1:A:2497:A:H2'	1:A:2498:C:H6	1.86	0.41
1:A:2727:A:C6	1:A:2756:U:C4	3.08	0.41
1:A:875:A:C2	3:C:194:MET:SD	3.14	0.41
1:A:87:C:H2'	29:3:28:LYS:O	2.21	0.41
4:D:156:LYS:NZ	4:D:160:ASP:OD2	2.49	0.41
6:F:15:GLU:O	6:F:16:PRO:O	2.39	0.41
15:O:115:VAL:HG23	37:O:8559:HOH:O	2.19	0.41
15:O:175:LEU:HD12	15:O:175:LEU:HA	1.89	0.41
18:R:16:ASN:HA	18:R:16:ASN:HD22	1.55	0.41
37:A:6976:HOH:O	21:U:2:LYS:HE2	2.19	0.41
26:Z:216:ARG:CD	37:Z:8157:HOH:O	2.64	0.41
27:1:31:ILE:O	27:1:35:LYS:HG3	2.20	0.41
1:A:1037:G:C2	1:A:1038:G:C8	3.09	0.41
1:A:1168:C:H5	37:A:7071:HOH:O	2.04	0.41
1:A:1211:G:O2'	1:A:1212:C:H5'	2.20	0.41
1:A:1261:A:O5'	1:A:1261:A:C8	2.74	0.41
1:A:1427:A:H61	1:A:1440:U:H1'	1.86	0.41
1:A:1804:A:H2'	1:A:1805:G:H8	1.86	0.41
1:A:2090:G:N2	1:A:2655:U:C2	2.89	0.41
1:A:2093:G:H5''	37:A:9062:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2637:A:H5'	37:A:3941:HOH:O	2.20	0.41
1:A:2727:A:N1	1:A:2756:U:C2	2.89	0.41
1:A:454:U:C2	37:A:8623:HOH:O	2.57	0.41
1:A:821:U:H2'	1:A:822:C:C6	2.56	0.41
1:A:951:A:H2'	1:A:952:G:H5'	2.03	0.41
2:B:3003:A:N6	2:B:3022:G:H1'	2.36	0.41
4:D:69:VAL:HA	4:D:70:PRO:HD3	1.90	0.41
10:J:136:VAL:HG23	37:J:8344:HOH:O	2.20	0.41
10:J:68:ALA:HB2	10:J:149:ALA:HB2	2.03	0.41
10:J:82:LYS:HZ2	10:J:82:LYS:HB2	1.86	0.41
1:A:1055:G:OP2	10:J:94:ARG:NH1	2.54	0.41
13:M:73:VAL:HG11	13:M:118:LEU:HD21	2.03	0.41
26:Z:130:ARG:HB2	26:Z:142:SER:O	2.20	0.41
1:A:1024:G:C5	1:A:1025:C:C4	3.09	0.40
1:A:12:U:H2'	1:A:13:G:H5'	2.02	0.40
1:A:154:C:P	14:N:188:ARG:HH12	2.44	0.40
1:A:1634:G:H2'	1:A:1635:U:H6	1.86	0.40
1:A:1681:G:H4'	1:A:1682:A:N3	2.36	0.40
1:A:2455:A:H2'	1:A:2456:A:O4'	2.21	0.40
1:A:685:C:O2	1:A:748:C:H4'	2.20	0.40
1:A:70:A:H4'	1:A:71:G:O5'	2.21	0.40
1:A:778:C:C4	1:A:779:U:C4	3.09	0.40
2:B:3050:G:C6	2:B:3051:A:N6	2.89	0.40
3:C:107:ASN:OD1	3:C:116:GLY:HA3	2.21	0.40
3:C:140:LEU:HB3	3:C:141:PRO:HD2	2.03	0.40
4:D:51:VAL:HG21	4:D:327:VAL:HG13	2.03	0.40
4:D:92:TYR:CD1	4:D:92:TYR:N	2.89	0.40
5:E:127:ARG:CZ	5:E:225:PRO:HG2	2.49	0.40
5:E:39:GLN:O	5:E:43:LYS:HD3	2.21	0.40
2:B:3057:A:C8	6:F:141:VAL:HG21	2.56	0.40
1:A:262:A:OP2	8:H:91:VAL:HG11	2.22	0.40
12:L:99:ASP:OD1	12:L:99:ASP:C	2.58	0.40
13:M:104:ASP:HB2	37:M:8448:HOH:O	2.21	0.40
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.51	0.40
14:N:62:VAL:C	14:N:63:VAL:HG23	2.41	0.40
15:O:72:GLU:H	15:O:171:HIS:CE1	2.39	0.40
16:P:22:GLY:CA	37:P:2823:HOH:O	2.69	0.40
19:S:149:GLU:HA	19:S:150:PRO:HD3	1.87	0.40
19:S:72:VAL:HG11	19:S:75:TRP:HB3	2.02	0.40
24:X:32:CYS:SG	24:X:33:THR:N	2.94	0.40
29:3:18:ASN:ND2	29:3:40:ARG:H	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:84:ARG:HD3	37:4:8551:HOH:O	2.21	0.40
1:A:1141:U:H2'	1:A:1142:C:H6	1.86	0.40
1:A:1309:U:O2'	1:A:1310:U:H5'	2.22	0.40
1:A:2001:G:C2'	1:A:2002:C:H5'	2.52	0.40
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.43	0.40
1:A:2090:G:H2'	1:A:2091:G:C8	2.56	0.40
1:A:2441:U:H4'	13:M:53:ARG:HD2	2.03	0.40
1:A:432:G:O2'	1:A:433:C:H5'	2.21	0.40
1:A:840:U:O2	1:A:2055:A:H1'	2.22	0.40
1:A:958:G:H2'	1:A:959:C:C6	2.55	0.40
2:B:3045:A:H2'	2:B:3046:C:H6	1.86	0.40
2:B:3091:C:H2'	2:B:3092:G:O4'	2.21	0.40
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.51	0.40
4:D:7:ARG:NH2	4:D:250:THR:O	2.54	0.40
6:F:35:ALA:C	6:F:37:ALA:N	2.74	0.40
7:G:139:GLU:CG	37:G:5919:HOH:O	2.69	0.40
1:A:2502:C:H4'	10:J:151:MET:HG2	2.03	0.40
1:A:1003:U:O2'	10:J:90:PHE:HE1	2.03	0.40
1:A:709:G:O2'	16:P:25:VAL:HG12	2.21	0.40
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.21	0.40
23:W:39:ALA:C	23:W:41:GLU:N	2.74	0.40
24:X:5:VAL:O	24:X:52:VAL:HG22	2.21	0.40
1:A:1058:A:H2'	1:A:1060:C:C5'	2.49	0.40
1:A:1068:C:OP2	37:A:3868:HOH:O	2.22	0.40
1:A:1495:C:C1'	1:A:1573:A:H1'	2.52	0.40
1:A:1593:C:O2'	1:A:1594:C:H5'	2.22	0.40
