



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 04:39 PM EDT

PDB ID : 2OTL  
Title : Girodazole bound to the large subunit of Haloarcula marismortui  
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.  
Deposited on : unknown  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

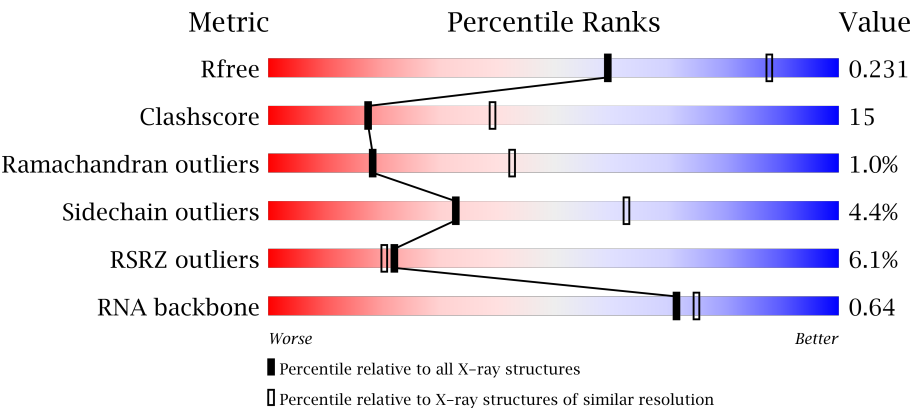
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

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. 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	0	2922	<div><div></div><div><div></div><div>49%</div><div>39%</div><div>6%</div><div>6%</div></div></div>
2	9	122	<div><div>3%</div><div><div></div><div>43%</div><div>44%</div><div>12%</div></div></div>
3	A	239	<div><div>12%</div><div><div></div><div>70%</div><div>26%</div><div>••</div></div></div>
4	B	337	<div><div></div><div><div></div><div>61%</div><div>35%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8060	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8514	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8529	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8578	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8537	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8705	-	-	-	X
36	CL	0	8713	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	O	8715	-	-	-	X
36	CL	J	8701	-	-	X	-
36	CL	M	8718	-	-	X	-

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			579	346	116	112	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

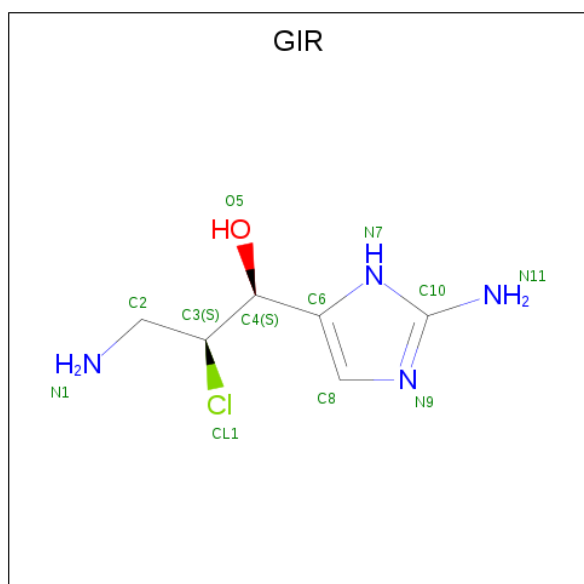
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 32 is GIRODAZOLE (three-letter code: GIR) (formula: C<sub>6</sub>H<sub>11</sub>ClN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	0	0
			12	6	1	4	1		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	J	3	Total 3	Cl 3	0	0
36	Q	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5893	Total O 5893 5893	0	0
38	9	145	Total O 145 145	0	0
38	A	118	Total O 118 118	0	0
38	B	147	Total O 147 147	0	0
38	C	163	Total O 163 163	0	0
38	D	48	Total O 48 48	0	0
38	E	46	Total O 46 46	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	69	Total O 69 69	0	0
38	J	58	Total O 58 58	0	0
38	K	58	Total O 58 58	0	0
38	L	81	Total O 81 81	0	0
38	M	115	Total O 115 115	0	0
38	N	58	Total O 58 58	0	0

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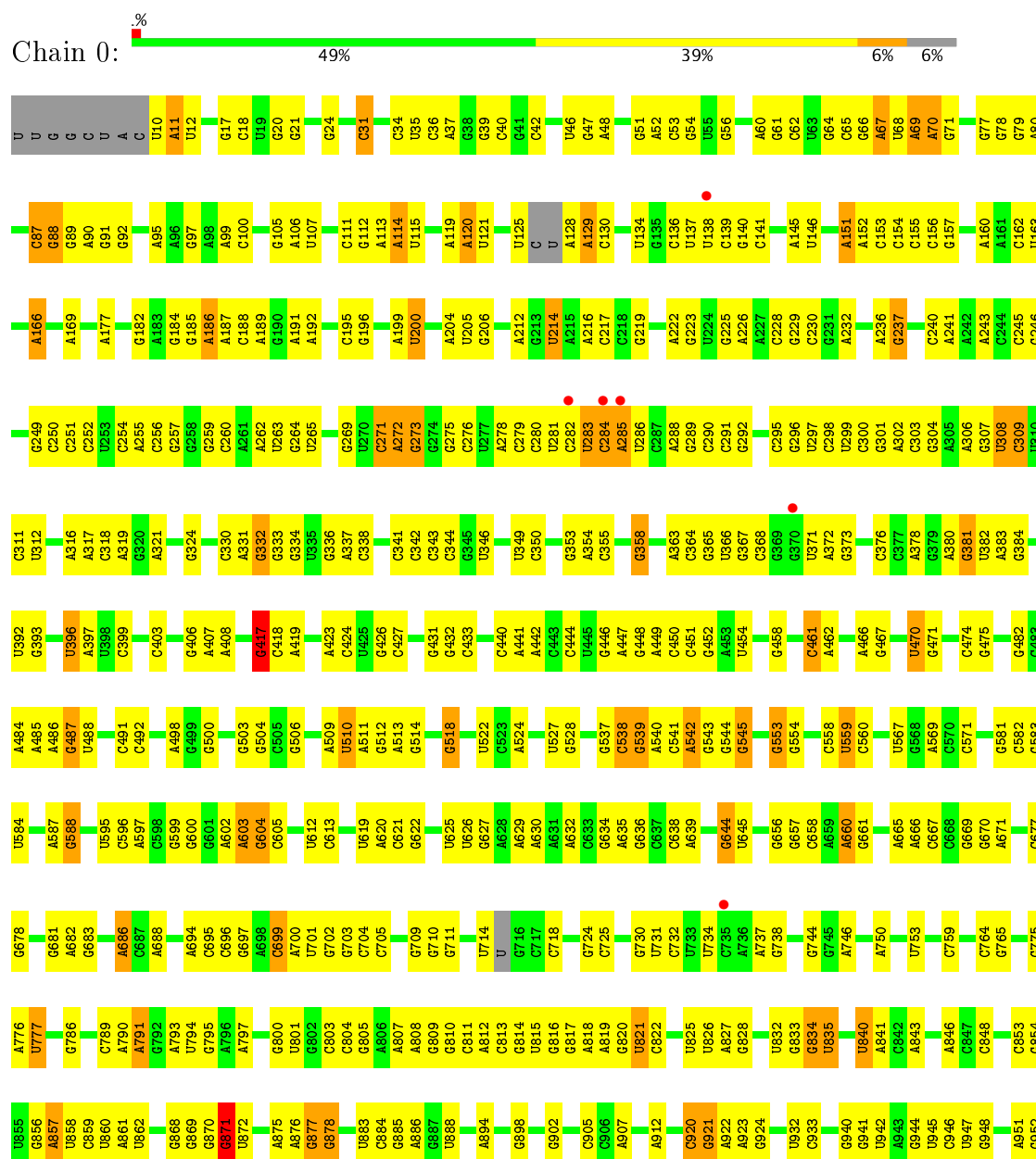
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	61	Total 61	O 61	0	0
38	Q	55	Total 55	O 55	0	0
38	R	81	Total 81	O 81	0	0
38	S	37	Total 37	O 37	0	0
38	T	39	Total 39	O 39	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	70	Total 70	O 70	0	0
38	X	26	Total 26	O 26	0	0
38	Y	99	Total 99	O 99	0	0
38	Z	32	Total 32	O 32	0	0
38	1	56	Total 56	O 56	0	0
38	2	40	Total 40	O 40	0	0
38	3	66	Total 66	O 66	0	0
38	I	4	Total 4	O 4	0	0

### 3 Residue-property plots

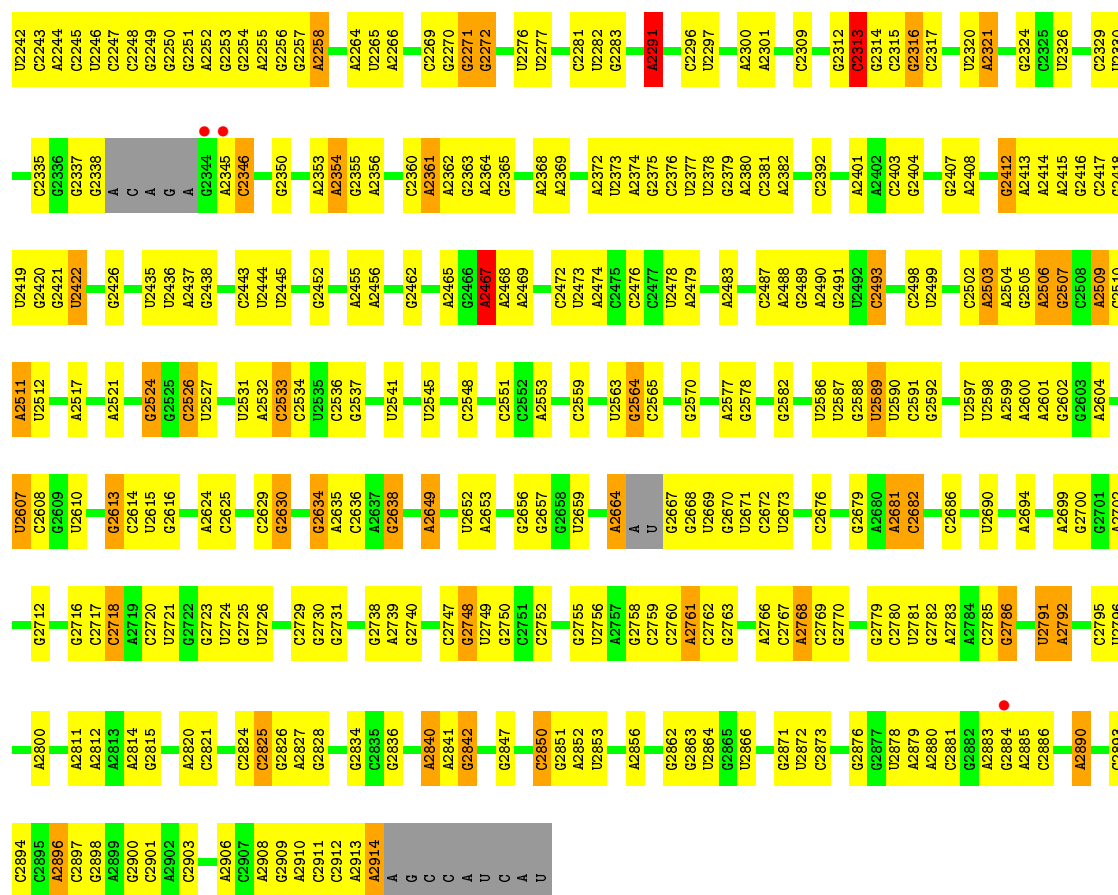
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 23S ribosomal RNA

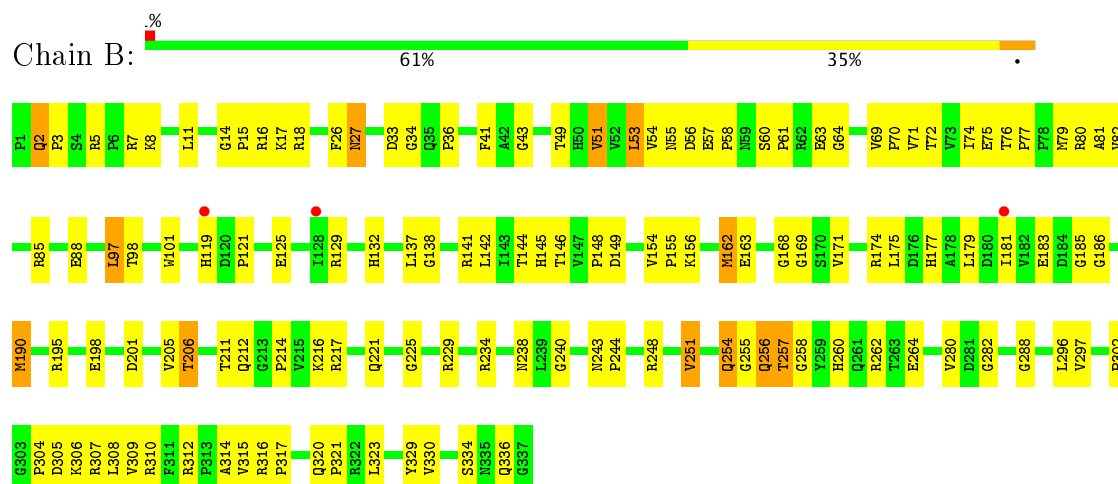




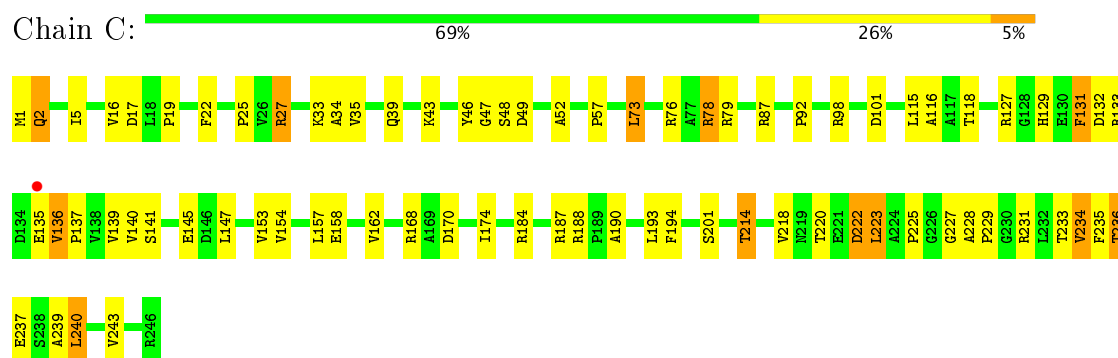
U	A2112	G2001	C1920	U1835	G1752	A1856	U1569	G1497	G1415	G1325	C1229	A1160	C1025	G953
A	G2113	C2002	A1921	A1836	C1753	A1857	A1572	U1500	G1416	A1328	A1230	A1161	G1027	U954
C	U2114	U2003	A1922	A1858	A1759	A1859	A1573	A1501	G1417	A1329	A1231	G1162	U1028	A955
C	U2115	U2004	G1925	A1840	G1765	G1860	C1574	A1502	U1418	A1330	A1232	G1163	U1029	G958
G	U2116	G2005	G1926	A1841	U1766	A1861	U1577	A1503	C1420	A1331	A1233	G1164	A1032	C959
C	C2119	U2008	A1927	C1842	U1767	C1862	C1578	A1504	C1421	U1332	U1234	G1165	C1044	G960
G	U2120	C2009	G1928	A1845	A1768	G1863	C1578	U1505	U1422	U1333	U1235	G1166	G1045	A961
C	C2128	A2010	G1929	U1846	C1769	G1864	C1578	U1506	C1423	C1334	A1236	G1167	C1044	C962
U	A2128	A2011	G1930	G1847	U1770	G1865	A1581	C1507	G1424	G1340	U1237	U1170	G1052	G968
A	U2012	U2012	A1930	G1848	U1770	C1866	C1582	U1508	G1425	G1341	U1237	U1171	G1053	G969
G	C2132	G2013	G1931	U1849	U1771	A1667	C1582	C1509	C1426	C1342	G1239	G1172	G1054	U970
C	U2133	C1936	C1936	A1850	G1772	U1668	G1586	G1512	A1427	C1343	A1242	A1173	G1055	G
G	G2134	U1937	U1937	G1851	G1773	A1669	U1587	G1512	U1432	C1343	A1242	A1173	G1055	G
G	A2135	U1938	U1938	A1852	G1774	G1670	U1587	C1513	G1433	G1344	C1243	A1174	U1056	U
G	G2136	C1939	U1939	C1853	G1774	U1671	G1589	C1514	G1433	U1244	U1244	A1175	A1057	U
C	A	C2029	C1940	G1854	G1777	G1672	C1592	A1515	A1434	U1350	C1245	G1176	A1058	U
C	C	G2033	A1941	C1855	A1778	G1672	C1592	C1516	U1435	A1352	A1246	G1177	G1059	C
A	U	U2034	C1856	C1856	A1779	C1679	C1593	U1517	C1436	C1353	A1252	G1178	C1060	C
C	U	C2039	A1857	C1857	G1780	G1680	C1594	G1520	U1440	U1266	A1252	U1180	U1066	C
C	G	A2039	G1862	G1862	G1781	G1681	C1594	C1521	G1441	C1263	C1254	U1181	A1067	C
A	U	G2044	G1863	G1863	A1782	A1682	U1596	A1522	A1442	U1359	C1254	C1182	U1067	U
G	C	G2045	G1863	G1863	A1783	G1683	A1597	G1523	G1443	C1360	C1262	C1183	G1072	C
U	C	G2046	G1868	G1868	U1784	A1684	A1598	U1524	G1444	C1361	U1266	C1184	A1078	C
C	C	C	G1949	G1866	G1785	A1685	A1603	G1525	G1445	U1362	U1266	U1185	A1078	G
A	A	A2054	G1950	C1867	G1786	G1866	A1604	G1526	U1446	C1366	C1267	U1186	A1079	A
C	G	U2063	G1951	U1874	U1788	C1867	G1605	A1527	U1447	U1279	C1268	U1187	C1080	G
C	C	U2064	U	C1877	G1789	C1692	A1606	A1528	U1447	C1377	G1269	A1188	A1081	A
A	U	U2065	A	G1878	C1790	A1607	A1607	G1529	C1460	U1380	U1285	A1189	A1086	G
U	U	U2066	C	U1879	U1791	U1702	C1613	A1533	C1451	U1383	C1289	G1190	A1087	G
U	U	C2065	C	C1880	G1795	U1702	G1614	C1534	G1452	U1388	G1290	A1191	A1088	A
G	C	C2066	U	A1881	A1796	A1710	C1614	G1535	G1453	G1389	A1294	A1192	A1088	G
A	A	C2071	U	C1882	A1797	A1711	G1619	C1536	U1454	C1390	U1298	A1193	C1102	U
A	G	G2072	G	U1883	C1798	A1712	C1620	C1537	U1454	C1391	G1298	A1194	C1102	C
U	C	G2073	C	G1884	C1798	G1713	C1620	C1538	G1460	C1395	U1298	G1195	C1102	G
A	A	A2074	C	A1885	C1803	A1717	U1625	U1539	U1461	C1397	A1308	G1196	U109	C
C	U	A2081	C	A1886	A1804	A1717	A1626	U1539	C1462	U1398	G1311	G1197	G1110	C
U	A	G2082	C	U1889	G1805	U1722	A1627	G1543	A1463	U1388	C1289	U1198	U1116	A
C	C	A2083	U	U1890	G1806	G1723	G1627	U1544	A1471	U1389	A1294	C1201	A1117	C
C	U	C2088	G1970	C1894	G1809	U1724	A1630	G1546	U1473	A1390	U1298	A1202	A1118	G999
A	A	A2089	G1971	A1895	G1810	C1725	C1633	C1553	C1474	G1391	G1298	G1203	U1120	C1000
G	G	G2090	U1972	G1896	A1811	G1730	G1634	U1554	C1477	A1392	G1298	C1204	U1130	U1001
U	C	C2091	A1973	C1731	G1812	C1731	U1635	G1555	U1478	C1393	U1306	U1205	U1131	C1004
G	G	G2092	G1974	U1897	G1812	C1731	G1636	G1556	A1479	C1394	U1307	G1212	G1138	A1005
A	A	A2096	C1975	C1818	C1818	A1732	A1637	G1557	C1474	C1395	A1308	G1213	U1137	A1006
U	C	U2097	G1976	G1819	G1819	A1733	A1641	G1558	G1484	C1396	A1308	G1214	G1135	A1007
U	C	U2098	U1977	G1820	G1820	C1734	A1642	C1559	A1485	C1397	G1311	G1215	U1009	C1008
G	A	A2101	G1978	A1821	A1821	C1735	A1642	U1559	U1485	G1398	G1311	G1216	U1136	U1009
C	C	G2102	G1979	A1822	A1822	U1741	C1643	U	G1489	A1399	G1312	G1217	G1137	C1010
U	U	A2103	U1980	G1823	G1823	A1742	C1644	U1561	C1400	C1399	A1312	G1218	U1138	A1013
C	A	C2104	A1910	C1824	C1824	A1742	U1645	C1562	G1490	C1400	U1307	G1219	G1139	A1014
G	C	C2105	U1992	U1825	U1825	G1743	U1645	G1563	G1491	G1401	G1315	G1219	C1140	C1015
C	A	C2106	U1915	G1744	G1744	G1744	G1649	C1564	A1492	A1406	G1316	G1216	C1156	U1016
C	C	G2110	C1916	G1745	G1745	G1745	C1650	C1565	A1493	A1407	A1321	G1217	C1157	U1016
A	A	G2111	U1917	A1746	A1746	A1746	U1654	C1566	A1494	U1408	G1322	U1218	G1158	G1024
G	G	G2112	U1918	A1747	A1747	A1747	U1655	G1568	A1495	A1414	A1414	U1219	G1159	C1025
U	G	G2113	A1919	A1748	A1748	A1748	G1655	G1568	A1496	A1414	A1414	U1219	G1159	C1025