1:A:1613:C:H2'	1:A:1614:G:O4'	2.21	0.40
1:A:1827:G:H2'	1:A:1828:G:C8	2.56	0.40
1:A:2453:G:H5''	37:M:8415:HOH:O	2.20	0.40
1:A:2456:A:H2'	1:A:2457:U:H6	1.84	0.40
1:A:466:A:H2'	1:A:467:G:O4'	2.22	0.40
3:C:130:THR:HG22	3:C:131:HIS:O	2.20	0.40
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.70	0.40
11:K:52:GLN:CG	11:K:53:ILE:N	2.85	0.40
12:L:40:THR:O	12:L:41:LYS:C	2.60	0.40
12:L:87:ARG:NE	37:L:4854:HOH:O	2.53	0.40
16:P:4:ASN:HB3	16:P:7:LEU:HB3	2.04	0.40
18:R:22:GLY:O	18:R:23:THR:C	2.59	0.40
18:R:42:LYS:HD2	18:R:42:LYS:HA	1.93	0.40
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.52	0.40
1:A:1730:G:C5'	1:A:1731:C:C6	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:A:N6	37:A:9721:HOH:O	2.42	0.40
1:A:2121:G:O2'	1:A:2122:C:H5'	2.21	0.40
1:A:2550:U:O2'	1:A:2551:C:H5'	2.21	0.40
1:A:282:C:H2'	1:A:283:U:O4'	2.20	0.40
1:A:538:C:H5''	1:A:539:G:C8	2.56	0.40
4:D:108:GLU:HB3	4:D:111:ARG:HD2	2.03	0.40
6:F:104:PHE:CE2	6:F:166:ILE:HD13	2.57	0.40
7:G:83:GLY:O	7:G:169:THR:N	2.41	0.40
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.40	0.40
16:P:99:GLU:CG	37:P:6044:HOH:O	2.68	0.40
16:P:99:GLU:HG3	37:P:6044:HOH:O	2.21	0.40
21:U:44:ALA:HA	21:U:62:VAL:HG12	2.03	0.40
25:Y:71:ARG:HD2	37:Y:7542:HOH:O	2.22	0.40
27:1:17:ARG:O	27:1:18:TYR:HB2	2.21	0.40
1:A:1224:G:H2'	1:A:1225:C:C6	2.56	0.40
1:A:1416:G:H2'	1:A:1417:G:H5'	2.03	0.40
1:A:1594:C:C5	17:Q:120:ARG:CZ	3.04	0.40
1:A:1706:G:C6	1:A:1707:G:C6	3.09	0.40
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.40
1:A:2552:C:C6	1:A:2577:A:N7	2.89	0.40
1:A:2564:G:OP2	1:A:2565:C:H5''	2.22	0.40
1:A:2598:U:H2'	1:A:2600:A:OP2	2.22	0.40
1:A:2812:A:H1'	37:A:5365:HOH:O	2.21	0.40
1:A:2823:G:H4'	1:A:2827:A:O4'	2.21	0.40
1:A:2270:G:C4'	3:C:223:ARG:HH12	2.31	0.40
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.52	0.40
6:F:173:GLU:HG3	6:F:174:VAL:N	2.37	0.40
6:F:59:GLY:C	6:F:61:PHE:N	2.75	0.40
7:G:138:ILE:HG23	7:G:139:GLU:N	2.36	0.40
8:H:26:THR:HG21	8:H:103:ALA:CB	2.52	0.40
10:J:163:PRO:HG2	37:J:8339:HOH:O	2.21	0.40
11:K:130:VAL:CG1	11:K:131:THR:N	2.84	0.40
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.50	0.40
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.80	0.40
15:O:149:GLU:O	15:O:152:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	204 (87%)	26 (11%)	5 (2%)	7	37
4	D	335/337 (99%)	303 (90%)	23 (7%)	9 (3%)	5	30
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	34	69
6	F	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	0	3
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	42
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	4	25
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	7	37
12	L	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	10	44
13	M	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	11	46
14	N	192/194 (99%)	174 (91%)	15 (8%)	3 (2%)	9	43
15	O	184/186 (99%)	164 (89%)	13 (7%)	7 (4%)	3	22
16	P	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17	56
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	22	61
18	R	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	14	51
19	S	148/154 (96%)	139 (94%)	8 (5%)	1 (1%)	22	61
20	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
21	U	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	56
22	V	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	7	38
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	26
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	61
25	Y	80/91 (88%)	71 (89%)	8 (10%)	1 (1%)	12	47
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	61 (86%)	8 (11%)	2 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6	35
All	All	3633/4235 (86%)	3285 (90%)	281 (8%)	67 (2%)	8	41

All (67) 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
11	K	143	LYS
13	M	21	ARG
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
3	C	132	ASP
4	D	34	GLY
4	D	169	GLY
4	D	184	ASP
6	F	16	PRO
6	F	20	LYS
6	F	61	PHE
6	F	171	ASP
10	J	40	PRO
10	J	138	PRO
11	K	5	GLU
14	N	140	ALA
14	N	165	SER
15	O	162	ASP
15	O	181	ASP
22	V	7	ASP

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Mol	Chain	Res	Type
30	4	57	GLY
4	D	107	SER
5	E	8	LEU
6	F	36	ASN
6	F	137	PRO
6	F	147	ALA
12	L	119	GLN
25	Y	77	PHE
6	F	11	HIS
6	F	82	GLU
6	F	170	TYR
11	K	7	ASP
14	N	18	GLY
15	O	65	ASP
15	O	167	ASP
17	Q	116	SER
27	1	81	LYS
30	4	56	PRO
3	C	69	LEU
3	C	119	ALA
4	D	206	THR
4	D	291	ASP
6	F	96	SER
8	H	64	PRO
12	L	126	SER
16	P	20	SER
4	D	2	GLN
4	D	185	GLY
21	U	53	GLY
10	J	72	VAL
23	W	40	PRO
27	1	41	VAL
19	S	81	PRO
18	R	54	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	14	46
4	D	282/282 (100%)	263 (93%)	19 (7%)	16	50
5	E	193/193 (100%)	175 (91%)	18 (9%)	9	33
6	F	117/147 (80%)	107 (92%)	10 (8%)	10	38
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	76
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	88
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	9	34
11	K	118/121 (98%)	108 (92%)	10 (8%)	10	38
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	74
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	69
14	N	166/166 (100%)	158 (95%)	8 (5%)	25	61
15	O	149/149 (100%)	143 (96%)	6 (4%)	31	66
16	P	93/93 (100%)	90 (97%)	3 (3%)	39	71
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	75
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	114 (97%)	3 (3%)	46	76
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	101 (96%)	4 (4%)	33	67
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	80
24	X	130/130 (100%)	122 (94%)	8 (6%)	18	53
25	Y	66/73 (90%)	61 (92%)	5 (8%)	13	45
26	Z	120/195 (62%)	112 (93%)	8 (7%)	16	50
27	1	56/56 (100%)	53 (95%)	3 (5%)	22	58
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
30	4	79/79 (100%)	78 (99%)	1 (1%)	69	87
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	24	60