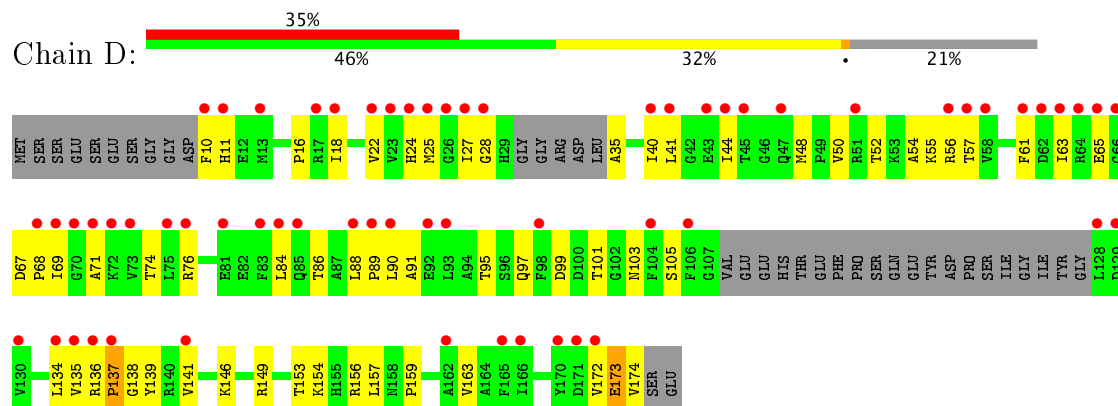
- Molecule 4: 50S ribosomal protein L3P



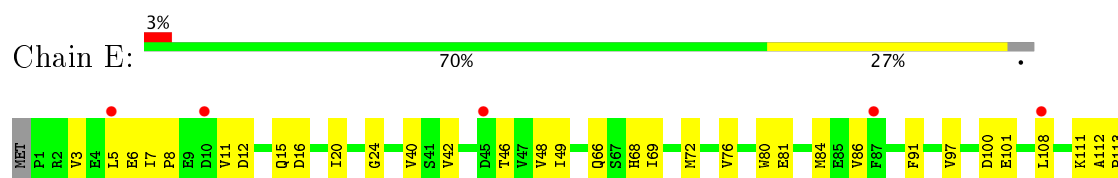
- Molecule 5: 50S ribosomal protein L4P



- Molecule 6: 50S ribosomal protein L5P

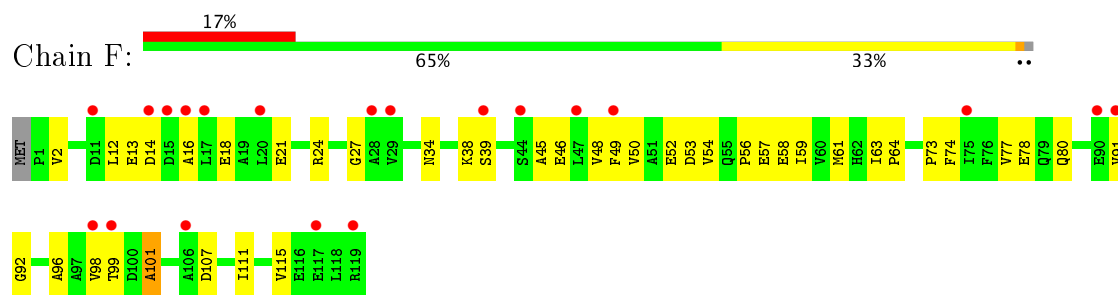


- Molecule 7: 50S ribosomal protein L6P

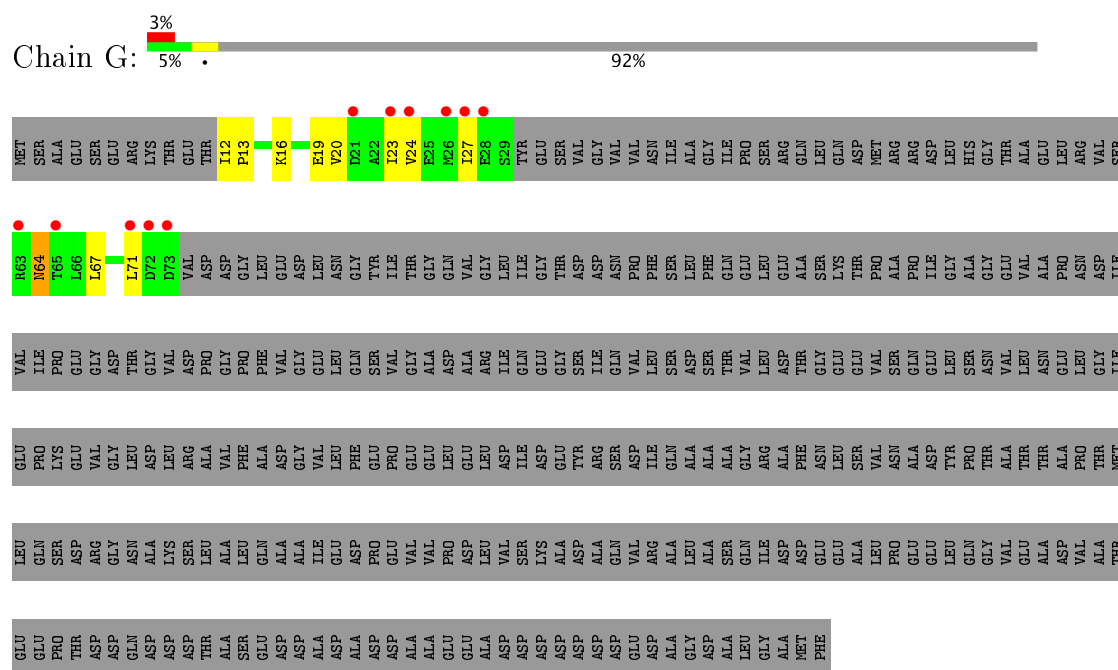




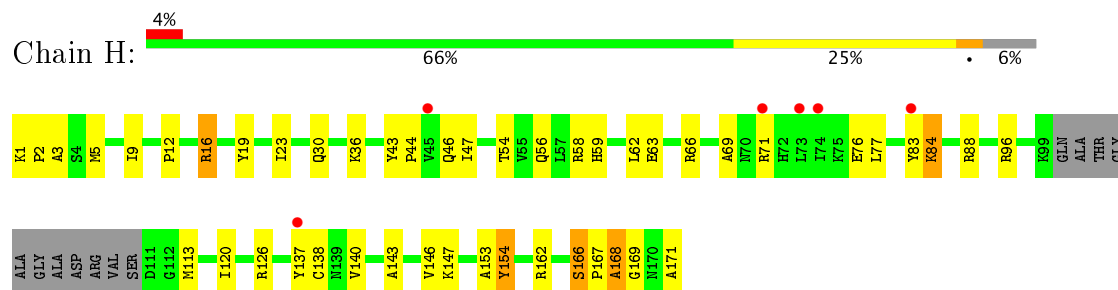
- Molecule 8: 50S ribosomal protein L7Ae



- Molecule 9: 50S ribosomal protein L10E

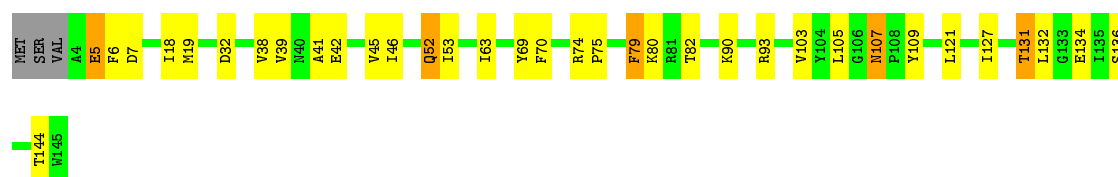


- Molecule 10: 50S ribosomal protein L10e

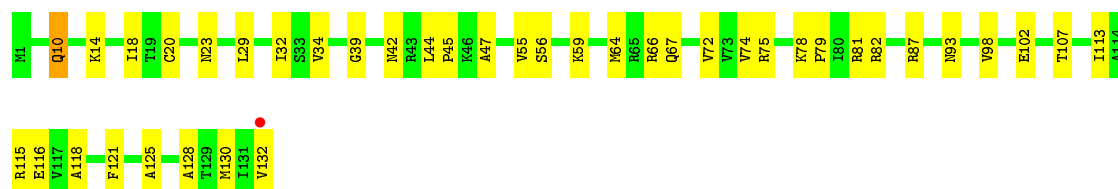


- Molecule 11: 50S ribosomal protein L13P

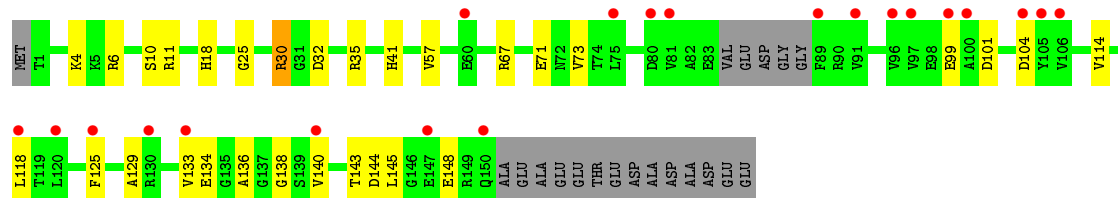




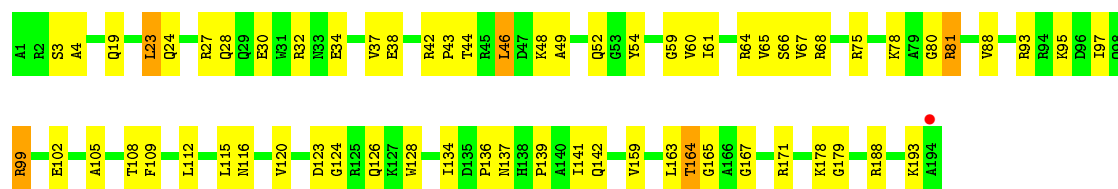
- Molecule 12: 50S ribosomal protein L14P



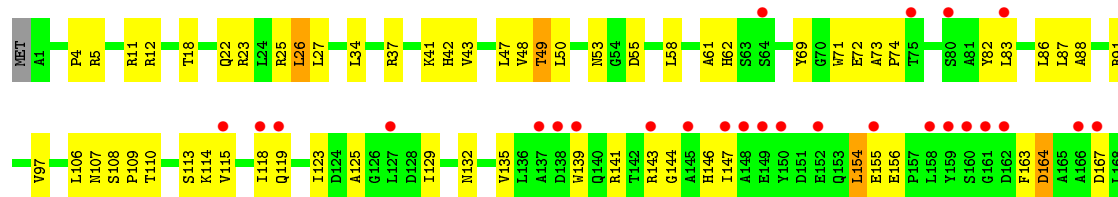
- Molecule 13: 50S ribosomal protein L15P



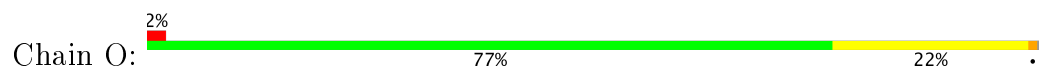
- Molecule 14: 50S ribosomal protein L15e



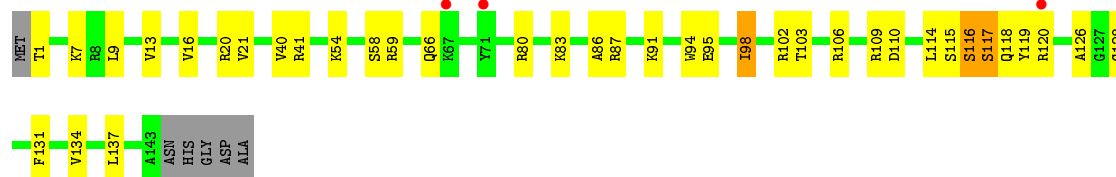
- Molecule 15: 50S ribosomal protein L18P



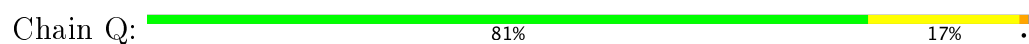
- Molecule 16: 50S ribosomal protein L18e



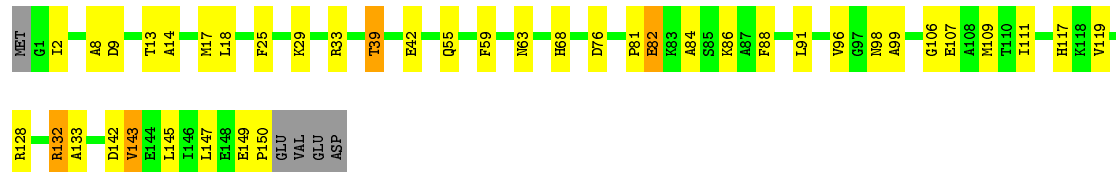
- Molecule 17: 50S ribosomal protein L19e



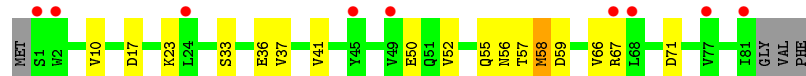
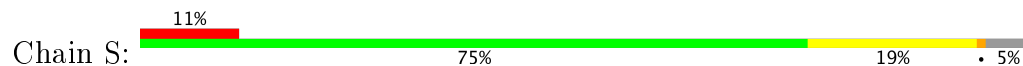
- Molecule 18: 50S ribosomal protein L21e



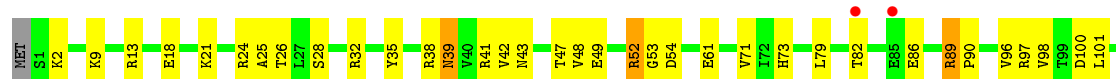
- Molecule 19: 50S ribosomal protein L22P

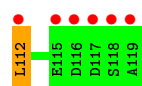


- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

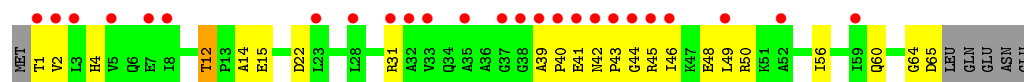




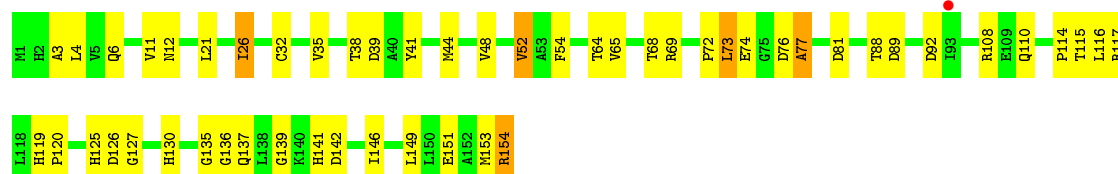
- Molecule 22: 50S ribosomal protein L24e



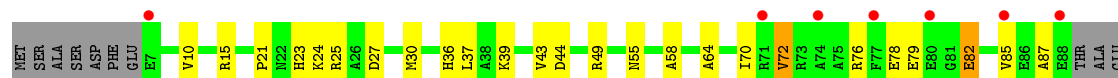
- Molecule 23: 50S ribosomal protein L29P



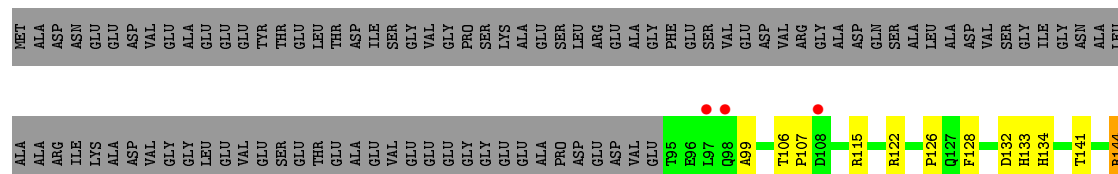
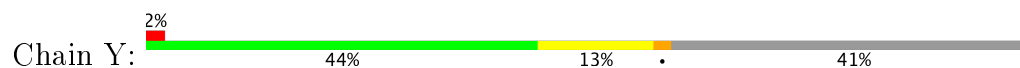
- Molecule 24: 50S ribosomal protein L30P