All (151) 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	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	67	GLN
5	E	78	ARG
5	E	91	PRO
5	E	94	THR
5	E	95	GLU
5	E	101	ASP
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG

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Mol	Chain	Res	Type
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
5	E	246	ARG
6	F	24	HIS
6	F	50	VAL
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
8	H	12	LEU
10	J	1	LYS
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	86	ARG
10	J	93	ILE
10	J	129	ASN
10	J	142	VAL
10	J	150	LYS
11	K	46	ILE
11	K	52	GLN
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

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Mol	Chain	Res	Type
11	K	127	ILE
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	46	LEU
14	N	48	ARG
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
16	P	28	ASP
16	P	97	SER
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
21	U	39	ASN
21	U	48	VAL
21	U	73	HIS
21	U	96	VAL
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL

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Mol	Chain	Res	Type
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	52	PRO
25	Y	72	VAL
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	186	ARG
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	44	PHE
27	1	64	ILE
29	3	18	ASN
30	4	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	238	ASN
4	D	260	HIS
4	D	318	ASN
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
5	E	163	HIS

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Mol	Chain	Res	Type
6	F	103	ASN
6	F	133	ASN
7	G	90	HIS
7	G	106	ASN
7	G	143	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
12	L	42	ASN
13	M	18	HIS
13	M	41	HIS
13	M	42	ASN
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	GLN
15	O	93	GLN
15	O	107	ASN
15	O	153	GLN
16	P	53	GLN
16	P	100	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN

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Mol	Chain	Res	Type
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	123	GLN
20	T	53	ASN
21	U	39	ASN
21	U	73	HIS
22	V	39	ASN
23	W	60	GLN
24	X	27	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	134	HIS
26	Z	149	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	70	GLN
28	2	8	GLN
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	15	ASN
30	4	30	GLN
30	4	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	245 (8%)	36 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	121/122 (99%)	14 (11%)	6 (4%)
All	All	2868/3044 (94%)	259 (9%)	42 (1%)

All (259) 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	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	A	885	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	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
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	1234	U
1	A	1238	C
1	A	1239	G

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Mol	Chain	Res	Type
1	A	1262	C
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	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C

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Mol	Chain	Res	Type
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
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	2006	C
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2291	A
1	A	2317	C
1	A	2321	A
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2465	A
1	A	2467	A
1	A	2469	A

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Mol	Chain	Res	Type
1	A	2476	C
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	2718	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U

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Mol	Chain	Res	Type
2	B	3003	A
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1261	A
1	A	1352	A
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1692	C
1	A	1814	G
1	A	1856	C
1	A	1942	A

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Mol	Chain	Res	Type
1	A	1979	G
1	A	2005	G
1	A	2011	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	2761	A
1	A	2791	U
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3043	G
2	B	3065	A
2	B	3103	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	ZIT	A	8600	-	54,54,54	1.75	11 (20%)	82,83,83	1.27	8 (9%)

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	ZIT	A	8600	-	-	1/72/107/107	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	8600	ZIT	C2-C3	4.53	1.65	1.55
31	A	8600	ZIT	C7-C6	4.33	1.61	1.54
31	A	8600	ZIT	C3A-N3A	4.23	1.57	1.48
31	A	8600	ZIT	C11-N10	3.47	1.54	1.49
31	A	8600	ZIT	C2B-C3B	3.18	1.60	1.52
31	A	8600	ZIT	C4A-C5A	2.96	1.57	1.51
31	A	8600	ZIT	C13-C14	2.57	1.59	1.54
31	A	8600	ZIT	C4-C5	2.55	1.61	1.55
31	A	8600	ZIT	O5A-C5A	2.26	1.49	1.44
31	A	8600	ZIT	C9-C8	2.21	1.61	1.53
31	A	8600	ZIT	C4A-C3A	2.09	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	8600	ZIT	C6-C5-C4	-4.02	108.35	114.05
31	A	8600	ZIT	O1A-C5-C6	3.07	110.17	106.39
31	A	8600	ZIT	C17-C2-C3	2.57	118.73	112.92
31	A	8600	ZIT	O1B-C3-C4	2.37	111.08	108.22
31	A	8600	ZIT	C21-N10-C9	2.34	113.83	110.28
31	A	8600	ZIT	C9-N10-C11	-2.23	108.26	112.05
31	A	8600	ZIT	C2A-C3A-N3A	2.19	117.17	110.83
31	A	8600	ZIT	O5A-C5A-C6A	-2.02	102.60	106.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