- Molecule 25: 50S ribosomal protein L31e



- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.08Å 300.60Å 575.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 85.94 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.36-2.70) 90.7 (85.94-2.41)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.248 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	4912 reflections (1.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, OMG, GIR, CL, NA, K, CD, OMU, UR3, 1MA, PSU

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	0	0.40	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.68	0/4528
3	A	0.36	0/1786	0.66	0/2408
4	B	0.33	0/2690	0.65	0/3652
5	C	0.39	0/1884	0.69	1/2551 (0.0%)
6	D	0.33	0/1111	0.55	0/1498
7	E	0.33	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.30	0/241	0.47	0/324
10	H	0.35	0/1287	0.66	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.38	0/1130	0.67	0/1509
14	M	0.38	0/1584	0.64	0/2119
15	N	0.33	0/1474	0.64	0/1999
16	O	0.35	0/874	0.59	0/1181
17	P	0.36	0/1147	0.55	0/1528
18	Q	0.36	0/749	0.70	0/1005
19	R	0.38	0/1172	0.65	0/1578
20	S	0.34	0/648	0.59	0/875
21	T	0.35	0/958	0.64	1/1289 (0.1%)
22	U	0.37	0/417	0.55	0/562
23	V	0.35	0/502	0.57	0/675
24	W	0.38	0/1219	0.64	0/1655
25	X	0.35	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.54	0/590	0.66	0/787
28	1	0.39	0/437	0.63	0/578
29	2	0.39	0/401	0.54	0/529
30	3	0.39	0/771	0.59	0/1024
31	I	0.33	0/526	0.55	0/716
All	All	0.39	0/98692	0.67	16/147577 (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	0	0	52

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1878	G	N9-C1'-C2'	-6.83	104.49	112.00
1	0	1979	G	C2'-C3'-O3'	6.63	124.31	113.70
1	0	1504	A	C1'-O4'-C4'	-6.20	104.94	109.90
1	0	1559	A	C2'-C3'-O3'	5.63	122.71	113.70
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10
1	0	2467	A	C1'-O4'-C4'	-5.54	105.47	109.90
1	0	2291	A	N9-C1'-C2'	5.51	121.16	114.00
1	0	1592	G	N9-C1'-C2'	5.51	121.16	114.00
1	0	871	G	C5'-C4'-O4'	-5.35	102.69	109.10
1	0	1118	A	N9-C1'-C2'	-5.33	106.13	112.00
1	0	1829	A	N9-C1'-C2'	-5.29	106.18	112.00
1	0	1819	G	C5'-C4'-C3'	5.28	124.44	116.00
5	C	73	LEU	CA-CB-CG	-5.16	103.44	115.30
1	0	841	A	C1'-O4'-C4'	-5.15	105.78	109.90
21	T	52	ARG	N-CA-C	5.05	124.63	111.00
1	0	206	G	C5'-C4'-C3'	-5.01	107.98	116.00

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1316	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1376	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1681	G	Sidechain
1	0	1744	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	2101	A	Sidechain
1	0	214	U	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2524	G	Sidechain
1	0	2526	C	Sidechain
1	0	2551	C	Sidechain
1	0	2564	G	Sidechain
1	0	2597	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	332	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	458	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	686	A	Sidechain
1	0	791	A	Sidechain
1	0	857	A	Sidechain
1	0	888	U	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	1361	0
2	9	2600	0	1326	97	0
3	A	1753	0	1766	74	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	70	0
6	D	1094	0	1085	45	0
7	E	1357	0	1266	33	0
8	F	890	0	843	36	0
9	G	240	0	231	10	0
10	H	1266	0	1268	41	0
11	J	1120	0	1098	41	0
12	K	992	0	1031	38	0
13	L	1118	0	1076	24	0
14	M	1560	0	1568	55	0
15	N	1445	0	1401	64	0
16	O	865	0	873	21	0
17	P	1136	0	1123	35	0
18	Q	735	0	729	13	0
19	R	1149	0	1122	40	0
20	S	641	0	605	12	0
21	T	950	0	923	38	0
22	U	410	0	364	17	0
23	V	499	0	511	20	0
24	W	1196	0	1137	54	0
25	X	654	0	653	23	0
26	Y	1130	0	1133	37	0
27	Z	579	0	540	46	0
28	1	430	0	426	20	0
29	2	396	0	413	25	0
30	3	755	0	729	27	0
31	I	519	0	500	27	0
32	0	12	0	10	0	0
33	0	107	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	4	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	4	0
36	L	1	0	0	0	0
36	M	1	0	0	2	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5893	0	0	185	0
38	1	56	0	0	1	0
38	2	40	0	0	3	0
38	3	66	0	0	5	0
38	9	145	0	0	9	0
38	A	118	0	0	10	0
38	B	147	0	0	15	0
38	C	163	0	0	14	0
38	D	48	0	0	8	0
38	E	46	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	23	0	0	3	0
38	G	19	0	0	0	0
38	H	69	0	0	6	0
38	I	4	0	0	1	0
38	J	58	0	0	4	0
38	K	58	0	0	4	0
38	L	81	0	0	8	0
38	M	115	0	0	5	0
38	N	58	0	0	5	0
38	O	44	0	0	6	0
38	P	61	0	0	1	0
38	Q	55	0	0	4	0
38	R	81	0	0	4	0
38	S	37	0	0	0	0
38	T	39	0	0	3	0
38	U	28	0	0	2	0
38	V	11	0	0	3	0
38	W	70	0	0	5	0
38	X	26	0	0	2	0
38	Y	99	0	0	10	0
38	Z	32	0	0	5	0
All	All	99016	0	59909	2306	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 15.

All (2306) 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)
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.29	1.15
1:0:871:G:H8	1:0:871:G:H5'	1.06	1.12
1:0:656:G:H5'	16:O:3:THR:HG22	1.16	1.12
2:9:3056:A:H2'	2:9:3057:A:H5''	1.31	1.10
5:C:236:THR:HG22	5:C:239:ALA:H	1.16	1.09
1:0:1559:A:H1'	38:O:5862:HOH:O	1.50	1.09
1:0:871:G:C8	1:0:871:G:H5'	1.86	1.08
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.69	1.07
1:0:1242:A:H5'	11:J:82:THR:HG23	1.35	1.06
1:0:1160:G:C5'	1:0:1161:A:H5'	1.85	1.06
1:0:282:C:H1'	1:0:368:C:N4	1.72	1.02
1:0:156:C:H5''	14:M:171:ARG:HD3	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:870:G:H2'	1:0:871:G:H5''	1.41	1.01
1:0:1603:A:H5'	1:0:1605:G:O4'	1.61	1.00
1:0:1160:G:H5'	1:0:1161:A:H5'	1.03	1.00
1:0:214:U:H5'	38:0:6131:HOH:O	1.61	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.44	0.99
1:0:1474:C:H6	1:0:1474:C:H5'	1.25	0.99
1:0:1160:G:H5'	1:0:1161:A:C5'	1.92	0.99
2:9:3076:G:H3'	2:9:3077:A:H5''	1.44	0.98
1:0:236:A:H4'	1:0:237:G:H5'	1.46	0.98
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.47	0.97
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.46	0.97
1:0:1118:A:H3'	1:0:1118:A:C8	1.99	0.96
1:0:1118:A:H3'	1:0:1118:A:H8	1.26	0.96
1:0:289:G:H22	1:0:363:A:H2	1.05	0.96
27:Z:41:ASN:HB3	27:Z:60:CYS:SG	2.05	0.95
1:0:1835:U:H5	1:0:1840:A:N7	1.62	0.95
1:0:2812:A:H2	1:0:2814:A:H62	1.14	0.94
1:0:2783:A:H3'	38:0:5224:HOH:O	1.67	0.94
1:0:541:C:H2'	1:0:542:A:H5''	1.48	0.93
1:0:2533:C:H5'	1:0:2533:C:H6	1.32	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.30	0.92
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.50	0.92
1:0:797:A:H4'	27:Z:10:ARG:N	1.85	0.92
17:P:115:SER:H	17:P:118:GLN:HE21	1.03	0.92
1:0:1372:A:H3'	38:0:7168:HOH:O	1.70	0.92
2:9:3006:C:H5''	15:N:37:ARG:HH12	1.30	0.92
1:0:1862:C:H1'	38:0:7198:HOH:O	1.68	0.92
11:J:127:ILE:HG22	36:J:8701:CL:CL	2.07	0.92
12:K:10:GLN:H	12:K:10:GLN:HE21	0.92	0.92
2:9:3054:A:O2'	2:9:3055:U:H5'	1.69	0.91
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.50	0.91
1:0:2506:A:HO2'	1:0:2507:G:H8	0.92	0.91
1:0:381:G:H5''	38:0:4317:HOH:O	1.71	0.90
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.90
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.51	0.90
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.19	0.90
1:0:1666:C:O2'	1:0:1667:A:H5''	1.72	0.90
1:0:182:G:H5'	38:0:5151:HOH:O	1.71	0.90
1:0:1205:U:H2'	1:0:1206:U:C5'	2.02	0.89
1:0:1206:U:H6	1:0:1206:U:H5'	1.37	0.89
1:0:871:G:H8	1:0:871:G:C5'	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.87	0.89
1:0:545:G:H8	1:0:545:G:H5'	1.35	0.89
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.88
1:0:2506:A:O2'	1:0:2507:G:H8	1.57	0.88
1:0:2672:C:H1'	38:B:8833:HOH:O	1.71	0.88
1:0:2850:C:H6	1:0:2850:C:H5'	1.37	0.88
1:0:56:G:H5''	23:V:50:ARG:HH12	1.39	0.87
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.54	0.87
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.16	0.87
2:9:3056:A:C2'	2:9:3057:A:H5''	2.05	0.87
1:0:541:C:C2'	1:0:542:A:H5''	2.05	0.86
1:0:753:U:H3'	38:0:5520:HOH:O	1.75	0.86
1:0:2824:C:H5''	1:0:2825:C:H5'	1.56	0.86
1:0:396:U:H1'	38:0:7600:HOH:O	1.75	0.86
1:0:558:C:O2'	1:0:559:U:H5''	1.75	0.86
1:0:656:G:H5'	16:O:3:THR:CG2	2.01	0.86
1:0:1116:U:HO2'	1:0:1118:A:H2	0.88	0.86
1:0:1450:C:H4'	1:0:1451:C:OP2	1.75	0.86
1:0:1187:U:HO2'	1:0:1189:A:H2	1.19	0.86
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.41	0.86
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.39	0.86
12:K:10:GLN:N	12:K:10:GLN:HE21	1.75	0.85
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.85
12:K:10:GLN:H	12:K:10:GLN:NE2	1.74	0.85
1:0:1184:C:H1'	38:0:7436:HOH:O	1.76	0.85
1:0:1189:A:H1'	1:0:1209:C:O4'	1.77	0.84
1:0:2421:G:H1'	38:0:7002:HOH:O	1.76	0.84
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.58	0.84
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.59	0.84
1:0:1474:C:C6	1:0:1474:C:H5'	2.12	0.84
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.43	0.84
1:0:2570:G:H5''	38:0:4909:HOH:O	1.78	0.83
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.61	0.83
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.58	0.83
1:0:1120:U:H6	1:0:1120:U:H5'	1.41	0.83
1:0:677:C:O2'	1:0:678:G:H5'	1.78	0.83
4:B:238:ASN:HD22	4:B:240:GLY:H	1.25	0.83
22:U:39:ASN:ND2	22:U:44:ARG:HH11	1.76	0.83
27:Z:42:CYS:SG	27:Z:59:TYR:HD2	2.00	0.83
1:0:877:G:H5'	1:0:878:G:OP1	1.79	0.83
36:0:8713:CL:CL	38:0:4680:HOH:O	2.33	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.61	0.83
1:0:282:C:O2'	1:0:283:U:H5'	1.79	0.82
29:2:41:HIS:H	29:2:45:ASN:HD22	1.28	0.82
1:0:1118:A:H62	1:0:1244:U:H3	1.24	0.82
1:0:2502:C:C2'	1:0:2503:A:H5'	2.10	0.82
1:0:2533:C:C6	1:0:2533:C:H5'	2.13	0.82
14:M:59:GLY:HA3	14:M:141:ILE:HD11	1.62	0.82
1:0:2769:C:O2'	1:0:2770:G:H5'	1.80	0.82
1:0:1119:G:N2	1:0:1246:A:C2	2.48	0.81
36:M:8718:CL:CL	38:M:8819:HOH:O	2.34	0.81
5:C:236:THR:HG22	5:C:239:ALA:N	1.96	0.81
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.61	0.81
1:0:1183:C:N4	1:0:1184:C:H41	1.79	0.81
1:0:21:G:H5'	19:R:2:ILE:HA	1.63	0.81
1:0:21:G:C5'	19:R:2:ILE:HA	2.11	0.81
1:0:1205:U:H2'	1:0:1206:U:H5''	1.60	0.81
1:0:2256:G:C2'	1:0:2257:G:H5'	2.11	0.81
27:Z:46:ARG:HD2	27:Z:59:TYR:HB2	1.60	0.81
1:0:870:G:C2'	1:0:871:G:H5''	2.09	0.80
1:0:2291:A:C8	1:0:2309:C:H5'	2.16	0.80
1:0:2251:G:H2'	1:0:2252:A:C8	2.16	0.80
1:0:2502:C:H2'	1:0:2503:A:H5'	1.62	0.80
1:0:1116:U:O2'	1:0:1118:A:H2	1.65	0.80
19:R:39:THR:HG22	19:R:42:GLU:H	1.46	0.80
23:V:2:VAL:HG21	23:V:45:ARG:NH2	1.96	0.80
2:9:3014:G:H8	2:9:3014:G:H5'	1.46	0.80
1:0:1919:A:H4'	38:0:4847:HOH:O	1.83	0.79
2:9:3049:G:O2'	2:9:3050:G:H5'	1.81	0.79
1:0:1771:U:H1'	27:Z:23:ARG:HH21	1.45	0.79
1:0:1603:A:H5''	1:0:1605:G:H5'	1.63	0.79
1:0:188:C:H5''	14:M:163:LEU:HD21	1.63	0.79
1:0:289:G:N2	1:0:363:A:H2	1.81	0.79
1:0:558:C:C2'	1:0:559:U:H5''	2.12	0.79
1:0:558:C:H2'	1:0:559:U:C5'	2.13	0.79
38:0:5215:HOH:O	12:K:39:GLY:HA2	1.82	0.79
1:0:2248:C:H3'	38:0:5439:HOH:O	1.82	0.79
1:0:272:A:H5'	1:0:273:G:OP2	1.83	0.79
36:0:8717:CL:CL	38:Y:8755:HOH:O	2.37	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
1:0:2890:A:H1'	22:U:56:ARG:NH2	1.98	0.78
1:0:199:A:H5''	38:0:3528:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2586:U:H3	1:0:2592:G:H22	1.32	0.78
1:0:2256:G:H2'	1:0:2257:G:H5'	1.65	0.78
3:A:36:ASP:HB2	3:A:83:GLY:HA3	1.65	0.78
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.64	0.78
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.64	0.78
1:0:31:C:H4'	38:0:7398:HOH:O	1.84	0.78
1:0:1835:U:C5	1:0:1840:A:N7	2.49	0.78
1:0:1130:U:H5'	38:0:7642:HOH:O	1.84	0.78
1:0:2001:G:O2'	1:0:2002:C:H5'	1.84	0.78
1:0:541:C:H2'	1:0:542:A:C5'	2.13	0.78
1:0:2491:G:H1'	38:0:6848:HOH:O	1.84	0.77
1:0:69:A:H5'	1:0:69:A:C8	2.20	0.77
1:0:69:A:H5'	1:0:69:A:H8	1.50	0.77
2:9:3058:G:H1'	38:D:3839:HOH:O	1.83	0.77
1:0:1279:U:O2	1:0:1279:U:H2'	1.85	0.77
1:0:603:A:H5''	1:0:604:G:OP1	1.84	0.77
26:Y:174:VAL:HG23	26:Y:177:LYS:HD2	1.67	0.77
1:0:2755:G:H1'	38:0:4679:HOH:O	1.84	0.76
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.76
1:0:2851:G:O2'	1:0:2852:A:H5'	1.85	0.76
5:C:139:VAL:HG13	38:C:8642:HOH:O	1.82	0.76
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.68	0.76
1:0:383:A:H4'	38:0:5323:HOH:O	1.85	0.76
23:V:2:VAL:HG21	23:V:45:ARG:HH21	1.46	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.33	0.76
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.68	0.76
1:0:1537:C:H1'	38:0:6566:HOH:O	1.85	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.76
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.68	0.76
1:0:338:C:H4'	5:C:174:ILE:CD1	2.16	0.76
1:0:1213:C:O2'	1:0:1214:G:H5'	1.84	0.76
1:0:2489:G:H1'	38:0:7254:HOH:O	1.85	0.76
1:0:1398:G:O2'	1:0:1399:A:H5'	1.86	0.75
1:0:2748:G:H2'	38:0:7511:HOH:O	1.85	0.75
1:0:1667:A:C8	1:0:1667:A:H5'	2.19	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.68	0.75
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.68	0.75
1:0:506:G:H22	1:0:509:A:H5'	1.49	0.75
1:0:2679:G:H2'	1:0:2681:A:OP2	1.86	0.75
1:0:2851:G:C2'	1:0:2852:A:H5'	2.17	0.75
30:3:65:THR:HG22	30:3:67:LEU:HG	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.16	0.75
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.69	0.75
24:W:6:GLN:HB2	24:W:26:ILE:CD1	2.17	0.75
1:0:1118:A:C8	1:0:1118:A:C3'	2.65	0.74
1:0:2768:A:H2'	1:0:2769:C:O4'	1.86	0.74
1:0:711:G:H1'	38:0:7076:HOH:O	1.86	0.74
4:B:179:LEU:O	4:B:183:GLU:HG2	1.87	0.74
1:0:2256:G:O2'	1:0:2257:G:H5'	1.88	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.67	0.74
1:0:1080:C:H4'	1:0:1081:A:OP1	1.87	0.74
1:0:292:G:H2'	1:0:358:G:N2	2.03	0.74
1:0:2256:G:H2'	1:0:2257:G:C5'	2.18	0.74
6:D:103:ASN:ND2	6:D:134:LEU:H	1.84	0.74
1:0:1657:A:H2'	1:0:1658:A:C8	2.23	0.74
1:0:1205:U:H2'	1:0:1206:U:H5'	1.68	0.74
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.70	0.74
1:0:1130:U:H2'	1:0:1131:G:O4'	1.87	0.73
1:0:2414:A:H2'	1:0:2415:A:C8	2.23	0.73
19:R:17:MET:SD	38:R:8745:HOH:O	2.46	0.73
1:0:2426:G:H1'	38:0:6084:HOH:O	1.89	0.73
36:J:8701:CL:CL	38:J:8752:HOH:O	2.44	0.73
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.18	0.73
1:0:558:C:H2'	1:0:559:U:H5'	1.71	0.73
2:9:3055:U:H4'	2:9:3056:A:C8	2.23	0.73
1:0:656:G:C5'	16:O:3:THR:HG22	2.08	0.73
24:W:88:THR:HG22	24:W:89:ASP:H	1.54	0.73
2:9:3039:U:H1'	2:9:3044:A:H61	1.51	0.73
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.89	0.73
1:0:661:G:C5	1:0:686:A:C2	2.76	0.72
1:0:281:U:H3'	38:0:7185:HOH:O	1.88	0.72
2:9:3092:G:H2'	2:9:3093:A:C8	2.25	0.72
1:0:797:A:C4'	27:Z:10:ARG:N	2.52	0.72
3:A:121:ALA:O	3:A:124:VAL:HG22	1.90	0.72
1:0:2252:A:C5	1:0:2253:G:H1'	2.25	0.72
11:J:19:MET:HE1	11:J:132:LEU:HD21	1.70	0.72
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.07	0.72
14:M:102:GLU:OE1	14:M:164:THR:HG21	1.89	0.72
1:0:1667:A:H2'	1:0:1668:U:C6	2.25	0.72
1:0:2769:C:C2'	1:0:2770:G:H5'	2.19	0.72
1:0:1168:C:H4'	38:0:5905:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:284:C:H4'	1:0:285:A:O5'	1.90	0.71
1:0:2840:A:OP1	4:B:211:THR:HG23	1.90	0.71
5:C:145:GLU:HG3	38:C:8573:HOH:O	1.90	0.71
1:0:2635:A:O2'	1:0:2636:C:H5'	1.89	0.71
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.54	0.71
1:0:1878:G:H1'	38:0:6112:HOH:O	1.91	0.71
1:0:1441:G:O2'	1:0:1442:A:H5'	1.90	0.71
1:0:1666:C:H2'	1:0:1667:A:H5'	1.72	0.71
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.72	0.71
15:N:144:GLY:O	15:N:147:ILE:HG22	1.91	0.71
1:0:1205:U:C2'	1:0:1206:U:H5''	2.21	0.70
1:0:2488:A:H61	1:0:2534:C:H42	1.36	0.70
1:0:403:C:H3'	38:0:6290:HOH:O	1.90	0.70
2:9:3054:A:HO2'	2:9:3055:U:H5'	1.55	0.70
17:P:115:SER:H	17:P:118:GLN:NE2	1.84	0.70
19:R:25:PHE:CE2	19:R:29:LYS:HE2	2.27	0.70
1:0:1342:C:C2'	1:0:1343:C:H5'	2.21	0.70
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.73	0.70
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.26	0.70
29:2:35:ARG:HB3	38:2:2691:HOH:O	1.92	0.70
38:0:7428:HOH:O	5:C:188:ARG:HD2	1.92	0.70
1:0:2524:G:H21	1:0:2526:C:N4	1.89	0.70
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.26	0.70
1:0:1164:U:H3	1:0:1192:A:H2	1.37	0.70
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.56	0.70
1:0:288:A:H61	1:0:364:C:H42	1.40	0.70
1:0:2320:U:H4'	1:0:2321:A:O4'	1.92	0.69
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.69
1:0:2237:G:H1'	38:0:4851:HOH:O	1.91	0.69
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.52	0.69
1:0:338:C:H4'	5:C:174:ILE:HD11	1.74	0.69
1:0:2827:A:H2'	1:0:2828:G:O4'	1.92	0.69
1:0:2054:A:N3	19:R:128:ARG:NH2	2.40	0.69
21:T:48:VAL:HG11	21:T:96:VAL:HG13	1.74	0.69
1:0:2420:G:O2'	1:0:2421:G:H5'	1.93	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.92	0.69
1:0:1701:A:H5'	38:0:6267:HOH:O	1.92	0.69
1:0:1942:A:H3'	38:0:7323:HOH:O	1.91	0.69
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.58	0.69
17:P:115:SER:N	17:P:118:GLN:HE21	1.86	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:59:ARG:NH2	17:P:66:GLN:HE22	1.90	0.69
1:0:1314:U:H2'	38:0:5871:HOH:O	1.94	0.68
14:M:164:THR:HG22	14:M:167:GLY:H	1.58	0.68
1:0:2716:G:H5''	4:B:206:THR:HG21	1.73	0.68
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.73	0.68
1:0:447:A:OP1	21:T:2:LYS:HG2	1.93	0.68
2:9:3064:C:H2'	2:9:3065:A:H5'	1.76	0.68
2:9:3014:G:C8	2:9:3014:G:H5'	2.28	0.68
38:0:5455:HOH:O	9:G:12:ILE:HA	1.92	0.68
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.09	0.68
1:0:703:G:O2'	1:0:704:C:H5'	1.93	0.68
2:9:3054:A:C2'	2:9:3055:U:H5'	2.24	0.68
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.23	0.68
1:0:1289:C:H3'	38:0:6391:HOH:O	1.93	0.68
1:0:380:A:H2'	38:0:7206:HOH:O	1.92	0.68
38:0:7198:HOH:O	3:A:11:ARG:HA	1.93	0.68
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.42	0.68
1:0:1167:G:H4'	31:I:135:LEU:HD22	1.75	0.68
27:Z:10:ARG:HA	38:Z:8615:HOH:O	1.94	0.68
1:0:1189:A:H1'	1:0:1209:C:C1'	2.24	0.67
1:0:702:G:O2'	1:0:703:G:H5'	1.95	0.67
1:0:2363:G:O2'	18:Q:11:ARG:HG3	1.94	0.67
1:0:156:C:H5''	14:M:171:ARG:CD	2.22	0.67
1:0:1771:U:H1'	27:Z:23:ARG:NH2	2.09	0.67
3:A:51:ARG:HB2	38:A:8801:HOH:O	1.92	0.67
1:0:2505:G:O2'	1:0:2506:A:H5'	1.95	0.67
36:0:8712:CL:CL	38:0:5118:HOH:O	2.49	0.67
1:0:1189:A:O2'	1:0:1208:C:H2'	1.95	0.67
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.94	0.67
1:0:2779:G:H21	7:E:143:GLN:NE2	1.92	0.67
1:0:2896:A:H5''	38:0:6091:HOH:O	1.94	0.67
1:0:544:G:C2'	1:0:545:G:H5''	2.24	0.67
1:0:871:G:C8	1:0:871:G:C5'	2.66	0.67
1:0:272:A:H3'	38:0:7500:HOH:O	1.94	0.67
1:0:558:C:C2'	1:0:559:U:C5'	2.72	0.67
2:9:3055:U:H4'	2:9:3056:A:H8	1.60	0.67
1:0:2533:C:H6	1:0:2533:C:C5'	2.06	0.67
31:I:131:THR:O	31:I:135:LEU:HG	1.94	0.67
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.77	0.66
1:0:1350:U:H4'	38:0:5116:HOH:O	1.93	0.66
4:B:238:ASN:HD22	4:B:240:GLY:N	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2559:C:H4'	38:0:7235:HOH:O	1.95	0.66
1:0:285:A:H2'	1:0:286:U:O4'	1.94	0.66
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.61	0.66
1:0:2269:C:C2'	1:0:2270:G:H5'	2.25	0.66