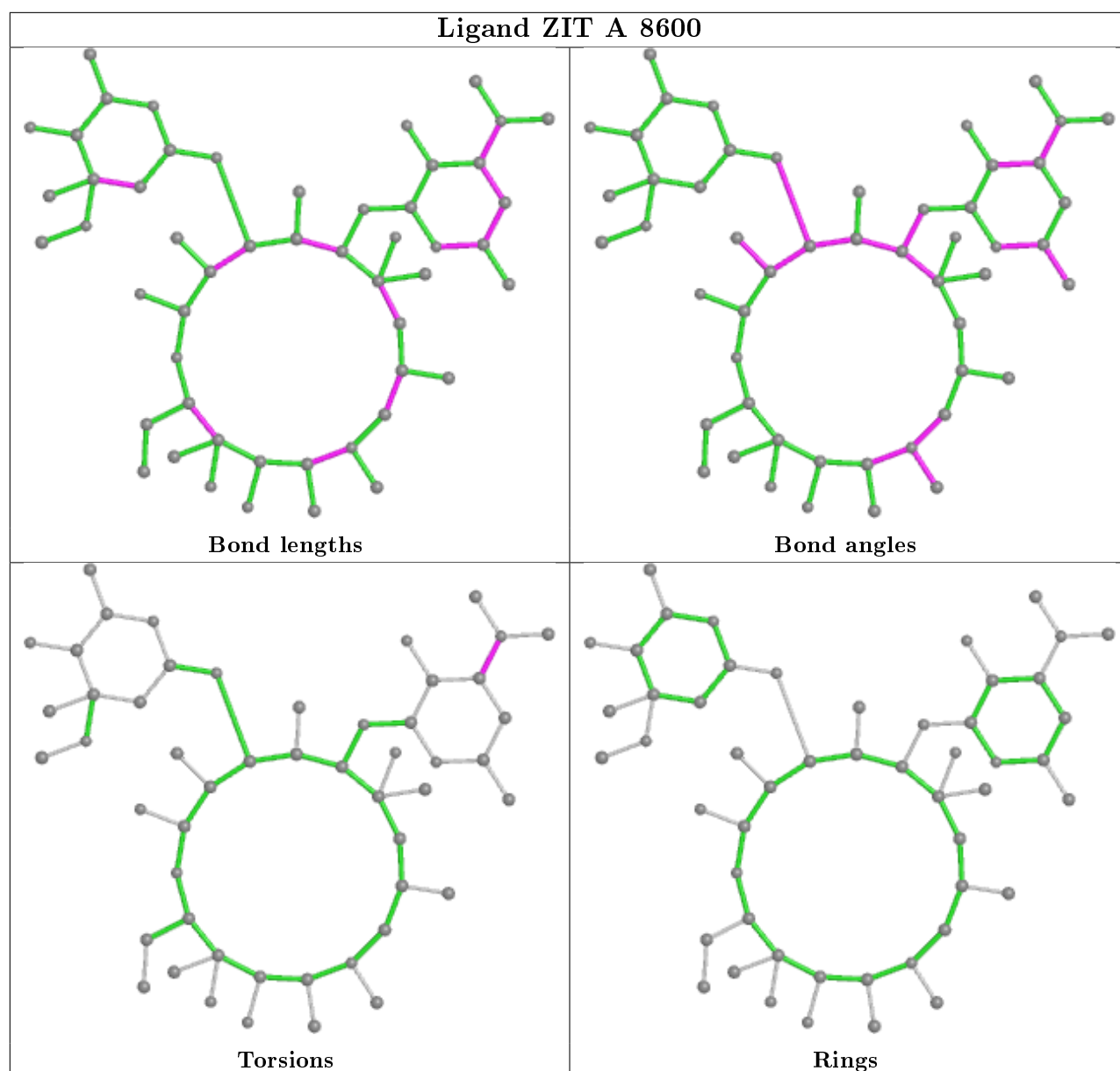
Mol	Chain	Res	Type	Atoms
31	A	8600	ZIT	C4A-C3A-N3A-C8A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	8600	ZIT	2	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.10	37 (1%) 77 65	27, 56, 101, 149	0
2	B	122/122 (100%)	0.07	6 (4%) 29 17	43, 71, 98, 158	0
3	C	237/239 (99%)	0.05	10 (4%) 36 23	38, 62, 93, 114	0
4	D	337/337 (100%)	-0.12	2 (0%) 89 83	29, 64, 90, 99	0
5	E	246/246 (100%)	-0.14	0 100 100	30, 58, 81, 92	0
6	F	140/176 (79%)	1.34	43 (30%) 0 0	61, 108, 124, 131	0
7	G	172/177 (97%)	0.33	4 (2%) 60 47	50, 76, 97, 102	0
8	H	119/119 (100%)	0.46	11 (9%) 9 5	62, 82, 106, 110	0
9	I	29/348 (8%)	1.64	11 (37%) 0 0	80, 100, 109, 109	0
10	J	156/167 (93%)	0.04	2 (1%) 77 65	43, 65, 94, 101	0
11	K	142/145 (97%)	-0.12	0 100 100	45, 57, 80, 97	0
12	L	132/132 (100%)	-0.15	0 100 100	38, 58, 80, 87	0
13	M	145/164 (88%)	0.46	15 (10%) 6 4	33, 77, 113, 123	0
14	N	194/194 (100%)	-0.16	2 (1%) 82 72	42, 56, 73, 84	0
15	O	186/186 (100%)	0.36	14 (7%) 14 8	52, 74, 114, 124	0
16	P	115/115 (100%)	0.05	0 100 100	52, 66, 84, 88	0
17	Q	143/148 (96%)	0.22	3 (2%) 63 49	45, 65, 80, 89	0
18	R	95/95 (100%)	-0.11	0 100 100	38, 54, 70, 82	0
19	S	150/154 (97%)	-0.21	0 100 100	40, 54, 74, 82	0
20	T	81/84 (96%)	-0.02	1 (1%) 79 67	55, 71, 90, 97	0
21	U	119/119 (100%)	0.42	4 (3%) 45 29	52, 69, 92, 103	0
22	V	53/66 (80%)	-0.02	0 100 100	51, 64, 82, 89	0
23	W	65/70 (92%)	1.11	13 (20%) 1 1	62, 83, 118, 124	0
24	X	154/154 (100%)	-0.36	0 100 100	38, 56, 76, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.12	1 (1%) 79 67	53, 67, 91, 107	0
26	Z	142/240 (59%)	-0.11	0 100 100	33, 56, 77, 94	0
27	1	73/73 (100%)	0.04	5 (6%) 17 10	59, 71, 87, 94	0
28	2	56/56 (100%)	-0.31	0 100 100	35, 46, 51, 52	0
29	3	46/48 (95%)	0.10	1 (2%) 62 48	44, 72, 96, 106	0
30	4	92/92 (100%)	0.35	4 (4%) 35 22	44, 66, 79, 90	0
All	All	6577/7279 (90%)	0.03	189 (2%) 51 36	27, 62, 101, 158	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3001	U	8.2
23	W	1	THR	7.5
9	I	27	ILE	5.8
6	F	57	THR	5.7
15	O	186	LEU	5.5
6	F	88	LEU	5.3
2	B	3024	U	5.2
21	U	119	ALA	5.2
2	B	3023	U	4.7
15	O	162	ASP	4.6
6	F	69	ILE	4.5
1	A	1173	A	4.5
1	A	1175	G	4.5
6	F	62	ASP	4.4
6	F	63	ILE	4.3
6	F	56	ARG	4.2
23	W	39	ALA	4.2
6	F	18	ILE	4.1
13	M	104	ASP	4.0
1	A	735	C	3.9
1	A	1172	G	3.9
13	M	59	GLU	3.8
6	F	25	MET	3.8
9	I	23	ILE	3.8
6	F	85	GLN	3.7
6	F	27	ILE	3.7
30	4	22	VAL	3.6
1	A	1198	U	3.6
15	O	160	SER	3.6