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.10	0.66
1:0:1524:U:OP1	1:0:1524:U:H4'	1.96	0.66
1:0:1804:A:H2'	1:0:1805:G:C8	2.29	0.66
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.60	0.66
13:L:148:GLU:HA	38:L:8769:HOH:O	1.96	0.66
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.66
1:0:1058:A:H2'	1:0:1060:C:H5''	1.77	0.66
1:0:56:G:H5''	23:V:50:ARG:NH1	2.09	0.66
10:H:169:GLY:HA3	38:H:8589:HOH:O	1.95	0.66
1:0:1187:U:O2'	1:0:1189:A:H2	1.79	0.66
2:9:3064:C:C2'	2:9:3065:A:H5'	2.26	0.66
6:D:99:ASP:HB3	6:D:103:ASN:H	1.61	0.65
6:D:103:ASN:HD22	6:D:134:LEU:H	1.44	0.65
1:0:1205:U:C2'	1:0:1206:U:C5'	2.74	0.65
15:N:113:SER:HB2	38:N:8754:HOH:O	1.95	0.65
1:0:2587:OMU:O3'	1:0:2587:OMU:HM22	1.96	0.65
1:0:447:A:O2'	1:0:448:G:H5'	1.97	0.65
4:B:297:VAL:HB	38:B:8804:HOH:O	1.95	0.65
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.78	0.65
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.79	0.65
1:0:282:C:H1'	1:0:368:C:H41	1.60	0.65
1:0:1187:U:H2'	38:0:6878:HOH:O	1.97	0.65
1:0:1730:G:H5'	1:0:1731:C:C5	2.32	0.65
1:0:2004:U:H4'	38:0:5302:HOH:O	1.96	0.65
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.77	0.65
1:0:1234:U:N3	4:B:244:PRO:HB3	2.11	0.65
5:C:16:VAL:HG12	5:C:17:ASP:H	1.61	0.65
1:0:2269:C:H2'	1:0:2270:G:H5'	1.77	0.65
4:B:51:VAL:CG1	4:B:53:LEU:HD13	2.26	0.65
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.78	0.65
15:N:132:ASN:O	15:N:135:VAL:HG12	1.96	0.65
1:0:560:C:H42	1:0:597:A:H61	1.43	0.65
29:2:39:ARG:HG2	38:2:3143:HOH:O	1.95	0.65
29:2:41:HIS:HD2	29:2:44:ARG:H	1.45	0.65
3:A:8:ARG:HG2	38:A:8751:HOH:O	1.97	0.65
6:D:65:GLU:HA	38:D:6752:HOH:O	1.97	0.65
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1926:G:H2'	1:0:1927:A:H8	1.61	0.65
1:0:2649:A:H5'	1:0:2649:A:H8	1.62	0.65
1:0:644:G:N3	1:0:644:G:H5'	2.11	0.65
27:Z:41:ASN:ND2	27:Z:60:CYS:SG	2.69	0.65
27:Z:27:ALA:HA	38:Z:8615:HOH:O	1.98	0.64
1:0:2248:C:H2'	1:0:2249:G:H8	1.62	0.64
20:S:33:SER:O	20:S:37:VAL:HG23	1.96	0.64
1:0:1528:A:H2'	1:0:1529:G:O4'	1.98	0.64
1:0:2509:A:OP2	1:0:2510:C:H5	1.80	0.64
1:0:450:C:OP1	5:C:184:ARG:NH2	2.30	0.64
1:0:1377:C:H6	1:0:1377:C:H5'	1.63	0.64
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.79	0.64
22:U:47:ARG:HG3	38:U:4381:HOH:O	1.96	0.64
23:V:1:THR:HG23	23:V:2:VAL:H	1.62	0.64
1:0:200:U:H2'	38:0:3441:HOH:O	1.98	0.64
1:0:1603:A:C5'	1:0:1605:G:H5'	2.27	0.64
1:0:1625:U:H4'	38:0:4662:HOH:O	1.97	0.64
1:0:545:G:C8	1:0:545:G:H5'	2.25	0.64
1:0:960:G:H2'	1:0:960:G:N3	2.12	0.64
10:H:166:SER:CB	10:H:167:PRO:HD3	2.27	0.64
13:L:136:ALA:HB3	38:L:8770:HOH:O	1.98	0.64
24:W:88:THR:HB	38:W:6679:HOH:O	1.98	0.64
5:C:132:ASP:HB3	38:C:8561:HOH:O	1.98	0.64
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.80	0.64
24:W:151:GLU:O	24:W:154:ARG:HB3	1.98	0.64
1:0:1120:U:H5'	1:0:1120:U:C6	2.31	0.64
1:0:1557:G:O2'	1:0:1558:C:H5'	1.97	0.64
1:0:1636:G:O2'	1:0:1637:A:H5'	1.97	0.64
1:0:2897:C:O2'	1:0:2898:G:H5'	1.98	0.64
1:0:1462:C:H2'	1:0:1463:A:C8	2.33	0.63
1:0:281:U:O2'	1:0:282:C:H5'	1.98	0.63
1:0:856:G:C8	38:0:5424:HOH:O	2.50	0.63
5:C:236:THR:H	5:C:239:ALA:HB3	1.61	0.63
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.27	0.63
1:0:1118:A:H2'	1:0:1120:U:H5''	1.80	0.63
1:0:2717:C:H2'	1:0:2718:C:C5'	2.25	0.63
2:9:3035:C:H5''	38:9:4078:HOH:O	1.98	0.63
2:9:3114:G:O6	15:N:11:ARG:HD3	1.98	0.63
22:U:52:THR:HG22	22:U:55:ALA:H	1.63	0.63
1:0:2244:A:H1'	38:M:8765:HOH:O	1.97	0.63
1:0:2521:A:OP2	10:H:3:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3003:A:N6	2:9:3022:G:H1'	2.13	0.63
14:M:164:THR:CG2	14:M:167:GLY:H	2.12	0.63
1:0:2850:C:C6	1:0:2850:C:H5'	2.25	0.63
1:0:814:G:H4'	38:0:3125:HOH:O	1.97	0.63
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.79	0.63
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63
1:0:669:G:O2'	1:0:670:G:H5'	1.99	0.63
2:9:3007:G:H5'	38:9:5071:HOH:O	1.98	0.63
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.64	0.63
1:0:475:G:OP1	5:C:73:LEU:HD22	1.98	0.63
2:9:3069:U:OP1	15:N:4:PRO:HG3	1.99	0.63
27:Z:46:ARG:CD	27:Z:59:TYR:HB2	2.29	0.63
1:0:777:U:O2'	28:1:11:LYS:HG2	1.99	0.63
11:J:41:ALA:HB3	38:J:8768:HOH:O	1.99	0.63
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.64	0.63
1:0:1185:U:H5'	38:0:7436:HOH:O	1.99	0.63
1:0:1474:C:C5'	1:0:1474:C:H6	2.07	0.63
1:0:308:U:C4	1:0:342:C:H1'	2.34	0.63
1:0:39:G:N2	1:0:444:C:C2	2.67	0.63
1:0:1593:C:H5'	17:P:116:SER:O	1.98	0.63
5:C:1:MET:HG2	5:C:2:GLN:H	1.63	0.62
1:0:1342:C:O2'	1:0:1343:C:H5'	1.98	0.62
1:0:1166:A:H1'	1:0:1192:A:C2	2.34	0.62
1:0:1450:C:C4'	1:0:1451:C:OP2	2.48	0.62
1:0:1804:A:H2'	1:0:1805:G:H8	1.64	0.62
1:0:657:G:OP1	5:C:27:ARG:NH2	2.30	0.62
1:0:67:A:H5''	1:0:69:A:C8	2.34	0.62
1:0:2629:C:H41	3:A:206:ARG:HH21	1.45	0.62
14:M:66:SER:HB3	14:M:128:TRP:CD1	2.33	0.62
1:0:1741:U:O2'	1:0:2723:G:H4'	1.99	0.62
1:0:185:G:H4'	1:0:186:A:H4'	1.79	0.62
1:0:396:U:O2'	1:0:418:C:H4'	1.99	0.62
4:B:168:GLY:H	4:B:174:ARG:HD3	1.63	0.62
4:B:280:VAL:HG13	4:B:334:SER:HA	1.80	0.62
1:0:1422:U:H2'	1:0:1423:C:H6	1.65	0.62
1:0:1603:A:H5'	1:0:1605:G:C4'	2.30	0.62
1:0:363:A:O2'	1:0:364:C:H5'	1.99	0.62
1:0:814:G:H8	38:0:7188:HOH:O	1.82	0.62
31:I:118:SER:HB2	31:I:123:ASN:HB2	1.82	0.62
1:0:1422:U:H2'	1:0:1423:C:C6	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:96:ALA:HA	38:F:3111:HOH:O	2.00	0.62
9:G:16:LYS:O	9:G:20:VAL:HG23	2.00	0.62
1:0:399:C:H5'	14:M:179:GLY:O	1.99	0.62
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.30	0.62
24:W:64:THR:O	24:W:68:THR:HG22	2.00	0.62
1:0:542:A:H5'	1:0:542:A:C8	2.27	0.62
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.82	0.62
10:H:9:ILE:HG23	10:H:126:ARG:CZ	2.29	0.62
14:M:59:GLY:CA	14:M:141:ILE:HD11	2.30	0.62
25:X:25:ARG:HD3	25:X:64:ALA:O	2.00	0.62
1:0:2681:A:H4'	1:0:2682:C:H5'	1.80	0.61
1:0:338:C:H5''	38:0:3795:HOH:O	2.00	0.61
1:0:349:U:O2'	1:0:350:C:H5'	2.00	0.61
2:9:3047:A:C2	2:9:3048:C:C2	2.88	0.61
1:0:1507:C:H4'	38:0:3600:HOH:O	2.00	0.61
1:0:1926:G:H2'	1:0:1927:A:C8	2.34	0.61
1:0:303:C:O2'	1:0:304:G:H5'	2.01	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.14	0.61
2:9:3061:C:H2'	2:9:3062:A:H8	1.64	0.61
3:A:211:LYS:HB2	38:A:8812:HOH:O	2.00	0.61
1:0:1787:C:H4'	1:0:2883:A:O4'	2.00	0.61
10:H:166:SER:HB2	10:H:167:PRO:CD	2.30	0.61
1:0:1159:G:H1	1:0:1208:C:H42	1.48	0.61
2:9:3107:C:H5	38:9:3167:HOH:O	1.84	0.61
4:B:36:PRO:HA	4:B:168:GLY:HA2	1.83	0.61
13:L:134:GLU:HG3	38:L:8754:HOH:O	2.00	0.61
1:0:2563:U:H2'	1:0:2565:C:O5'	2.01	0.61
1:0:264:G:H1'	1:0:265:U:H5	1.65	0.61
2:9:3042:C:H5'	2:9:3043:G:OP2	2.00	0.61
1:0:1641:A:H2'	1:0:1642:A:H5'	1.83	0.61
1:0:656:G:OP2	16:O:37:ARG:HD2	2.00	0.61
38:0:6854:HOH:O	14:M:178:LYS:HB2	2.00	0.61
1:0:1160:G:O2'	1:0:1190:G:H1'	2.01	0.61
1:0:1525:G:H5'	1:0:1526:A:OP2	2.01	0.61
1:0:2729:C:H2'	1:0:2730:G:H8	1.65	0.61
1:0:2880:A:H2'	1:0:2881:C:H5'	1.83	0.61
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.96	0.61
1:0:1342:C:H2'	1:0:1343:C:H5'	1.83	0.61
1:0:2812:A:C2	1:0:2814:A:N6	2.66	0.61
2:9:3049:G:C2'	2:9:3050:G:H5'	2.31	0.61
1:0:2316:G:H4'	38:0:6084:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:371:U:H2'	1:0:372:A:H8	1.66	0.60
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.83	0.60
1:0:1278:A:H4'	1:0:1279:U:C4	2.36	0.60
1:0:1768:C:C2'	1:0:1769:C:H5'	2.31	0.60
4:B:168:GLY:N	4:B:174:ARG:HD3	2.17	0.60
1:0:553:G:P	26:Y:204:ARG:HH22	2.25	0.60
27:Z:39:CYS:CB	27:Z:57:CYS:SG	2.88	0.60
1:0:2252:A:H2'	1:0:2253:G:H5'	1.84	0.60
1:0:2769:C:H2'	1:0:2770:G:C5'	2.30	0.60
4:B:264:GLU:HG3	4:B:302:PRO:HD3	1.83	0.60
19:R:99:ALA:HB1	19:R:109:MET:CE	2.30	0.60
19:R:14:ALA:HB3	19:R:147:LEU:HB2	1.82	0.60
25:X:25:ARG:HD2	38:X:5356:HOH:O	2.00	0.60
1:0:1167:G:H2'	1:0:1168:C:O4'	2.02	0.60
1:0:2526:C:O2'	1:0:2527:U:H5'	2.01	0.60
1:0:65:C:O2'	1:0:66:G:H5'	2.01	0.60
1:0:21:G:H4'	19:R:2:ILE:HG22	1.83	0.60
4:B:137:LEU:HG	38:B:8776:HOH:O	2.01	0.60
1:0:125:U:H3'	38:0:3762:HOH:O	2.00	0.60
1:0:407:A:H5'	38:0:6019:HOH:O	2.00	0.60
1:0:2365:G:H4'	18:Q:45:PRO:O	2.01	0.60
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.60
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.84	0.60
16:O:42:GLU:HB2	38:O:2176:HOH:O	2.00	0.60
23:V:44:GLY:O	23:V:48:GLU:HG2	2.01	0.60
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.83	0.60
1:0:1132:A:N6	1:0:1229:C:H2'	2.17	0.60
1:0:638:C:H2'	1:0:639:A:C8	2.37	0.60
4:B:248:ARG:O	4:B:251:VAL:HG13	2.02	0.60
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.84	0.60
1:0:1391:G:H2'	1:0:1392:A:H5'	1.84	0.60
1:0:1945:G:O2'	1:0:1946:C:H5'	2.01	0.60
1:0:354:A:H2'	1:0:355:C:H6	1.66	0.60
23:V:64:GLY:O	23:V:65:ASP:HB2	2.02	0.60
38:0:5662:HOH:O	27:Z:17:ARG:HD3	2.02	0.60
1:0:1299:G:O6	13:L:6:ARG:HD3	2.02	0.59
30:3:70:ARG:HD3	38:3:8767:HOH:O	2.02	0.59
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.36	0.59
23:V:39:ALA:N	23:V:40:PRO:HD2	2.17	0.59
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.02	0.59
19:R:9:ASP:O	19:R:13:THR:HB	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1741:U:H5'	1:0:1742:A:OP1	2.03	0.59
1:0:283:U:C5	1:0:284:C:N3	2.71	0.59
1:0:111:C:O2'	28:1:20:ARG:HG2	2.03	0.59
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.59
5:C:22:PHE:HA	5:C:116:ALA:HA	1.83	0.59
1:0:136:C:H2'	1:0:137:U:O4'	2.03	0.59
1:0:1634:G:H3'	38:0:3886:HOH:O	2.01	0.59
1:0:212:A:O4'	1:0:214:U:C6	2.56	0.59
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.67	0.59
1:0:962:C:H1'	15:N:5:ARG:NH1	2.18	0.59
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.37	0.59
1:0:1937:U:O2'	1:0:1938:G:H5'	2.03	0.59
2:9:3028:U:H2'	2:9:3029:C:C6	2.38	0.59
18:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.59
10:H:58:ARG:HG3	10:H:58:ARG:HH11	1.68	0.59
1:0:2416:G:H2'	1:0:2417:C:C6	2.37	0.59
1:0:283:U:H5	1:0:284:C:H42	1.49	0.59
29:2:18:ASN:ND2	29:2:40:ARG:H	2.00	0.59
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.85	0.59
25:X:43:VAL:HG12	25:X:44:ASP:H	1.66	0.59
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.42	0.59
1:0:812:A:H2'	1:0:813:C:C6	2.38	0.59
1:0:1181:A:H5'	31:I:94:GLU:OE2	2.03	0.59
15:N:164:ASP:OD1	15:N:167:ASP:HA	2.03	0.59
1:0:2781:U:C2'	1:0:2782:G:H5'	2.33	0.59
1:0:426:G:H2'	1:0:427:C:O4'	2.02	0.59
6:D:50:VAL:O	6:D:71:ALA:HA	2.03	0.59
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.03	0.59
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.33	0.59
24:W:72:PRO:HG2	24:W:77:ALA:HB3	1.84	0.59
1:0:1211:G:O2'	1:0:1212:C:H5'	2.03	0.59
1:0:1625:U:H3'	1:0:1625:U:C6	2.38	0.59
1:0:1790:C:H2'	1:0:1791:U:H6	1.68	0.59
1:0:2000:G:O2'	1:0:2001:G:H5'	2.03	0.59
1:0:2010:A:H2'	38:0:5952:HOH:O	2.01	0.59
1:0:236:A:C4'	1:0:237:G:H5'	2.26	0.59
1:0:2610:U:H4'	38:B:8726:HOH:O	2.03	0.59
1:0:559:U:C5	1:0:560:C:C5	2.91	0.59
1:0:1625:U:H3'	1:0:1625:U:H6	1.68	0.58
1:0:1834:C:H2'	1:0:1840:A:N6	2.18	0.58
9:G:64:ASN:N	9:G:64:ASN:HD22	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:24:GLN:NE2	14:M:27:ARG:HH11	2.00	0.58
1:0:944:G:H21	24:W:44:MET:CE	2.15	0.58
1:0:1773:G:C8	27:Z:16:ALA:HA	2.38	0.58
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.58
1:0:2135:A:O2'	1:0:2136:G:H5'	2.03	0.58
1:0:902:G:N7	13:L:18:HIS:HD2	2.00	0.58
6:D:25:MET:HE2	6:D:41:LEU:HG	1.85	0.58
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.85	0.58
1:0:2346:C:O2'	6:D:52:THR:HG21	2.03	0.58
1:0:1008:C:H5''	10:H:16:ARG:HH12	1.67	0.58
11:J:127:ILE:CG2	36:J:8701:CL:CL	2.85	0.58
1:0:1400:C:C2'	1:0:1401:G:H5'	2.33	0.58
2:9:3001:U:O3'	2:9:3003:A:H5'	2.03	0.58
14:M:59:GLY:HA3	14:M:141:ILE:CD1	2.34	0.58
1:0:449:A:N7	5:C:43:LYS:HG2	2.18	0.58
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.86	0.58
1:0:1174:A:C5	1:0:1201:C:H4'	2.38	0.58
1:0:1613:C:H2'	1:0:1614:G:O4'	2.03	0.58
1:0:1477:C:H5'	1:0:1868:G:C5'	2.34	0.58
7:E:100:ASP:HB2	38:E:2789:HOH:O	2.04	0.58
1:0:1595:G:O2'	1:0:1596:U:H5'	2.04	0.58
1:0:524:A:H5''	19:R:29:LYS:HD3	1.86	0.58
1:0:635:A:H2'	1:0:636:G:H5''	1.86	0.58
8:F:38:LYS:NZ	14:M:3:SER:HA	2.17	0.58
31:I:113:HIS:NE2	31:I:121:LEU:HD22	2.18	0.58
21:T:86:GLU:HG3	38:T:6653:HOH:O	2.02	0.58
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.68	0.58
1:0:1120:U:H6	1:0:1120:U:C5'	2.16	0.58
1:0:1730:G:C5'	1:0:1731:C:C6	2.87	0.58
1:0:1829:A:N6	27:Z:18:TYR:HA	2.19	0.58
1:0:2300:A:H4'	1:0:2301:A:O5'	2.04	0.58
1:0:821:U:H2'	1:0:822:C:H6	1.68	0.58
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.03	0.58
19:R:111:ILE:HG23	19:R:145:LEU:HD11	1.86	0.58
25:X:78:GLU:HG2	25:X:79:GLU:H	1.68	0.58
1:0:1849:G:H1'	1:0:2011:A:N1	2.19	0.58
3:A:48:ASP:HB3	38:A:8801:HOH:O	2.03	0.58
8:F:91:VAL:HG12	8:F:92:GLY:N	2.19	0.58
1:0:120:A:H2'	1:0:120:A:N3	2.19	0.57
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.85	0.57
8:F:101:ALA:HA	38:F:5413:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:66:ARG:HD3	38:H:8579:HOH:O	2.04	0.57
14:M:64:ARG:HD2	38:M:8778:HOH:O	2.04	0.57
21:T:71:VAL:CG1	21:T:90:PRO:HB3	2.29	0.57
1:0:2649:A:H5'	1:0:2649:A:C8	2.39	0.57
1:0:2781:U:H2'	1:0:2782:G:H5'	1.85	0.57
1:0:820:G:C6	3:A:171:LYS:HB2	2.39	0.57
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.57
5:C:2:GLN:HB3	38:C:8536:HOH:O	2.03	0.57
12:K:23:ASN:HD21	12:K:107:THR:HB	1.68	0.57
19:R:132:ARG:HG2	19:R:133:ALA:N	2.19	0.57
1:0:848:C:H5'	38:0:7251:HOH:O	2.03	0.57
11:J:131:THR:HG22	11:J:134:GLU:H	1.69	0.57
1:0:2472:C:O2'	1:0:2634:G:H4'	2.04	0.57
1:0:297:U:H2'	1:0:298:C:H6	1.69	0.57
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.20	0.57
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.87	0.57
2:9:3057:A:H8	6:D:141:VAL:HG21	1.70	0.57
6:D:57:THR:HG23	6:D:63:ILE:HA	1.86	0.57
10:H:63:GLU:HA	38:H:8579:HOH:O	2.04	0.57
2:9:3001:U:H5''	2:9:3003:A:OP1	2.05	0.57
4:B:162:MET:CE	4:B:308:LEU:HD21	2.35	0.57
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.70	0.57
11:J:5:GLU:HA	38:J:8729:HOH:O	2.04	0.57
1:0:1768:C:H2'	1:0:1769:C:H5'	1.87	0.57
1:0:2667:G:H1'	1:0:2914:A:N3	2.20	0.57
1:0:475:G:H5'	5:C:73:LEU:HD23	1.86	0.57
21:T:47:THR:HB	21:T:100:ASP:HB3	1.86	0.57
26:Y:99:ALA:HB2	26:Y:233:TYR:CE2	2.40	0.57
1:0:1666:C:C2'	1:0:1667:A:C5'	2.83	0.57
1:0:1681:G:H5''	1:0:1682:A:H5'	1.86	0.57
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.57
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.86	0.57
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.57
1:0:1586:G:O2'	1:0:1587:U:H5'	2.04	0.57
1:0:1916:C:O2'	1:0:1917:G:H5'	2.04	0.57
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.86	0.57
1:0:128:A:H3'	1:0:128:A:C8	2.40	0.57
4:B:258:GLY:H	4:B:260:HIS:CE1	2.23	0.57
1:0:1080:C:O5'	1:0:1080:C:H6	1.88	0.56
1:0:2909:G:O2'	1:0:2910:A:H5'	2.05	0.56
1:0:354:A:H2'	1:0:355:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:775:G:OP1	28:1:16:HIS:HE1	1.88	0.56
1:0:820:G:H5'	1:0:821:U:H5'	1.87	0.56
6:D:16:PRO:HG3	6:D:157:LEU:HD11	1.86	0.56
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.69	0.56
26:Y:187:VAL:HB	38:Y:8769:HOH:O	2.04	0.56
1:0:1116:U:O2'	1:0:1118:A:C2	2.48	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
2:9:3045:A:H2'	2:9:3046:C:H6	1.70	0.56
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.39	0.56
17:P:7:LYS:HD3	17:P:21:VAL:CG2	2.35	0.56
1:0:1135:G:H5'	38:0:5924:HOH:O	2.04	0.56
1:0:2768:A:O2'	1:0:2769:C:H5'	2.05	0.56
1:0:2851:G:H2'	1:0:2852:A:H5'	1.86	0.56
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.86	0.56
14:M:164:THR:HG22	14:M:167:GLY:N	2.20	0.56
21:T:48:VAL:HG11	21:T:96:VAL:CG1	2.35	0.56
38:0:7009:HOH:O	3:A:211:LYS:HG3	2.05	0.56
4:B:168:GLY:HA3	4:B:174:ARG:HB3	1.87	0.56
6:D:25:MET:CE	6:D:41:LEU:HG	2.35	0.56
15:N:49:THR:HB	15:N:58:LEU:HD11	1.85	0.56
1:0:1181:A:H2'	1:0:1182:C:H5'	1.88	0.56
1:0:1909:A:H2'	1:0:1910:A:C8	2.39	0.56
1:0:1925:G:O2'	1:0:1926:G:H5'	2.06	0.56
1:0:2435:U:H1'	38:0:5427:HOH:O	2.06	0.56
1:0:474:C:O2'	5:C:73:LEU:HD21	2.06	0.56
13:L:133:VAL:HA	38:L:8770:HOH:O	2.06	0.56
1:0:1496:G:H5'	1:0:1572:A:H1'	1.88	0.56
1:0:1768:C:H2'	1:0:1769:C:O4'	2.06	0.56
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.87	0.56
1:0:832:U:H2'	1:0:833:G:C8	2.41	0.56
7:E:132:THR:HB	38:E:2227:HOH:O	2.06	0.56
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.21	0.56
31:I:87:THR:HG22	31:I:88:GLY:H	1.70	0.56
18:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.06	0.56
1:0:1992:U:OP2	12:K:66:ARG:HD2	2.06	0.56
1:0:2324:G:H4'	1:0:2418:G:O2'	2.04	0.56
1:0:92:G:H4'	23:V:44:GLY:HA3	1.87	0.56
2:9:3048:C:H4'	15:N:141:ARG:NH2	2.20	0.56
1:0:2083:A:H3'	38:0:7551:HOH:O	2.05	0.56
1:0:2089:A:O2'	1:0:2090:G:H5'	2.06	0.56
1:0:2717:C:O2'	1:0:2718:C:H5"	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:583:G:H2'	1:0:584:U:C6	2.40	0.56
4:B:88:GLU:HB3	4:B:97:LEU:HG	1.87	0.56
9:G:20:VAL:O	9:G:24:VAL:HG23	2.06	0.56
20:S:57:THR:HG22	20:S:59:ASP:H	1.70	0.56
21:T:48:VAL:HG22	21:T:98:VAL:HA	1.87	0.56
1:0:1701:A:H4'	1:0:1702:U:C5'	2.34	0.56
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.88	0.56
2:9:3045:A:C5	2:9:3046:C:C5	2.94	0.56
11:J:75:PRO:HB3	11:J:132:LEU:HB3	1.87	0.56
22:U:17:THR:HG22	22:U:18:GLY:N	2.21	0.56
1:0:538:C:OP2	26:Y:134:HIS:HE1	1.88	0.56
1:0:1730:G:C5'	1:0:1731:C:H6	2.19	0.56
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.56
1:0:793:A:H5''	17:P:83:LYS:HG2	1.88	0.56
1:0:1206:U:C5'	1:0:1206:U:H6	2.14	0.56
1:0:1506:U:H6	1:0:1506:U:H5'	1.70	0.56
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.88	0.56
14:M:80:GLY:O	14:M:81:ARG:HD3	2.05	0.56
1:0:2276:U:H2'	1:0:2277:U:C6	2.41	0.55
1:0:2064:U:H4'	1:0:2653:A:OP1	2.06	0.55
1:0:816:G:H5'	1:0:1598:A:H4'	1.88	0.55
5:C:233:THR:HG22	5:C:234:VAL:N	2.21	0.55
1:0:1213:C:C2'	1:0:1214:G:H5'	2.37	0.55
3:A:55:VAL:HG12	3:A:67:LEU:HD22	1.88	0.55
12:K:14:LYS:CB	12:K:45:PRO:HG2	2.36	0.55
1:0:1555:G:H4'	1:0:1630:A:H2	1.71	0.55
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.55
1:0:2769:C:H2'	1:0:2770:G:H5'	1.88	0.55
5:C:39:GLN:O	5:C:43:LYS:HD3	2.07	0.55
19:R:39:THR:HG23	19:R:107:GLU:O	2.07	0.55
1:0:1086:A:C6	24:W:11:VAL:HG11	2.41	0.55
26:Y:144:ARG:CZ	38:Y:8815:HOH:O	2.54	0.55
1:0:2269:C:H2'	1:0:2270:G:C5'	2.36	0.55
1:0:2421:G:H3'	1:0:2422:U:H5''	1.88	0.55
1:0:2748:G:H5'	38:0:7511:HOH:O	2.07	0.55
1:0:2900:G:H2'	1:0:2901:C:O4'	2.07	0.55
2:9:3095:C:O2'	2:9:3096:C:H5'	2.06	0.55
3:A:65:ARG:O	3:A:66:ARG:HG3	2.07	0.55
1:0:2545:U:OP2	4:B:2:GLN:HG3	2.07	0.55
1:0:263:U:C2	8:F:59:ILE:CD1	2.89	0.55
29:2:41:HIS:CD2	29:2:43:ARG:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.88	0.55
22:U:6:CYS:HB2	22:U:32:CYS:HB3	1.87	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.72	0.55
24:W:125:HIS:HE1	38:W:3071:HOH:O	1.89	0.55
1:0:1730:G:H5''	1:0:1731:C:H6	1.71	0.55
1:0:343:C:O2'	1:0:344:C:H5'	2.06	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
38:0:4358:HOH:O	4:B:225:GLY:HA3	2.05	0.55
4:B:51:VAL:HG22	4:B:330:VAL:HG22	1.89	0.55
1:0:1829:A:H61	27:Z:18:TYR:HD2	1.54	0.55
1:0:731:U:H2'	1:0:732:C:C6	2.42	0.55
27:Z:42:CYS:SG	27:Z:42:CYS:O	2.65	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.55
5:C:79:ARG:O	5:C:87:ARG:HG2	2.07	0.55
2:9:3044:A:O4'	6:D:76:ARG:NE	2.39	0.55
1:0:1209:C:C2	1:0:1210:G:C8	2.95	0.55
1:0:1329:A:N1	36:0:8713:CL:CL	2.77	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.06	0.55
8:F:61:MET:HB3	14:M:19:GLN:OE1	2.07	0.55
1:0:1479:A:H5''	38:0:3736:HOH:O	2.06	0.54
12:K:55:VAL:HG12	12:K:56:SER:N	2.22	0.54
38:0:4617:HOH:O	3:A:6:GLY:HA3	2.06	0.54
38:0:4058:HOH:O	4:B:27:ASN:HB2	2.07	0.54
1:0:2897:C:H2'	1:0:2898:G:H8	1.70	0.54
2:9:3076:G:C3'	2:9:3077:A:H5''	2.30	0.54
6:D:146:LYS:NZ	15:N:107:ASN:HD21	2.06	0.54
1:0:262:A:OP2	8:F:91:VAL:HG11	2.08	0.54
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.89	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.07	0.54
1:0:2488:A:H2	38:0:7254:HOH:O	1.89	0.54
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.54
1:0:960:G:N3	1:0:960:G:C2'	2.70	0.54
30:3:73:GLU:HB3	38:3:8757:HOH:O	2.07	0.54
8:F:14:ASP:O	8:F:18:GLU:HG3	2.07	0.54
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.07	0.54
10:H:171:ALA:HA	38:H:8568:HOH:O	2.07	0.54
13:L:138:GLY:HA3	38:L:8751:HOH:O	2.07	0.54
20:S:57:THR:HG22	20:S:59:ASP:N	2.23	0.54
26:Y:189:ASN:HD22	26:Y:189:ASN:C	2.09	0.54
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1733:A:H4'	4:B:212:GLN:HA	1.89	0.54
24:W:4:LEU:O	24:W:32:CYS:HA	2.07	0.54
1:0:1315:G:H1'	26:Y:211:ALA:HB3	1.89	0.54
27:Z:56:GLN:HA	27:Z:62:TYR:O	2.07	0.54
1:0:1400:C:H1'	38:0:4132:HOH:O	2.08	0.54
1:0:1878:G:O2'	1:0:1879:U:H6	1.90	0.54
1:0:2878:U:H2'	1:0:2879:A:O4'	2.07	0.54
1:0:1174:A:C6	1:0:1201:C:H4'	2.42	0.54
1:0:1343:C:H2'	1:0:1344:G:O5'	2.07	0.54
2:9:3057:A:C8	6:D:141:VAL:HG21	2.43	0.54
11:J:42:GLU:O	11:J:131:THR:HG23	2.08	0.54
21:T:38:ARG:HG3	21:T:38:ARG:HH11	1.73	0.54
24:W:68:THR:HG23	24:W:69:ARG:HG2	1.90	0.54
1:0:960:G:H4'	38:0:7405:HOH:O	2.07	0.54
5:C:236:THR:HA	38:C:8645:HOH:O	2.07	0.54
14:M:65:VAL:HG21	14:M:105:ALA:HB2	1.89	0.54
1:0:1236:A:H2'	1:0:1237:U:O4'	2.08	0.54
1:0:816:G:C6	1:0:817:G:N1	2.76	0.54
1:0:2001:G:C2'	1:0:2002:C:H5'	2.38	0.54
1:0:2467:A:O2'	1:0:2468:A:H2'	2.08	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.90	0.54
1:0:2468:A:H61	30:3:48:ASN:HD21	1.55	0.54
1:0:157:G:H4'	14:M:95:LYS:HE2	1.90	0.53
1:0:1873:G:H3'	38:0:5204:HOH:O	2.09	0.53
1:0:2251:G:H2'	1:0:2252:A:H8	1.68	0.53
1:0:2419:U:H5''	1:0:2420:G:H5'	1.89	0.53
1:0:559:U:H2'	1:0:560:C:O4'	2.08	0.53
1:0:709:G:O2'	16:O:25:VAL:HG12	2.08	0.53
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.53
4:B:36:PRO:HA	4:B:168:GLY:CA	2.37	0.53
4:B:54:VAL:HB	38:B:8812:HOH:O	2.08	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.40	0.53
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.37	0.53
24:W:125:HIS:HD2	24:W:127:GLY:H	1.56	0.53
27:Z:41:ASN:CB	27:Z:60:CYS:SG	2.88	0.53
1:0:1016:U:H1'	38:0:3654:HOH:O	2.08	0.53
1:0:1168:C:H1'	38:0:7388:HOH:O	2.09	0.53
1:0:1521:C:H2'	1:0:1522:A:H8	1.73	0.53
1:0:1921:A:C6	1:0:1922:A:C2	2.95	0.53
1:0:2768:A:H3'	38:0:4423:HOH:O	2.07	0.53
28:1:25:LYS:HG3	29:2:49:GLU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:27:ASN:H	4:B:27:ASN:HD22	1.57	0.53
1:0:1119:G:H8	11:J:52:GLN:HE22	1.56	0.53
1:0:2507:G:H2'	1:0:2510:C:H42	1.73	0.53
2:9:3031:C:H2'	2:9:3032:G:O4'	2.07	0.53
3:A:199:HIS:HD2	3:A:201:PHE:H	1.55	0.53
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.91	0.53
24:W:139:GLY:O	24:W:141:HIS:HD2	1.91	0.53
24:W:65:VAL:HG12	24:W:116:LEU:HD13	1.90	0.53
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.09	0.53
1:0:2502:C:H2'	1:0:2503:A:C5'	2.37	0.53
1:0:284:C:C6	1:0:284:C:OP2	2.62	0.53
1:0:544:G:H2'	1:0:545:G:C5'	2.38	0.53
1:0:711:G:C2	1:0:718:C:C2	2.97	0.53
5:C:153:VAL:O	5:C:157:LEU:HG	2.08	0.53
9:G:19:GLU:O	9:G:23:ILE:HG13	2.08	0.53
1:0:155:C:OP2	14:M:188:ARG:HD3	2.08	0.53
16:O:88:LYS:HB3	38:O:7061:HOH:O	2.07	0.53
17:P:9:LEU:O	17:P:13:VAL:HG12	2.08	0.53
21:T:101:LEU:HD13	21:T:112:LEU:HD11	1.90	0.53
1:0:1471:A:H2'	1:0:1472:C:C6	2.43	0.53
1:0:1782:G:O2'	1:0:1783:A:H5'	2.09	0.53
1:0:407:A:H2'	1:0:408:A:C8	2.43	0.53
12:K:32:ILE:HD11	12:K:56:SER:HB2	1.91	0.53
16:O:73:ASP:HA	16:O:92:VAL:O	2.08	0.53
1:0:1641:A:C2'	1:0:1642:A:H5'	2.39	0.53
1:0:2248:C:H2'	1:0:2249:G:C8	2.42	0.53
1:0:371:U:H2'	1:0:372:A:C8	2.42	0.53
1:0:47:G:N3	1:0:114:A:C2	2.77	0.53
17:P:134:VAL:O	17:P:137:LEU:HB3	2.09	0.53
1:0:1505:U:H6	1:0:1505:U:H5'	1.73	0.53
1:0:1603:A:C5'	1:0:1605:G:O4'	2.48	0.53
1:0:281:U:H2'	1:0:282:C:O4'	2.08	0.53
1:0:602:A:O2'	1:0:605:C:H4'	2.09	0.53
29:2:20:ARG:HD3	38:2:5444:HOH:O	2.08	0.53
19:R:33:ARG:NH2	38:R:8729:HOH:O	2.41	0.53
27:Z:39:CYS:SG	27:Z:40:PRO:N	2.82	0.53
1:0:2613:G:O2'	1:0:2614:C:H5'	2.09	0.53
1:0:2712:G:H5'	38:0:5215:HOH:O	2.09	0.53
1:0:2271:G:H5'	38:0:4749:HOH:O	2.09	0.53
1:0:810:G:H2'	1:0:811:C:C6	2.44	0.53
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:57:GLU:O	8:F:61:MET:HG3	2.09	0.53
11:J:107:ASN:C	11:J:107:ASN:HD22	2.12	0.53
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.41	0.53
21:T:48:VAL:CG1	21:T:96:VAL:HG13	2.39	0.53
1:0:1588:G:C6	1:0:1589:G:N1	2.77	0.53
1:0:1759:A:N3	1:0:1818:C:H2'	2.24	0.53
1:0:353:G:H2'	1:0:354:A:C8	2.44	0.53
1:0:451:C:O2'	1:0:452:G:H5'	2.09	0.53
1:0:512:G:O3'	1:0:513:A:H8	1.92	0.53
2:9:3034:A:H2'	2:9:3035:C:O4'	2.09	0.53
3:A:94:LEU:N	3:A:94:LEU:HD23	2.24	0.53
13:L:143:THR:HG22	13:L:144:ASP:N	2.24	0.53
1:0:746:A:C6	16:O:65:LEU:HD13	2.44	0.53
1:0:1118:A:N6	1:0:1244:U:H3	2.01	0.52
1:0:1279:U:C2'	1:0:1279:U:O2	2.56	0.52
1:0:2045:G:H2'	1:0:2046:G:O4'	2.09	0.52
1:0:661:G:C4	1:0:686:A:C2	2.97	0.52
4:B:305:ASP:O	4:B:306:LYS:HB2	2.10	0.52
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.91	0.52
1:0:944:G:H21	24:W:44:MET:HE2	1.73	0.52
1:0:1903:U:O2'	1:0:1904:A:C8	2.61	0.52
1:0:2690:U:O2'	7:E:111:LYS:HE3	2.08	0.52
4:B:16:ARG:NH1	38:B:8816:HOH:O	2.41	0.52
1:0:2720:C:O2	12:K:87:ARG:NH2	2.41	0.52
1:0:1544:U:H2'	1:0:1545:C:H6	1.74	0.52
1:0:567:U:H5''	38:W:5817:HOH:O	2.09	0.52
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.39	0.52
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.91	0.52
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.91	0.52
1:0:1166:A:N3	1:0:1166:A:H2'	2.25	0.52
1:0:138:U:OP2	1:0:139:C:H5	1.93	0.52
1:0:1592:G:O2'	1:0:1593:C:O4'	2.28	0.52
1:0:1702:U:H5'	38:0:3423:HOH:O	2.08	0.52
1:0:1730:G:H5'	1:0:1731:C:H5	1.75	0.52
1:0:1916:C:N4	1:0:1917:G:C6	2.77	0.52
1:0:2254:G:O2'	1:0:2255:A:H5'	2.08	0.52
1:0:2421:G:H3'	1:0:2422:U:C5'	2.39	0.52
1:0:2758:G:H2'	1:0:2759:C:C6	2.45	0.52
1:0:299:U:C2	1:0:300:C:C6	2.98	0.52
6:D:135:VAL:HG22	6:D:136:ARG:H	1.74	0.52
38:0:4228:HOH:O	19:R:17:MET:HE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:39:ASN:HD21	22:U:44:ARG:HH11	1.55	0.52
1:0:2265:U:H2'	1:0:2266:A:C8	2.45	0.52
1:0:31:C:H2'	38:0:7659:HOH:O	2.09	0.52
1:0:42:C:H1'	38:0:4672:HOH:O	2.10	0.52
1:0:714:U:H3'	38:0:6924:HOH:O	2.10	0.52
2:9:3002:U:OP2	2:9:3003:A:H5'	2.10	0.52
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.91	0.52
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.91	0.52
4:B:17:LYS:O	4:B:260:HIS:HD2	1.91	0.52
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.44	0.52
15:N:114:LYS:O	15:N:118:ILE:HG13	2.09	0.52
25:X:76:ARG:NH1	25:X:76:ARG:HG3	2.18	0.52
1:0:1087:G:H4'	1:0:1088:A:OP1	2.10	0.52
1:0:1200:A:H2'	38:0:5753:HOH:O	2.09	0.52
1:0:1252:A:H2'	1:0:1253:C:O4'	2.10	0.52
1:0:1400:C:H2'	1:0:1401:G:H5'	1.90	0.52
1:0:1625:U:C3'	1:0:1625:U:C6	2.93	0.52
1:0:232:A:H4'	38:0:6075:HOH:O	2.10	0.52
1:0:2360:C:H1'	38:0:3525:HOH:O	2.09	0.52
1:0:318:C:H5	38:0:3720:HOH:O	1.92	0.52
7:E:11:VAL:HG12	7:E:12:ASP:N	2.25	0.52
1:0:1180:U:H2'	1:0:1181:A:O4'	2.09	0.52
1:0:1562:C:H3'	1:0:1563:G:C8	2.44	0.52
1:0:2667:G:N3	1:0:2827:A:H2	2.07	0.52
1:0:558:C:H2'	1:0:559:U:H5''	1.79	0.52
1:0:694:A:H2'	1:0:695:C:H5'	1.91	0.52
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.58	0.52
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.52
2:9:3044:A:H1'	6:D:76:ARG:NH2	2.24	0.52
10:H:120:ILE:HD12	10:H:120:ILE:N	2.25	0.52
24:W:81:ASP:OD1	24:W:92:ASP:HB2	2.09	0.52
1:0:1644:C:C2	1:0:1645:U:C6	2.98	0.52
1:0:332:G:O2'	1:0:333:G:H5'	2.10	0.52
1:0:958:G:O2'	1:0:959:C:H5'	2.10	0.52
29:2:18:ASN:HD21	29:2:40:ARG:H	1.58	0.52
21:T:61:GLU:HG2	38:T:3851:HOH:O	2.08	0.52
1:0:1167:G:O2'	1:0:1168:C:H5'	2.09	0.52
1:0:11:A:H5'	1:0:12:U:OP2	2.09	0.52
1:0:1568:G:O2'	1:0:1569:U:H5'	2.10	0.52
1:0:2436:U:H5'	30:3:68:LYS:HE2	1.92	0.52
1:0:2064:U:H5'	1:0:2652:U:H4'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2699:A:H2'	1:0:2700:G:O4'	2.10	0.52
1:0:282:C:O2'	1:0:283:U:C5'	2.53	0.52
1:0:695:C:O2'	1:0:696:C:H5'	2.10	0.52
4:B:320:GLN:HE21	4:B:321:PRO:CD	2.23	0.52
14:M:123:ASP:OD1	14:M:126:GLN:HG2	2.10	0.52
19:R:33:ARG:NH1	38:R:8741:HOH:O	2.39	0.52
1:0:1497:G:H4'	1:0:1627:G:O2'	2.11	0.52
1:0:1666:C:C2'	1:0:1667:A:H5''	2.39	0.52
1:0:1825:U:O2'	1:0:1826:C:H5'	2.10	0.52
1:0:1890:U:H4'	1:0:2010:A:C6	2.45	0.52
1:0:2702:A:H2	38:E:2401:HOH:O	1.92	0.52
3:A:36:ASP:OD2	3:A:85:SER:HB2	2.10	0.52
7:E:8:PRO:HB2	7:E:11:VAL:HG23	1.92	0.52