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Mol	Chain	Res	Type	RSRZ
6	F	58	VAL	3.6
8	H	106	THR	3.6
13	M	60	GLU	3.6
15	O	179	LEU	3.5
6	F	10	PHE	3.5
1	A	282	C	3.5
13	M	105	TYR	3.5
1	A	1162	G	3.4
1	A	1190	G	3.4
1	A	2237	G	3.4
3	C	36	ASP	3.4
23	W	38	GLY	3.3
20	T	81	ILE	3.3
23	W	3	LEU	3.2
15	O	149	GLU	3.2
6	F	70	GLY	3.2
6	F	87	ALA	3.2
1	A	1171	A	3.2
15	O	138	ASP	3.2
3	C	82	VAL	3.1
3	C	85	ASP	3.1
23	W	59	ILE	3.1
6	F	17	ARG	3.1
9	I	24	VAL	3.1
1	A	1948	G	3.1
6	F	128	LEU	3.1
6	F	84	LEU	3.0
23	W	8	ILE	3.0
9	I	26	MET	3.0
13	M	61	ALA	3.0
1	A	1199	A	3.0
1	A	960	G	3.0
13	M	123	ASP	3.0
23	W	40	PRO	3.0
6	F	44	ILE	3.0
7	G	45	ASP	3.0
1	A	1951	G	2.9
23	W	52	ALA	2.9
27	1	11	THR	2.9
1	A	1186	C	2.9
2	B	3025	G	2.9
1	A	1177	A	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1204	C	2.8
6	F	166	ILE	2.8
6	F	54	ALA	2.8
1	A	2345	A	2.8
6	F	104	PHE	2.8
21	U	112	LEU	2.8
10	J	59	ASN	2.8
6	F	66	GLY	2.7
21	U	42	VAL	2.7
8	H	17	LEU	2.7
6	F	132	VAL	2.7
1	A	138	U	2.7
6	F	45	THR	2.7
6	F	130	VAL	2.7
7	G	10	ASP	2.7
15	O	158	LEU	2.7
6	F	26	GLY	2.6
9	I	13	PRO	2.6
7	G	100	ASP	2.6
13	M	102	ASP	2.6
17	Q	1	THR	2.6
1	A	284	C	2.6
3	C	35	GLY	2.6
21	U	37	GLN	2.6
9	I	15	TRP	2.5
1	A	1188	A	2.5
13	M	99	GLU	2.5
3	C	91	GLY	2.5
6	F	75	LEU	2.5
1	A	1525	G	2.5
1	A	285	A	2.5
6	F	102	GLY	2.5
6	F	107	GLY	2.5
6	F	134	LEU	2.5
27	1	21	LYS	2.5
4	D	97	LEU	2.4
13	M	106	VAL	2.4
17	Q	77	ALA	2.4
9	I	28	GLU	2.4
1	A	1197	G	2.4
6	F	55	LYS	2.4
30	4	92	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	93	LEU	2.4
23	W	58	THR	2.4
1	A	1163	G	2.4
8	H	49	PHE	2.4
6	F	24	HIS	2.4
13	M	100	ALA	2.4
15	O	152	GLU	2.4
1	A	2238	A	2.4
9	I	16	LYS	2.4
6	F	71	ALA	2.4
23	W	62	GLU	2.4
15	O	159	TYR	2.4
9	I	20	VAL	2.3
1	A	736	A	2.3
3	C	154	ALA	2.3
1	A	1205	U	2.3
6	F	65	GLU	2.3
23	W	9	ARG	2.3
13	M	111	ALA	2.3
4	D	1	PRO	2.3
1	A	1193	A	2.3
6	F	53	LYS	2.3
15	O	147	ILE	2.3
15	O	150	TYR	2.3
8	H	108	LEU	2.2
29	3	35	ARG	2.2
6	F	72	LYS	2.2
3	C	236	GLY	2.2
13	M	108	VAL	2.2
8	H	44	SER	2.2
8	H	26	THR	2.2
2	B	3002	U	2.2
14	N	87	MET	2.2
9	I	65	THR	2.2
27	1	38	LYS	2.2
8	H	20	LEU	2.2
6	F	170	TYR	2.2
13	M	80	ASP	2.2
15	O	167	ASP	2.2
6	F	29	HIS	2.2
8	H	22	VAL	2.2
30	4	35	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	3122	C	2.1
8	H	98	VAL	2.1
1	A	1167	G	2.1
13	M	120	LEU	2.1
13	M	62	ALA	2.1
3	C	84	VAL	2.1
15	O	157	PRO	2.1
8	H	90	GLU	2.1
23	W	7	GLU	2.1
6	F	171	ASP	2.1
1	A	1201	C	2.1
15	O	163	PHE	2.1
3	C	37	VAL	2.1
1	A	1185	U	2.1
6	F	67	ASP	2.1
17	Q	63	ARG	2.1
30	4	8	ASN	2.1
1	A	281	U	2.1
10	J	83	PHE	2.1
1	A	602	A	2.1
9	I	67	LEU	2.1
27	1	22	ILE	2.0
25	Y	76	ARG	2.0
8	H	19	ALA	2.0
27	1	44	PHE	2.0
3	C	110	SER	2.0
23	W	63	GLU	2.0
1	A	1184	C	2.0
7	G	108	LEU	2.0
1	A	368	C	2.0
6	F	41	LEU	2.0
14	N	194	ALA	2.0
1	A	258	G	2.0
6	F	106	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8329	1/1	0.28	0.45	70,70,70,70	0
34	NA	A	8374	1/1	0.32	1.54	89,89,89,89	0
34	NA	A	8384	1/1	0.40	1.14	90,90,90,90	0
34	NA	S	8386	1/1	0.51	0.45	97,97,97,97	0
34	NA	A	8363	1/1	0.55	0.91	79,79,79,79	0
34	NA	A	8341	1/1	0.57	0.31	63,63,63,63	0
35	CL	R	8511	1/1	0.61	0.59	102,102,102,102	0
34	NA	A	8326	1/1	0.63	1.00	92,92,92,92	0
34	NA	A	8364	1/1	0.64	0.23	52,52,52,52	0
35	CL	A	8515	1/1	0.65	0.88	110,110,110,110	0
34	NA	A	8303	1/1	0.66	0.40	54,54,54,54	0
34	NA	A	8375	1/1	0.67	0.28	86,86,86,86	0
34	NA	A	8328	1/1	0.69	0.28	61,61,61,61	0
35	CL	O	8507	1/1	0.71	0.52	84,84,84,84	0
34	NA	J	8322	1/1	0.71	0.43	62,62,62,62	0
32	MG	A	8066	1/1	0.72	0.69	48,48,48,48	0
34	NA	A	8371	1/1	0.74	0.33	48,48,48,48	0
32	MG	A	8041	1/1	0.75	0.26	69,69,69,69	0
34	NA	A	8377	1/1	0.75	0.34	68,68,68,68	0
34	NA	A	8385	1/1	0.75	0.67	73,73,73,73	0
34	NA	A	8305	1/1	0.76	0.25	46,46,46,46	0
34	NA	A	8340	1/1	0.76	0.61	56,56,56,56	0
34	NA	A	8332	1/1	0.76	0.16	50,50,50,50	0
35	CL	A	8510	1/1	0.77	0.34	97,97,97,97	0
34	NA	A	8354	1/1	0.78	0.61	54,54,54,54	0
32	MG	A	8053	1/1	0.78	0.15	40,40,40,40	0
32	MG	A	8024	1/1	0.79	0.48	79,79,79,79	0
32	MG	A	8096	1/1	0.79	0.10	64,64,64,64	0
34	NA	A	8357	1/1	0.79	0.07	64,64,64,64	0
34	NA	T	8312	1/1	0.79	0.25	51,51,51,51	0
35	CL	A	8522	1/1	0.80	0.70	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	U	8073	1/1	0.80	0.08	62,62,62,62	0
34	NA	B	8351	1/1	0.80	0.15	54,54,54,54	0
35	CL	A	8503	1/1	0.80	0.50	74,74,74,74	0
34	NA	A	8368	1/1	0.81	0.25	65,65,65,65	0
34	NA	A	8366	1/1	0.81	0.40	79,79,79,79	0
34	NA	S	8337	1/1	0.81	0.22	58,58,58,58	0
34	NA	A	8381	1/1	0.81	0.15	61,61,61,61	0
34	NA	B	8383	1/1	0.81	0.52	40,40,40,40	0
32	MG	A	8011	1/1	0.81	0.08	44,44,44,44	0
34	NA	A	8323	1/1	0.81	0.45	57,57,57,57	0
34	NA	A	8373	1/1	0.81	0.52	67,67,67,67	0
34	NA	A	8310	1/1	0.81	0.21	29,29,29,29	0
35	CL	A	8513	1/1	0.82	0.15	67,67,67,67	0
35	CL	A	8505	1/1	0.82	0.43	92,92,92,92	0
35	CL	P	8508	1/1	0.82	0.35	97,97,97,97	0