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.13	0.52
24:W:88:THR:HG22	24:W:89:ASP:N	2.22	0.52
38:0:6265:HOH:O	27:Z:49:ARG:HD3	2.10	0.52
1:0:1644:C:H2'	1:0:1645:U:H6	1.74	0.51
1:0:166:A:N7	13:L:25:GLY:HA2	2.25	0.51
1:0:1940:C:H1'	38:0:7323:HOH:O	2.11	0.51
1:0:2281:C:C2'	1:0:2282:U:H5'	2.39	0.51
1:0:2588:OMG:H3'	1:0:2589:U:H5''	1.92	0.51
1:0:2781:U:H2'	1:0:2782:G:C5'	2.39	0.51
1:0:87:C:H2'	29:2:28:LYS:O	2.10	0.51
6:D:101:THR:O	6:D:157:LEU:HB3	2.10	0.51
8:F:56:PRO:HG2	14:M:44:THR:HA	1.92	0.51
1:0:1242:A:C5'	11:J:82:THR:HG23	2.25	0.51
20:S:50:GLU:HB3	20:S:67:ARG:HH21	1.74	0.51
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.43	0.51
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.11	0.51
1:0:2134:G:C6	1:0:2258:A:C8	2.97	0.51
1:0:64:G:H2'	1:0:65:C:O4'	2.11	0.51
1:0:681:G:N3	1:0:681:G:H5'	2.25	0.51
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.93	0.51
1:0:1477:C:H5'	1:0:1868:G:H5''	1.92	0.51
1:0:1878:G:O2'	1:0:1879:U:P	2.69	0.51
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.51
1:0:2252:A:C2'	1:0:2253:G:H5'	2.40	0.51
1:0:2730:G:O2'	1:0:2731:G:H5'	2.11	0.51
1:0:2781:U:O2'	1:0:2782:G:H5'	2.09	0.51
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.44	0.51
38:0:7333:HOH:O	3:A:177:HIS:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:GLY:O	3:A:36:ASP:HB3	2.10	0.51
4:B:177:HIS:O	4:B:181:ILE:HG13	2.11	0.51
6:D:154:LYS:HD2	6:D:154:LYS:H	1.76	0.51
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.91	0.51
13:L:125:PHE:CE1	13:L:140:VAL:HG13	2.45	0.51
18:Q:14:LEU:HB3	38:Q:3971:HOH:O	2.09	0.51
1:0:1496:G:H1	1:0:1509:C:H42	1.57	0.51
1:0:195:C:H2'	1:0:196:G:H5'	1.93	0.51
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.76	0.51
23:V:42:ASN:HB3	38:V:7247:HOH:O	2.10	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.51
1:0:1778:A:H2'	1:0:1779:A:H5'	1.92	0.51
1:0:2249:G:C2	1:0:2253:G:C6	2.98	0.51
1:0:2739:A:C4	1:0:2740:G:C8	2.99	0.51
1:0:920:C:H5'	1:0:921:G:C4	2.46	0.51
10:H:36:LYS:HA	10:H:84:LYS:NZ	2.25	0.51
1:0:1165:G:O2'	1:0:1174:A:H1'	2.10	0.51
1:0:1819:G:H5'	38:0:4709:HOH:O	2.10	0.51
2:9:3001:U:H4'	2:9:3003:A:OP1	2.11	0.51
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.92	0.51
11:J:19:MET:CE	11:J:132:LEU:HD11	2.41	0.51
11:J:45:VAL:HG11	11:J:121:LEU:HD22	1.91	0.51
1:0:1711:A:O2'	1:0:1712:A:H5'	2.10	0.51
1:0:1916:C:C5	1:0:1917:G:N7	2.79	0.51
1:0:1973:A:H8	1:0:1973:A:H5'	1.76	0.51
1:0:2256:G:C2'	1:0:2257:G:C5'	2.83	0.51
1:0:2312:G:H2'	1:0:2313:C:H5'	1.93	0.51
1:0:2598:U:O2	1:0:2600:A:H8	1.94	0.51
2:9:3039:U:C2'	2:9:3040:C:OP1	2.59	0.51
2:9:3043:G:H5'	38:9:1987:HOH:O	2.09	0.51
3:A:36:ASP:HB2	3:A:83:GLY:CA	2.38	0.51
15:N:115:VAL:HG23	38:N:8754:HOH:O	2.11	0.51
1:0:2404:G:OP1	18:Q:68:GLY:HA3	2.11	0.51
23:V:1:THR:HG23	23:V:2:VAL:HG23	1.92	0.51
1:0:1060:C:H6	1:0:1060:C:H5'	1.76	0.51
1:0:1515:A:O2'	1:0:1516:C:H5'	2.11	0.51
1:0:1523:G:H2'	1:0:1524:U:C6	2.45	0.51
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.11	0.51
1:0:2768:A:H5''	38:0:4423:HOH:O	2.11	0.51
1:0:553:G:H2'	1:0:554:G:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:702:G:HO2'	1:0:703:G:H5'	1.76	0.51
5:C:16:VAL:HG12	5:C:17:ASP:N	2.24	0.51
5:C:49:ASP:HB3	5:C:52:ALA:HB2	1.92	0.51
21:T:28:SER:O	21:T:32:ARG:HG3	2.10	0.51
1:0:1517:U:C2	1:0:1670:G:N2	2.79	0.51
1:0:1803:C:H2'	1:0:1804:A:C8	2.46	0.51
1:0:1936:C:H2'	1:0:1937:U:H6	1.75	0.51
1:0:2002:C:H2'	1:0:2003:U:H5'	1.92	0.51
1:0:2010:A:C2'	38:0:5952:HOH:O	2.58	0.51
1:0:2883:A:H2'	1:0:2884:G:O4'	2.11	0.51
1:0:319:A:H4'	1:0:338:C:C5	2.46	0.51
1:0:396:U:OP2	30:3:38:ARG:HD2	2.09	0.51
1:0:567:U:C5'	38:W:5817:HOH:O	2.59	0.51
2:9:3074:G:H1	2:9:3107:C:H42	1.57	0.51
3:A:57:ALA:HA	3:A:67:LEU:HD23	1.93	0.51
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.93	0.51
11:J:74:ARG:NH1	11:J:144:THR:HG21	2.26	0.51
13:L:145:LEU:O	13:L:148:GLU:HG3	2.11	0.51
14:M:60:VAL:C	14:M:61:ILE:HD12	2.32	0.51
23:V:56:ILE:O	23:V:60:GLN:HG3	2.11	0.51
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.11	0.51
1:0:417:G:P	38:0:7393:HOH:O	2.68	0.51
1:0:571:C:H6	1:0:571:C:O5'	1.94	0.51
1:0:2629:C:N4	3:A:206:ARG:HH21	2.09	0.51
31:I:125:ALA:O	31:I:129:VAL:HG23	2.11	0.51
22:U:46:ALA:HA	38:U:3805:HOH:O	2.10	0.51
26:Y:216:ARG:HD2	38:Y:8768:HOH:O	2.10	0.51
1:0:1181:A:H2'	1:0:1182:C:C5'	2.41	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.41	0.50
1:0:2054:A:C2	19:R:128:ARG:NH2	2.79	0.50
1:0:2509:A:H2'	1:0:2510:C:O4'	2.11	0.50
1:0:2769:C:H2'	1:0:2770:G:O4'	2.11	0.50
1:0:696:C:O2'	1:0:697:G:H5'	2.11	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.11	0.50
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.47	0.50
6:D:18:ILE:HD13	6:D:84:LEU:HD12	1.93	0.50
14:M:115:LEU:HD13	14:M:116:ASN:HB2	1.92	0.50
17:P:20:ARG:NH1	17:P:54:LYS:HD3	2.25	0.50
25:X:30:MET:HE1	25:X:55:ASN:HA	1.93	0.50
27:Z:60:CYS:SG	27:Z:62:TYR:HB2	2.51	0.50
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2039:A:H4'	1:0:2760:C:O2'	2.12	0.50
24:W:130:HIS:O	24:W:136:GLY:HA3	2.11	0.50
30:3:62:THR:HB	38:3:8747:HOH:O	2.10	0.50
2:9:3002:U:OP2	2:9:3002:U:H4'	2.11	0.50
38:0:9690:HOH:O	4:B:254:GLN:HG3	2.10	0.50
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.92	0.50
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.93	0.50
1:0:1119:G:H8	11:J:52:GLN:NE2	2.08	0.50
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.41	0.50
24:W:4:LEU:CD2	24:W:54:PHE:HB3	2.39	0.50
1:0:1503:U:H2'	1:0:1504:A:O4'	2.11	0.50
1:0:1765:G:H1'	1:0:1780:G:N2	2.27	0.50
1:0:2681:A:H4'	1:0:2682:C:C5'	2.40	0.50
1:0:2786:G:H2'	38:0:7166:HOH:O	2.11	0.50
1:0:821:U:H2'	1:0:822:C:C6	2.47	0.50
2:9:3028:U:H3'	2:9:3029:C:C6	2.46	0.50
8:F:38:LYS:HZ1	14:M:3:SER:HA	1.76	0.50
12:K:132:VAL:HG11	22:U:22:VAL:HG22	1.93	0.50
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.46	0.50
1:0:500:G:H21	19:R:98:ASN:HD21	1.59	0.50
38:K:7438:HOH:O	22:U:20:MET:HE1	2.10	0.50
1:0:1209:C:H2'	1:0:1210:G:H8	1.76	0.50
1:0:290:C:O2'	1:0:291:C:H5'	2.12	0.50
1:0:858:U:H2'	1:0:859:C:H6	1.76	0.50
2:9:3012:C:H5'	2:9:3070:U:O4'	2.11	0.50
4:B:43:GLY:HA3	4:B:76:THR:HG22	1.93	0.50
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.80	0.50
14:M:30:GLU:O	14:M:34:GLU:HG3	2.11	0.50
15:N:72:GLU:HB3	15:N:163:PHE:CE1	2.47	0.50
1:0:2065:C:O2'	1:0:2066:C:H5'	2.12	0.50
1:0:2505:G:C2'	1:0:2506:A:H5'	2.42	0.50
1:0:661:G:C6	1:0:686:A:C2	2.99	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.93	0.50
2:9:3036:C:C5	2:9:3037:C:C5	3.00	0.50
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.94	0.50
5:C:118:THR:O	5:C:136:VAL:HG13	2.11	0.50
5:C:5:ILE:HG12	38:C:8627:HOH:O	2.11	0.50
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.50
11:J:107:ASN:HD22	11:J:109:TYR:H	1.59	0.50
23:V:4:HIS:HB3	38:V:6622:HOH:O	2.12	0.50
24:W:139:GLY:O	24:W:141:HIS:CD2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:43:VAL:HG12	25:X:44:ASP:N	2.26	0.50
1:0:1882:C:O2'	1:0:2012:U:OP2	2.30	0.50
1:0:2452:G:H1'	38:0:5984:HOH:O	2.12	0.50
1:0:299:U:H2'	1:0:300:C:H6	1.76	0.50
1:0:346:U:H4'	38:0:6822:HOH:O	2.12	0.50
1:0:581:G:O2'	1:0:582:C:H5'	2.12	0.50
1:0:657:G:H2'	1:0:658:C:C6	2.46	0.50
1:0:877:G:C5'	1:0:878:G:OP1	2.56	0.50
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.93	0.50
10:H:167:PRO:O	10:H:168:ALA:HB2	2.12	0.50
1:0:1535:G:H2'	1:0:1536:C:C6	2.47	0.50
1:0:1687:C:O2	28:1:9:GLY:HA2	2.12	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:1811:A:C2	1:0:2752:C:H1'	2.47	0.50
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.50
1:0:105:G:O2'	1:0:106:A:H5'	2.12	0.49
1:0:1494:A:C4	1:0:1495:C:C5	3.00	0.49
1:0:2264:A:H2'	1:0:2265:U:C6	2.47	0.49
28:1:10:LYS:HG3	38:1:2979:HOH:O	2.11	0.49
38:0:9072:HOH:O	4:B:214:PRO:HD2	2.11	0.49
11:J:52:GLN:HG3	11:J:53:ILE:N	2.27	0.49
16:O:39:THR:O	16:O:115:ARG:NH2	2.45	0.49
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.93	0.49
1:0:1185:U:O2'	1:0:1186:C:H5'	2.12	0.49
1:0:1942:A:O2'	1:0:1943:C:H5'	2.12	0.49
1:0:2896:A:N3	1:0:2896:A:H2'	2.28	0.49
1:0:35:U:H5'	5:C:47:GLY:O	2.12	0.49
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.93	0.49
7:E:101:GLU:HB3	7:E:117:THR:HA	1.94	0.49
26:Y:212:ARG:HD2	38:Y:8803:HOH:O	2.12	0.49
1:0:1181:A:C2'	1:0:1182:C:H5'	2.42	0.49
1:0:1201:C:H5''	38:0:6139:HOH:O	2.12	0.49
1:0:1268:C:O2'	1:0:1269:G:H5'	2.12	0.49
1:0:1396:C:H1'	17:P:1:THR:O	2.12	0.49
1:0:1930:A:H2'	1:0:1931:A:C8	2.47	0.49
1:0:2241:C:O2'	1:0:2242:U:H5'	2.13	0.49
1:0:2533:C:C6	1:0:2533:C:C5'	2.90	0.49
1:0:255:A:H2'	1:0:256:C:O4'	2.11	0.49
1:0:553:G:O4'	1:0:1325:G:H5'	2.12	0.49
1:0:699:C:C2	1:0:744:G:C2	3.00	0.49
20:S:56:ASN:O	29:2:8:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3003:A:OP2	2:9:3025:G:N2	2.44	0.49
12:K:115:ARG:HG3	12:K:116:GLU:N	2.26	0.49
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.92	0.49
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.95	0.49
1:0:121:U:OP2	29:2:10:ARG:NH2	2.43	0.49
1:0:1432:U:H5'	38:0:9190:HOH:O	2.12	0.49
1:0:1903:U:O2'	1:0:1904:A:N7	2.45	0.49
1:0:2766:A:O2'	1:0:2767:C:H5'	2.13	0.49
1:0:583:G:H2'	1:0:584:U:H6	1.75	0.49
2:9:3045:A:C4	2:9:3046:C:C6	2.99	0.49
5:C:140:VAL:HB	38:C:8645:HOH:O	2.11	0.49
7:E:80:TRP:O	7:E:134:SER:HA	2.12	0.49
1:0:113:A:OP2	1:0:114:A:H2'	2.12	0.49
1:0:1183:C:N4	1:0:1184:C:N4	2.56	0.49
1:0:1626:A:H2'	1:0:1627:G:H5'	1.94	0.49
1:0:1664:A:H8	1:0:1664:A:OP1	1.95	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.43	0.49
1:0:39:G:C2	1:0:444:C:N3	2.80	0.49
1:0:876:A:N3	1:0:876:A:H2'	2.27	0.49
3:A:68:ILE:HG13	38:A:8782:HOH:O	2.12	0.49
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.94	0.49
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.35	0.49
27:Z:46:ARG:O	27:Z:57:CYS:HA	2.13	0.49
1:0:88:G:H5'	1:0:88:G:H8	1.77	0.49
1:0:1874:U:OP1	3:A:51:ARG:HD2	2.13	0.49
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.28	0.49
31:I:123:ASN:HA	31:I:126:LYS:HD2	1.94	0.49
25:X:10:VAL:HG11	25:X:36:HIS:HE1	1.76	0.49
1:0:1400:C:O2'	1:0:1401:G:H5'	2.12	0.49
1:0:1771:U:O2	27:Z:19:GLY:HA2	2.12	0.49
1:0:832:U:H2'	1:0:833:G:H8	1.76	0.49
1:0:2436:U:C5'	30:3:68:LYS:HE2	2.42	0.49
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.45	0.49
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.94	0.49
1:0:275:G:N2	1:0:376:C:C2	2.81	0.49
1:0:275:G:C2	1:0:376:C:N3	2.80	0.49
4:B:125:GLU:O	4:B:129:ARG:HG3	2.13	0.49
1:0:2826:G:C6	1:0:2913:A:N6	2.81	0.49
1:0:431:G:O2'	1:0:432:G:H5'	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
3:A:192:VAL:HB	38:A:8790:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:254:GLN:HG2	4:B:255:GLY:N	2.27	0.49
20:S:57:THR:C	20:S:59:ASP:H	2.16	0.49
1:0:1186:C:N4	1:0:1187:U:C4	2.80	0.49
1:0:222:A:H2'	1:0:223:G:O4'	2.12	0.49
1:0:2314:G:C2'	1:0:2315:C:H5'	2.43	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.13	0.49
1:0:506:G:N2	1:0:509:A:H5'	2.24	0.49
1:0:660:A:H4'	1:0:661:G:O5'	2.13	0.49
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.95	0.49
1:0:475:G:H5'	5:C:73:LEU:CD2	2.42	0.49
1:0:119:A:H2'	1:0:120:A:H5''	1.95	0.48
1:0:2346:C:O5'	1:0:2346:C:H6	1.96	0.48
1:0:302:A:O2'	1:0:303:C:H5'	2.12	0.48
1:0:834:G:H4'	1:0:835:U:OP2	2.13	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.48
1:0:1380:U:H5'	38:0:9209:HOH:O	2.13	0.48
1:0:1925:G:H5'	30:3:29:ARG:HH12	1.78	0.48
1:0:2071:C:H5'	38:0:9520:HOH:O	2.13	0.48
1:0:2578:G:C8	1:0:2578:G:H5'	2.45	0.48
1:0:462:A:C8	29:2:37:HIS:CE1	3.01	0.48
3:A:109:GLU:HG2	3:A:116:GLY:N	2.28	0.48
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.25	0.48
6:D:25:MET:HE1	6:D:40:ILE:HG13	1.95	0.48
38:9:3472:HOH:O	15:N:41:LYS:HD3	2.14	0.48
17:P:115:SER:OG	17:P:118:GLN:HG3	2.13	0.48
1:0:1188:A:C6	1:0:1189:A:C6	3.01	0.48
1:0:152:A:H2'	1:0:153:C:C6	2.48	0.48
1:0:1829:A:H5''	38:0:3074:HOH:O	2.13	0.48
1:0:922:A:N7	1:0:2281:C:H5'	2.28	0.48
1:0:2824:C:C5'	1:0:2825:C:H5'	2.37	0.48
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.95	0.48
4:B:79:MET:CE	4:B:144:THR:HG21	2.43	0.48
7:E:149:GLU:HG3	7:E:167:TYR:HA	1.94	0.48
8:F:107:ASP:O	8:F:111:ILE:HG13	2.13	0.48
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.42	0.48
14:M:49:ALA:C	14:M:54:TYR:HB3	2.33	0.48
15:N:154:LEU:O	15:N:155:GLU:HB3	2.13	0.48
21:T:25:ALA:CB	21:T:96:VAL:HG12	2.43	0.48
1:0:1184:C:O2'	1:0:1185:U:OP2	2.28	0.48
1:0:790:A:H1'	1:0:1710:A:H2'	1.95	0.48
1:0:1753:C:H4'	38:0:5991:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:C5'	2.43	0.48
1:0:2493:C:O2	1:0:2493:C:H2'	2.12	0.48
1:0:485:A:N3	1:0:487:G:H5''	2.29	0.48
1:0:491:C:O2'	1:0:492:C:H5'	2.13	0.48
3:A:37:VAL:HG22	38:A:8792:HOH:O	2.14	0.48
4:B:85:ARG:NH1	38:B:8833:HOH:O	2.46	0.48
7:E:154:ILE:HD11	7:E:157:LYS:HB2	1.95	0.48
11:J:38:VAL:HB	11:J:103:VAL:HG22	1.95	0.48
24:W:88:THR:HG23	24:W:110:GLN:NE2	2.29	0.48
1:0:1311:G:C2	1:0:1312:G:C8	3.01	0.48
1:0:1477:C:O2'	1:0:1478:U:H5'	2.14	0.48
1:0:1537:C:O2'	1:0:1538:C:H5'	2.13	0.48
1:0:2791:U:H1'	1:0:2792:A:H5''	1.94	0.48
1:0:2880:A:C2'	1:0:2881:C:H5'	2.43	0.48
1:0:522:U:O2'	1:0:1366:C:H5'	2.14	0.48
30:3:17:HIS:O	30:3:18:GLN:HG3	2.13	0.48
2:9:3058:G:H3'	2:9:3059:C:C6	2.47	0.48
2:9:3041:C:H4'	6:D:48:MET:HB2	1.96	0.48
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.78	0.48
10:H:77:LEU:HD12	10:H:83:TYR:CD2	2.49	0.48
26:Y:99:ALA:HB2	26:Y:233:TYR:CZ	2.48	0.48
1:0:1936:C:H2'	1:0:1937:U:C6	2.48	0.48
1:0:2504:A:H4'	10:H:71:ARG:NH1	2.28	0.48
1:0:2729:C:H2'	1:0:2730:G:C8	2.47	0.48
1:0:677:C:C2'	1:0:678:G:H5'	2.44	0.48
1:0:858:U:H2'	1:0:859:C:C6	2.48	0.48
1:0:95:A:H5''	1:0:97:G:O4'	2.13	0.48
3:A:99:ILE:O	3:A:131:HIS:HE1	1.97	0.48
4:B:315:VAL:HG23	4:B:316:ARG:HG2	1.95	0.48
4:B:79:MET:HE1	38:B:8825:HOH:O	2.14	0.48
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.94	0.48
1:0:316:A:H5'	21:T:54:ASP:OD2	2.13	0.48
24:W:38:THR:HG22	24:W:39:ASP:N	2.28	0.48
27:Z:42:CYS:SG	27:Z:59:TYR:CD2	2.92	0.48
27:Z:49:ARG:HH21	27:Z:52:THR:HA	1.78	0.48
1:0:1545:C:H2'	1:0:1546:G:O4'	2.13	0.48
1:0:1574:C:H6	1:0:1574:C:O5'	1.96	0.48
1:0:1878:G:H5''	38:0:5160:HOH:O	2.12	0.48