34	NA	A	8367	1/1	0.83	0.24	38,38,38,38	0
32	MG	A	8116	1/1	0.83	0.10	54,54,54,54	0
34	NA	A	8330	1/1	0.84	0.29	57,57,57,57	0
35	CL	A	8520	1/1	0.84	0.19	65,65,65,65	0
32	MG	A	8088	1/1	0.84	0.13	64,64,64,64	0
34	NA	A	8316	1/1	0.84	0.41	61,61,61,61	0
31	ZIT	A	8600	52/52	0.84	0.30	81,91,95,96	0
32	MG	A	8092	1/1	0.84	0.32	95,95,95,95	0
32	MG	A	8087	1/1	0.85	0.10	75,75,75,75	0
32	MG	1	8105	1/1	0.85	0.43	38,38,38,38	0
32	MG	A	8071	1/1	0.86	0.13	85,85,85,85	0
32	MG	A	8099	1/1	0.86	0.17	55,55,55,55	0
35	CL	4	8504	1/1	0.86	0.54	93,93,93,93	0
34	NA	A	8342	1/1	0.86	0.38	51,51,51,51	0
34	NA	A	8308	1/1	0.86	0.23	53,53,53,53	0
34	NA	A	8365	1/1	0.87	0.58	76,76,76,76	0
32	MG	A	8001	1/1	0.87	0.10	41,41,41,41	0
34	NA	A	8325	1/1	0.87	0.25	62,62,62,62	0
34	NA	A	8352	1/1	0.87	0.32	56,56,56,56	0
32	MG	A	8067	1/1	0.87	0.21	51,51,51,51	0
34	NA	A	8372	1/1	0.87	0.48	87,87,87,87	0
32	MG	A	8114	1/1	0.88	0.26	47,47,47,47	0
32	MG	A	8112	1/1	0.88	0.22	50,50,50,50	0
32	MG	A	8050	1/1	0.88	0.25	67,67,67,67	0
34	NA	A	8313	1/1	0.88	0.23	66,66,66,66	0
34	NA	A	8355	1/1	0.88	0.49	60,60,60,60	0
34	NA	A	8307	1/1	0.88	0.40	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	U	8343	1/1	0.89	0.26	38,38,38,38	0
32	MG	A	8106	1/1	0.89	0.14	71,71,71,71	0
34	NA	A	8333	1/1	0.89	0.13	51,51,51,51	0
32	MG	A	8082	1/1	0.89	0.22	83,83,83,83	0
32	MG	A	8049	1/1	0.89	0.18	74,74,74,74	0
35	CL	A	8517	1/1	0.89	0.16	52,52,52,52	0
32	MG	A	8113	1/1	0.90	0.15	53,53,53,53	0
35	CL	L	8512	1/1	0.90	0.13	55,55,55,55	0
32	MG	A	8017	1/1	0.90	0.06	42,42,42,42	0
32	MG	A	8089	1/1	0.90	0.11	70,70,70,70	0
32	MG	A	8111	1/1	0.90	0.08	62,62,62,62	0
34	NA	A	8349	1/1	0.90	0.32	57,57,57,57	0
34	NA	A	8356	1/1	0.90	0.70	78,78,78,78	0
34	NA	M	8380	1/1	0.90	0.67	75,75,75,75	0
34	NA	A	8318	1/1	0.90	0.67	45,45,45,45	0
32	MG	A	8100	1/1	0.90	0.15	88,88,88,88	0
34	NA	A	8378	1/1	0.90	1.11	48,48,48,48	0
36	CD	P	8405	1/1	0.91	0.09	152,152,152,152	0
32	MG	A	8040	1/1	0.91	0.10	63,63,63,63	0
34	NA	E	8304	1/1	0.91	0.20	32,32,32,32	0
35	CL	A	8514	1/1	0.91	0.18	57,57,57,57	0
32	MG	4	8078	1/1	0.91	0.06	54,54,54,54	0
34	NA	A	8302	1/1	0.91	0.24	52,52,52,52	0
34	NA	A	8336	1/1	0.91	0.15	85,85,85,85	0
35	CL	C	8509	1/1	0.91	0.27	69,69,69,69	0
34	NA	A	8360	1/1	0.91	0.86	59,59,59,59	0
34	NA	A	8321	1/1	0.91	0.47	42,42,42,42	0
34	NA	A	8382	1/1	0.91	0.29	74,74,74,74	0
32	MG	L	8069	1/1	0.91	0.16	79,79,79,79	0
35	CL	S	8506	1/1	0.91	0.27	69,69,69,69	0
32	MG	A	8057	1/1	0.91	0.18	54,54,54,54	0
32	MG	A	8093	1/1	0.91	0.09	59,59,59,59	0
32	MG	A	8097	1/1	0.92	0.31	45,45,45,45	0
32	MG	A	8064	1/1	0.92	0.45	36,36,36,36	0
32	MG	A	8101	1/1	0.92	0.15	60,60,60,60	0
32	MG	A	8052	1/1	0.92	0.13	58,58,58,58	0
34	NA	A	8311	1/1	0.92	0.15	63,63,63,63	0
34	NA	A	8331	1/1	0.93	0.19	55,55,55,55	0
34	NA	A	8369	1/1	0.93	0.33	55,55,55,55	0
32	MG	A	8021	1/1	0.93	0.09	32,32,32,32	0
35	CL	K	8521	1/1	0.93	0.17	64,64,64,64	0
34	NA	C	8345	1/1	0.93	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8090	1/1	0.93	0.16	47,47,47,47	0
32	MG	A	8042	1/1	0.93	0.23	52,52,52,52	0
34	NA	A	8314	1/1	0.93	0.17	48,48,48,48	0
35	CL	D	8519	1/1	0.93	0.43	65,65,65,65	0
32	MG	A	8108	1/1	0.93	0.13	85,85,85,85	0
32	MG	A	8059	1/1	0.94	0.15	56,56,56,56	0
34	NA	A	8362	1/1	0.94	0.68	62,62,62,62	0
32	MG	A	8033	1/1	0.94	0.11	36,36,36,36	0
32	MG	A	8063	1/1	0.94	0.10	92,92,92,92	0
32	MG	A	8075	1/1	0.94	0.11	56,56,56,56	0
34	NA	A	8376	1/1	0.94	0.28	49,49,49,49	0
32	MG	A	8091	1/1	0.94	0.07	58,58,58,58	0
32	MG	Z	8109	1/1	0.94	0.17	61,61,61,61	0
32	MG	A	8008	1/1	0.94	0.13	61,61,61,61	0
34	NA	R	8348	1/1	0.94	0.07	39,39,39,39	0
32	MG	A	8086	1/1	0.94	0.12	56,56,56,56	0
34	NA	A	8359	1/1	0.94	0.51	75,75,75,75	0
32	MG	A	8043	1/1	0.94	0.14	56,56,56,56	0
35	CL	N	8518	1/1	0.94	0.20	65,65,65,65	0
32	MG	A	8056	1/1	0.94	0.10	61,61,61,61	0
32	MG	A	8039	1/1	0.94	0.06	67,67,67,67	0
32	MG	B	8095	1/1	0.95	0.08	98,98,98,98	0
34	NA	A	8361	1/1	0.95	0.51	46,46,46,46	0
34	NA	A	8324	1/1	0.95	0.09	48,48,48,48	0
32	MG	A	8070	1/1	0.95	0.19	46,46,46,46	0
35	CL	K	8502	1/1	0.95	0.15	87,87,87,87	0
32	MG	A	8076	1/1	0.95	0.09	75,75,75,75	0
32	MG	A	8010	1/1	0.95	0.09	43,43,43,43	0
32	MG	A	8102	1/1	0.95	0.28	75,75,75,75	0
32	MG	A	8009	1/1	0.95	0.05	46,46,46,46	0
32	MG	A	8054	1/1	0.95	0.06	52,52,52,52	0
32	MG	A	8083	1/1	0.95	0.08	51,51,51,51	0
32	MG	A	8110	1/1	0.95	0.08	35,35,35,35	0
34	NA	A	8306	1/1	0.95	0.52	41,41,41,41	0
34	NA	K	8346	1/1	0.95	0.15	33,33,33,33	0
32	MG	A	8074	1/1	0.95	0.04	52,52,52,52	0
32	MG	A	8012	1/1	0.95	0.10	35,35,35,35	0
34	NA	A	8334	1/1	0.95	0.19	45,45,45,45	0
32	MG	A	8037	1/1	0.95	0.12	61,61,61,61	0
32	MG	A	8020	1/1	0.95	0.07	36,36,36,36	0
34	NA	A	8370	1/1	0.95	0.20	42,42,42,42	0
34	NA	A	8301	1/1	0.95	0.17	42,42,42,42	0

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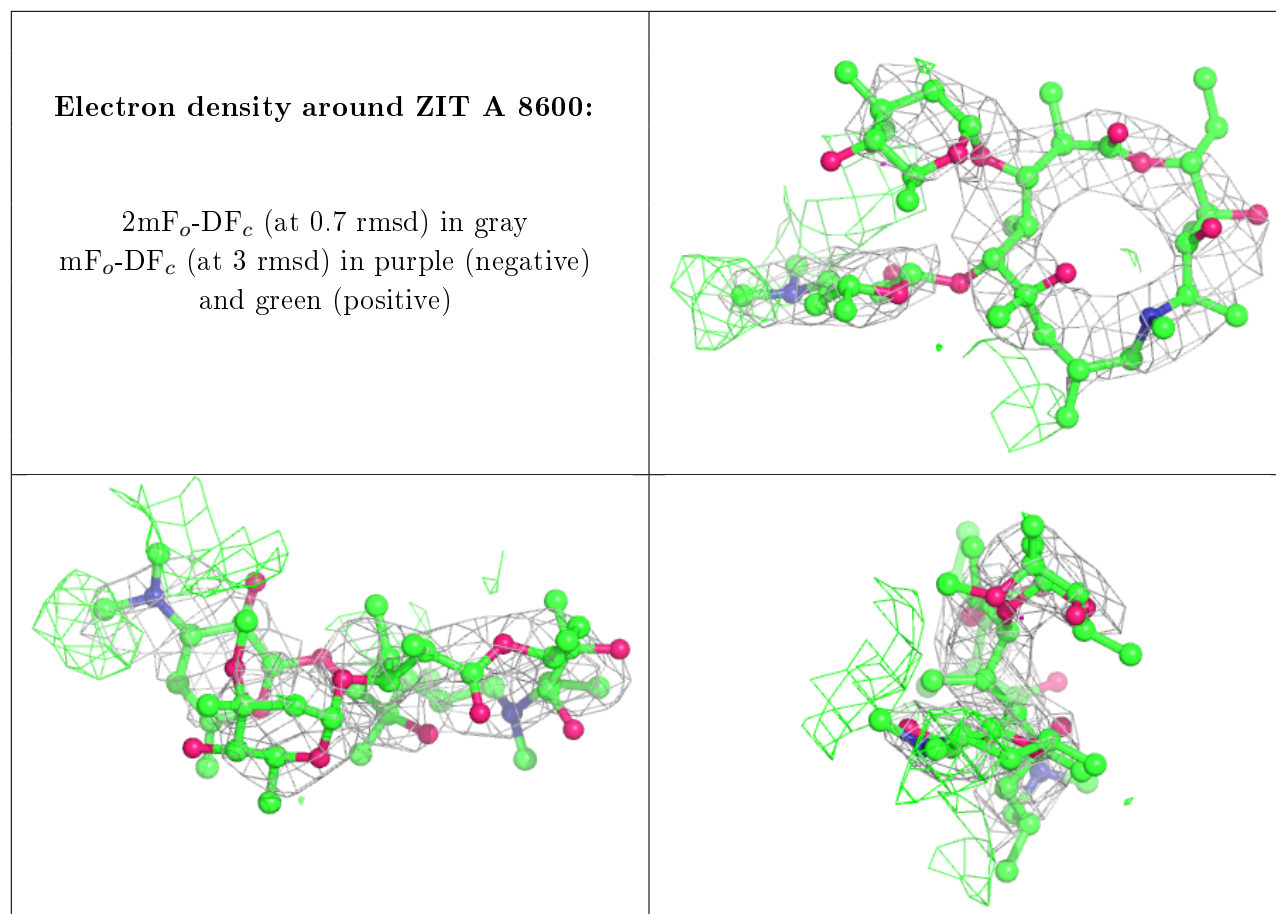
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8103	1/1	0.95	0.19	76,76,76,76	0
34	NA	A	8353	1/1	0.95	0.12	46,46,46,46	0
34	NA	A	8379	1/1	0.95	0.17	52,52,52,52	0
34	NA	A	8327	1/1	0.95	0.09	44,44,44,44	0
32	MG	A	8068	1/1	0.95	0.05	56,56,56,56	0
32	MG	A	8060	1/1	0.95	0.20	51,51,51,51	0
34	NA	A	8335	1/1	0.96	0.27	61,61,61,61	0
33	K	A	8201	1/1	0.96	0.16	70,70,70,70	0
32	MG	A	8013	1/1	0.96	0.20	56,56,56,56	0
32	MG	A	8016	1/1	0.96	0.13	50,50,50,50	0
34	NA	A	8358	1/1	0.96	0.65	107,107,107,107	0
35	CL	K	8501	1/1	0.96	0.33	81,81,81,81	0
32	MG	A	8027	1/1	0.96	0.05	51,51,51,51	0
32	MG	A	8022	1/1	0.96	0.05	55,55,55,55	0
32	MG	A	8084	1/1	0.96	0.05	41,41,41,41	0
36	CD	4	8404	1/1	0.96	0.11	75,75,75,75	0
32	MG	A	8046	1/1	0.96	0.09	72,72,72,72	0
32	MG	A	8038	1/1	0.96	0.08	29,29,29,29	0
32	MG	A	8005	1/1	0.96	0.12	60,60,60,60	0
32	MG	A	8006	1/1	0.96	0.04	54,54,54,54	0
32	MG	A	8094	1/1	0.96	0.09	66,66,66,66	0
32	MG	A	8051	1/1	0.96	0.13	66,66,66,66	0
32	MG	A	8035	1/1	0.96	0.08	60,60,60,60	0
34	NA	A	8344	1/1	0.96	0.08	39,39,39,39	0
32	MG	A	8061	1/1	0.96	0.04	37,37,37,37	0
32	MG	A	8048	1/1	0.96	0.08	41,41,41,41	0
34	NA	J	8309	1/1	0.96	0.15	43,43,43,43	0
32	MG	A	8072	1/1	0.96	0.11	65,65,65,65	0
32	MG	A	8002	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8081	1/1	0.96	0.12	67,67,67,67	0
32	MG	A	8007	1/1	0.97	0.09	42,42,42,42	0
34	NA	A	8320	1/1	0.97	0.12	32,32,32,32	0
32	MG	A	8085	1/1	0.97	0.15	68,68,68,68	0
32	MG	A	8034	1/1	0.97	0.03	32,32,32,32	0
35	CL	K	8516	1/1	0.97	0.26	53,53,53,53	0
32	MG	A	8107	1/1	0.97	0.04	60,60,60,60	0
36	CD	1	8403	1/1	0.97	0.12	77,77,77,77	0
32	MG	A	8004	1/1	0.97	0.11	60,60,60,60	0
32	MG	A	8079	1/1	0.97	0.08	42,42,42,42	0
32	MG	A	8045	1/1	0.97	0.10	58,58,58,58	0
32	MG	A	8036	1/1	0.97	0.07	46,46,46,46	0
32	MG	A	8077	1/1	0.97	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8315	1/1	0.97	0.31	62,62,62,62	0
32	MG	A	8032	1/1	0.97	0.15	63,63,63,63	0
32	MG	A	8015	1/1	0.97	0.09	57,57,57,57	0
32	MG	A	8026	1/1	0.97	0.09	49,49,49,49	0
32	MG	A	8003	1/1	0.97	0.10	26,26,26,26	0
32	MG	A	8080	1/1	0.97	0.13	65,65,65,65	0
32	MG	A	8104	1/1	0.97	0.07	50,50,50,50	0
32	MG	A	8062	1/1	0.97	0.09	61,61,61,61	0
32	MG	A	8028	1/1	0.97	0.04	57,57,57,57	0
32	MG	A	8029	1/1	0.98	0.12	50,50,50,50	0
32	MG	A	8044	1/1	0.98	0.21	58,58,58,58	0
32	MG	A	8058	1/1	0.98	0.18	62,62,62,62	0
32	MG	A	8115	1/1	0.98	0.06	43,43,43,43	0
32	MG	D	8055	1/1	0.98	0.10	51,51,51,51	0
32	MG	A	8019	1/1	0.98	0.06	24,24,24,24	0
32	MG	A	8025	1/1	0.98	0.05	54,54,54,54	0
34	NA	S	8338	1/1	0.98	0.09	49,49,49,49	0
34	NA	A	8350	1/1	0.98	0.22	43,43,43,43	0
33	K	A	8202	1/1	0.98	0.14	61,61,61,61	0
34	NA	A	8339	1/1	0.98	0.06	33,33,33,33	0
34	NA	N	8347	1/1	0.98	0.12	23,23,23,23	0
32	MG	A	8047	1/1	0.98	0.17	81,81,81,81	0
32	MG	A	8023	1/1	0.98	0.03	33,33,33,33	0
34	NA	A	8317	1/1	0.98	0.04	43,43,43,43	0
32	MG	A	8018	1/1	0.98	0.11	54,54,54,54	0
32	MG	A	8030	1/1	0.99	0.10	40,40,40,40	0
32	MG	A	8117	1/1	0.99	0.10	33,33,33,33	0
32	MG	C	8065	1/1	0.99	0.05	40,40,40,40	0
32	MG	A	8098	1/1	0.99	0.25	52,52,52,52	0
36	CD	2	8402	1/1	0.99	0.08	70,70,70,70	0
34	NA	A	8319	1/1	0.99	0.14	57,57,57,57	0
32	MG	A	8014	1/1	0.99	0.07	24,24,24,24	0
36	CD	V	8401	1/1	1.00	0.11	75,75,75,75	0
32	MG	A	8031	1/1	1.00	0.03	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.