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.79	0.48
1:0:2825:C:H4'	1:0:2826:G:O5'	2.13	0.48
1:0:297:U:H2'	1:0:298:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:69:A:H2'	1:0:70:A:OP2	2.13	0.48
1:0:710:G:O2'	1:0:711:G:H5'	2.13	0.48
1:0:78:G:C6	1:0:79:G:C6	3.02	0.48
4:B:148:PRO:HD2	38:B:8777:HOH:O	2.14	0.48
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.96	0.48
25:X:37:LEU:CD1	25:X:85:VAL:HG21	2.34	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:1596:U:H2'	1:0:1598:A:OP2	2.14	0.48
1:0:1682:A:H5''	38:0:9448:HOH:O	2.12	0.48
28:1:28:HIS:HD2	28:1:30:LYS:H	1.61	0.48
21:T:41:ARG:HG2	21:T:41:ARG:HH11	1.78	0.48
24:W:38:THR:HG22	24:W:39:ASP:H	1.79	0.48
1:0:1672:G:H8	38:0:3113:HOH:O	1.95	0.48
1:0:2281:C:H2'	1:0:2282:U:H5'	1.96	0.48
1:0:319:A:H4'	1:0:338:C:C4	2.49	0.48
1:0:39:G:C2	1:0:444:C:C2	3.02	0.48
30:3:69:TYR:CZ	30:3:80:ARG:HD2	2.49	0.48
31:I:100:LEU:HD23	31:I:104:GLN:OE1	2.14	0.48
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.95	0.48
1:0:306:A:P	21:T:38:ARG:HH21	2.37	0.48
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.14	0.48
1:0:1189:A:H1'	1:0:1209:C:H1'	1.96	0.48
1:0:152:A:O2'	1:0:153:C:H5'	2.14	0.48
1:0:1636:G:C2'	1:0:1637:A:H5'	2.43	0.48
1:0:1789:G:H2'	1:0:1790:C:O5'	2.14	0.48
1:0:1886:A:H61	1:0:2016:U:H3	1.60	0.48
1:0:228:C:H2'	1:0:229:G:H5'	1.96	0.48
1:0:407:A:H3'	38:0:4457:HOH:O	2.13	0.48
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.95	0.48
6:D:135:VAL:HG22	6:D:136:ARG:N	2.28	0.48
38:0:7653:HOH:O	14:M:78:LYS:HD3	2.13	0.48
38:0:4610:HOH:O	16:O:35:LYS:HD3	2.14	0.48
1:0:317:A:OP1	21:T:52:ARG:O	2.31	0.48
1:0:961:A:C6	1:0:1010:C:C5	3.01	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:1244:U:H5	38:J:8744:HOH:O	1.96	0.47
1:0:128:A:C8	1:0:128:A:C3'	2.96	0.47
1:0:1477:C:C5'	1:0:1868:G:H5''	2.44	0.47
1:0:1669:A:H2	38:0:3699:HOH:O	1.97	0.47
1:0:307:G:H3'	1:0:342:C:OP2	2.13	0.47
1:0:441:A:H1'	1:0:442:A:N7	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:559:U:C2'	1:0:560:C:H5'	2.44	0.47
1:0:853:C:H2'	1:0:854:G:O4'	2.14	0.47
1:0:951:A:O2'	1:0:952:G:H5'	2.14	0.47
1:0:968:G:O2'	1:0:969:G:H5'	2.14	0.47
8:F:111:ILE:O	8:F:115:VAL:HG23	2.14	0.47
8:F:21:GLU:O	8:F:24:ARG:HG2	2.14	0.47
38:0:7398:HOH:O	21:T:9:LYS:HB2	2.14	0.47
1:0:1183:C:H42	1:0:1184:C:H41	1.56	0.47
1:0:1565:C:O4'	1:0:2738:G:H1'	2.14	0.47
1:0:1588:G:C6	1:0:1589:G:C6	3.03	0.47
1:0:1909:A:N1	1:0:2128:G:H1'	2.29	0.47
1:0:2238:A:H3'	38:0:6652:HOH:O	2.14	0.47
1:0:2795:C:O2'	1:0:2796:U:H5'	2.14	0.47
1:0:283:U:H5	1:0:284:C:N4	2.11	0.47
1:0:392:U:H4'	14:M:193:LYS:HB3	1.95	0.47
2:9:3028:U:H3'	2:9:3029:C:H6	1.78	0.47
17:P:115:SER:O	17:P:117:SER:N	2.45	0.47
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.47
1:0:1850:U:H2'	1:0:1851:G:H8	1.78	0.47
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.47
1:0:569:A:H5''	1:0:587:A:N1	2.29	0.47
1:0:807:A:H2'	1:0:808:A:O4'	2.15	0.47
28:1:22:CYS:SG	28:1:24:GLU:HB2	2.55	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
13:L:73:VAL:HG11	13:L:118:LEU:HD21	1.97	0.47
17:P:94:TRP:CZ2	17:P:98:ILE:HG13	2.49	0.47
23:V:39:ALA:N	23:V:40:PRO:CD	2.77	0.47
1:0:1182:C:H1'	1:0:1192:A:H8	1.80	0.47
1:0:1419:U:H2'	1:0:1685:A:C2	2.48	0.47
1:0:1594:C:O2'	1:0:1607:A:H4'	2.15	0.47
1:0:307:G:C5	1:0:324:G:C2	3.03	0.47
1:0:696:C:HO2'	1:0:697:G:H5'	1.78	0.47
1:0:734:U:O2'	1:0:737:A:N6	2.47	0.47
2:9:3053:G:O2'	2:9:3054:A:H5'	2.15	0.47
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.44	0.47
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.44	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.29	0.47
8:F:99:THR:HA	38:F:3461:HOH:O	2.15	0.47
24:W:119:HIS:HD2	24:W:120:PRO:O	1.97	0.47
27:Z:42:CYS:C	27:Z:44:GLU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1586:G:C5	1:0:1587:U:C5	3.02	0.47
1:0:1593:C:OP1	17:P:117:SER:HB3	2.14	0.47
1:0:2329:C:O2'	1:0:2330:U:H5'	2.14	0.47
1:0:475:G:C5'	5:C:73:LEU:HD23	2.44	0.47
1:0:470:U:O2'	28:1:16:HIS:HD2	1.97	0.47
30:3:70:ARG:HA	38:3:8767:HOH:O	2.15	0.47
13:L:129:ALA:O	13:L:133:VAL:HG23	2.15	0.47
38:0:9546:HOH:O	24:W:119:HIS:HE1	1.97	0.47
1:0:1032:A:N3	1:0:1032:A:H2'	2.29	0.47
1:0:1577:U:O2'	1:0:1578:C:H5'	2.14	0.47
1:0:1790:C:H2'	1:0:1791:U:C6	2.48	0.47
1:0:236:A:H4'	1:0:237:G:OP1	2.14	0.47
1:0:840:U:H2'	19:R:128:ARG:HH12	1.79	0.47
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.96	0.47
23:V:46:ILE:HA	23:V:49:LEU:HD12	1.96	0.47
26:Y:133:HIS:HD2	38:Y:8782:HOH:O	1.97	0.47
1:0:1209:C:O2	1:0:1210:G:C8	2.68	0.47
1:0:407:A:C2	1:0:408:A:C4	3.03	0.47
1:0:883:U:C2'	1:0:883:U:O2	2.62	0.47
28:1:21:ARG:HD2	28:1:39:PHE:HB2	1.96	0.47
4:B:79:MET:HE3	4:B:144:THR:HG21	1.96	0.47
4:B:72:THR:HB	38:B:8804:HOH:O	2.14	0.47
5:C:236:THR:HG21	38:C:8573:HOH:O	2.15	0.47
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.62	0.47
1:0:1512:G:O2'	1:0:1513:C:H5'	2.15	0.47
1:0:1886:A:H4'	38:Z:8606:HOH:O	2.14	0.47
1:0:603:A:H1'	1:0:605:C:C2	2.49	0.47
1:0:894:A:C2	5:C:87:ARG:NH2	2.83	0.47
28:1:25:LYS:HD2	29:2:49:GLU:H	1.80	0.47
5:C:25:PRO:HG2	38:C:8524:HOH:O	2.15	0.47
6:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.47
31:I:112:LYS:O	31:I:116:LEU:HG	2.15	0.47
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.15	0.47
1:0:111:C:O2'	1:0:112:G:H5'	2.15	0.47
1:0:1352:A:N1	5:C:48:SER:HB3	2.30	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.47
1:0:1925:G:H5''	30:3:29:ARG:HH22	1.80	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.70	0.47
1:0:56:G:N3	1:0:70:A:C2	2.82	0.47
1:0:945:U:H2'	1:0:946:C:C6	2.50	0.47
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:ARG:NE	38:A:8785:HOH:O	2.47	0.47
4:B:41:PHE:HB3	4:B:190:MET:HE3	1.97	0.47
5:C:147:LEU:HA	38:C:8613:HOH:O	2.15	0.47
26:Y:141:THR:HG23	38:Y:8790:HOH:O	2.14	0.47
1:O:1217:G:C6	1:O:1218:U:C4	3.03	0.47
1:O:1373:G:H1'	38:O:6128:HOH:O	2.14	0.47
1:O:146:U:H5	38:O:3305:HOH:O	1.97	0.47
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.12	0.47
38:O:9208:HOH:O	3:A:11:ARG:HD3	2.15	0.47
15:N:22:GLN:HG2	15:N:26:LEU:HD22	1.97	0.47
31:I:87:THR:HG22	31:I:88:GLY:N	2.30	0.47
13:L:30:ARG:NH2	38:L:8722:HOH:O	2.45	0.47
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.44	0.47
24:W:137:GLN:NE2	24:W:141:HIS:HE1	2.01	0.47
1:O:1307:A:H2'	1:O:1308:A:C8	2.50	0.46
1:O:1362:U:H5'	38:O:3261:HOH:O	2.14	0.46
1:O:2415:A:H2'	1:O:2416:G:H5'	1.97	0.46
1:O:2885:A:H2'	1:O:2886:C:C6	2.50	0.46
1:O:886:A:OP2	1:O:2113:G:H5'	2.16	0.46
1:O:330:C:H5	5:C:170:ASP:OD2	1.98	0.46
1:O:263:U:C4	8:F:54:VAL:HG13	2.50	0.46
12:K:64:MET:HA	12:K:67:GLN:HE21	1.80	0.46
19:R:132:ARG:CZ	38:R:8780:HOH:O	2.63	0.46
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.97	0.46
1:O:1014:A:H2'	1:O:1015:C:H5'	1.96	0.46
1:O:106:A:H2'	1:O:107:U:O4'	2.16	0.46
1:O:1589:G:N2	1:O:1605:G:H1'	2.31	0.46
1:O:1855:G:H4'	1:O:1856:C:O5'	2.15	0.46
1:O:1877:G:C6	1:O:1878:G:C6	3.03	0.46
1:O:2506:A:N6	1:O:2511:A:O2'	2.48	0.46
1:O:2893:C:O2'	1:O:2894:C:H5'	2.14	0.46
1:O:46:U:H4'	1:O:47:G:OP2	2.15	0.46
1:O:638:C:H2'	1:O:639:A:H8	1.80	0.46
30:3:69:TYR:CE1	30:3:80:ARG:HD2	2.50	0.46
2:9:3054:A:H5''	38:D:3359:HOH:O	2.15	0.46
2:9:3114:G:H2'	2:9:3115:C:C6	2.51	0.46
5:C:233:THR:HG22	5:C:234:VAL:H	1.80	0.46
31:I:99:ASP:OD1	31:I:138:THR:HB	2.15	0.46
15:N:34:LEU:HD22	15:N:129:ILE:HD13	1.97	0.46
15:N:141:ARG:HG3	15:N:146:HIS:ND1	2.30	0.46
3:A:170:VAL:HG21	27:Z:26:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:138:U:H5''	1:0:139:C:OP2	2.15	0.46
1:0:1527:A:H1'	1:0:1528:A:C8	2.50	0.46
1:0:1753:C:O2	4:B:229:ARG:NH2	2.47	0.46
1:0:1883:U:O2'	1:0:1884:G:H5'	2.15	0.46
1:0:1916:C:H2'	1:0:1917:G:O4'	2.16	0.46
1:0:278:A:H2'	1:0:279:C:O4'	2.15	0.46
1:0:407:A:H8	38:0:4457:HOH:O	1.99	0.46
1:0:69:A:H8	1:0:69:A:C5'	2.22	0.46
1:0:812:A:H2'	1:0:813:C:O4'	2.14	0.46
1:0:819:A:H5''	38:Z:8619:HOH:O	2.16	0.46
2:9:3013:A:O2'	2:9:3014:G:H5''	2.16	0.46
2:9:3091:C:H2'	2:9:3092:G:O4'	2.16	0.46
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.48	0.46
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.16	0.46
4:B:310:ARG:HD2	38:B:8848:HOH:O	2.14	0.46
6:D:54:ALA:HB1	38:D:4069:HOH:O	2.14	0.46
1:0:1299:G:N7	13:L:6:ARG:NH1	2.64	0.46
15:N:154:LEU:C	15:N:156:GLU:H	2.18	0.46
15:N:42:HIS:HB3	15:N:62:HIS:HE1	1.80	0.46
17:P:13:VAL:HG11	17:P:40:VAL:CG1	2.46	0.46
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.46
24:W:11:VAL:O	24:W:12:ASN:HB2	2.16	0.46
24:W:125:HIS:CD2	24:W:127:GLY:H	2.34	0.46
1:0:1218:U:H2'	1:0:1219:U:H6	1.80	0.46
1:0:1850:U:O4'	1:0:1941:A:C2	2.69	0.46
1:0:1916:C:C4	1:0:1917:G:C5	3.03	0.46
1:0:299:U:N3	1:0:300:C:C5	2.83	0.46
1:0:308:U:C4	1:0:342:C:C1'	2.99	0.46
3:A:89:ALA:HB3	38:A:8817:HOH:O	2.15	0.46
7:E:68:HIS:O	7:E:72:MET:HG3	2.14	0.46
14:M:159:VAL:HG12	36:M:8718:CL:CL	2.53	0.46
1:0:1130:U:H2'	1:0:1131:G:C4'	2.44	0.46
1:0:1343:C:C2'	1:0:1344:G:O5'	2.63	0.46
1:0:1562:C:N4	38:0:5862:HOH:O	2.48	0.46
1:0:2862:G:H4'	4:B:336:GLN:O	2.16	0.46
11:J:75:PRO:HD3	11:J:136:SER:OG	2.16	0.46
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.98	0.46
13:L:143:THR:HG22	13:L:144:ASP:H	1.81	0.46
14:M:134:ILE:O	14:M:136:PRO:HD3	2.16	0.46
15:N:71:TRP:HE3	15:N:175:LEU:HD22	1.80	0.46
15:N:47:LEU:HD12	15:N:97:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:35:VAL:HG23	24:W:41:TYR:CD2	2.51	0.46
1:0:1119:G:N2	1:0:1246:A:H2	2.08	0.46
1:0:1414:A:H2'	1:0:1415:G:O4'	2.16	0.46
1:0:134:U:C2	1:0:145:A:C2	3.04	0.46
1:0:1902:G:O2'	1:0:1903:U:H5'	2.15	0.46
1:0:2237:G:O2'	1:0:2238:A:C8	2.68	0.46
1:0:245:C:H2'	1:0:246:G:H5'	1.97	0.46
1:0:396:U:P	30:3:38:ARG:HH11	2.38	0.46
10:H:9:ILE:HD12	10:H:54:THR:HG22	1.98	0.46
1:0:2866:U:C5	22:U:50:GLU:HB2	2.50	0.46
27:Z:39:CYS:HB2	27:Z:57:CYS:SG	2.53	0.46
1:0:1314:U:H5''	1:0:1316:G:O4'	2.16	0.46
1:0:1834:C:H2'	1:0:1840:A:H62	1.81	0.46
1:0:2408:A:H2	38:3:8713:HOH:O	1.98	0.46
1:0:2604:A:H5'	38:0:5788:HOH:O	2.15	0.46
1:0:51:G:O2'	1:0:52:A:H5'	2.16	0.46
2:9:3078:G:H5'	38:9:4932:HOH:O	2.16	0.46
2:9:3081:C:C2'	2:9:3082:U:H5'	2.45	0.46
5:C:19:PRO:HD2	5:C:240:LEU:HD22	1.98	0.46
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.50	0.46
18:Q:94:GLN:O	18:Q:95:GLU:HB2	2.16	0.46
1:0:372:A:H2'	1:0:373:G:C8	2.51	0.46
1:0:423:A:C4	1:0:424:C:C6	3.04	0.46
1:0:657:G:H2'	1:0:658:C:H6	1.79	0.46
28:1:25:LYS:HD2	29:2:49:GLU:N	2.30	0.46
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.50	0.46
5:C:133:ARG:NH2	38:C:8623:HOH:O	2.49	0.46
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.97	0.46
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.46
10:H:2:PRO:HD2	10:H:5:MET:SD	2.56	0.46
17:P:83:LYS:O	17:P:86:ALA:HB3	2.16	0.46
25:X:30:MET:CE	25:X:58:ALA:HB3	2.46	0.46
1:0:1523:G:C6	1:0:1524:U:O4	2.69	0.46
1:0:1634:G:H2'	1:0:1635:U:C6	2.50	0.46
1:0:2246:U:N3	1:0:2256:G:C2	2.84	0.46
1:0:2478:U:O2'	1:0:2479:A:H5'	2.16	0.46
1:0:80:A:H3'	21:T:43:ASN:OD1	2.15	0.46
1:0:776:A:OP1	28:1:28:HIS:HE1	1.99	0.46
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.46
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.15	0.46
9:G:23:ILE:O	9:G:27:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:107:ASN:ND2	11:J:109:TYR:H	2.14	0.46
1:0:2413:A:N7	15:N:109:PRO:HB3	2.31	0.46
15:N:48:VAL:HG12	15:N:49:THR:N	2.30	0.46
17:P:87:ARG:HG2	38:P:181:HOH:O	2.15	0.46
21:T:35:TYR:CG	21:T:112:LEU:HD22	2.51	0.46
21:T:38:ARG:NH1	21:T:38:ARG:HG3	2.31	0.46
21:T:48:VAL:HG13	21:T:97:ARG:O	2.15	0.46
23:V:39:ALA:C	23:V:41:GLU:H	2.19	0.46
1:0:1004:C:H1'	38:0:4835:HOH:O	2.15	0.46
1:0:1594:C:O2'	1:0:1595:G:H5'	2.16	0.46
1:0:185:G:H4'	1:0:186:A:OP1	2.15	0.46
1:0:2320:U:OP2	30:3:1:MET:HA	2.15	0.46
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.46
1:0:2361:A:H5''	38:0:9001:HOH:O	2.16	0.46
1:0:303:C:H2'	1:0:304:G:O4'	2.16	0.46
1:0:786:G:OP1	1:0:1489:G:H4'	2.16	0.46
1:0:820:G:C5	3:A:171:LYS:HB2	2.50	0.46
4:B:119:HIS:O	4:B:121:PRO:HD3	2.15	0.46
8:F:58:GLU:OE1	14:M:27:ARG:NH2	2.46	0.46
8:F:56:PRO:CG	14:M:44:THR:HA	2.46	0.46
1:0:1197:G:N2	38:0:6222:HOH:O	2.48	0.45
1:0:1484:G:H2'	38:0:9098:HOH:O	2.16	0.45
1:0:271:C:C2	1:0:273:G:O4'	2.69	0.45
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.99	0.45
7:E:15:GLN:HB3	7:E:42:VAL:HG23	1.97	0.45
1:0:1163:G:N2	38:0:4723:HOH:O	2.50	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.45
1:0:861:A:H2'	1:0:862:U:C6	2.51	0.45
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.55	0.45
1:0:2716:G:C5'	4:B:206:THR:HG21	2.44	0.45
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.45
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.16	0.45
25:X:43:VAL:HG11	25:X:82:GLU:HA	1.98	0.45
1:0:1160:G:HO2'	1:0:1190:G:H8	1.63	0.45
1:0:1634:G:H2'	1:0:1635:U:H6	1.82	0.45
1:0:1787:C:O2'	1:0:1788:U:H5'	2.16	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
1:0:858:U:C5	38:0:5424:HOH:O	2.56	0.45
1:0:955:A:C2	1:0:1013:A:C4	3.04	0.45
10:H:69:ALA:HB2	10:H:153:ALA:HB2	1.99	0.45
16:O:32:ARG:HB2	38:O:4656:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.32	0.45
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.45	0.45
1:0:1391:G:C2'	1:0:1392:A:H5'	2.46	0.45
1:0:1566:C:O2'	1:0:1567:A:H5'	2.15	0.45
1:0:1568:G:C2'	1:0:1569:U:H5'	2.46	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.43	0.45
1:0:1886:A:N6	1:0:2016:U:H3	2.15	0.45
1:0:1896:G:C6	1:0:1897:U:C4	3.04	0.45
1:0:2002:C:H2'	1:0:2003:U:C5'	2.47	0.45
1:0:2252:A:C6	1:0:2253:G:H1'	2.51	0.45
1:0:2255:A:O2'	1:0:2256:G:H5'	2.17	0.45
1:0:2269:C:O2'	1:0:2270:G:H5'	2.16	0.45
1:0:2506:A:O2'	1:0:2507:G:C8	2.43	0.45
1:0:251:C:O2'	1:0:252:C:H5'	2.15	0.45
1:0:259:G:O2'	1:0:260:C:H5'	2.17	0.45
1:0:2638:G:H1'	38:0:4577:HOH:O	2.17	0.45
1:0:284:C:C4'	1:0:285:A:O5'	2.62	0.45
1:0:289:G:O2'	1:0:290:C:H5'	2.16	0.45
1:0:612:U:H2'	1:0:613:C:C6	2.52	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.52	0.45
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.46	0.45
2:9:3001:U:C4'	2:9:3003:A:OP1	2.64	0.45
10:H:9:ILE:HG12	10:H:56:GLN:HG3	1.98	0.45
10:H:9:ILE:HD12	10:H:54:THR:CG2	2.46	0.45
13:L:10:SER:O	13:L:11:ARG:HB3	2.16	0.45
15:N:110:THR:HB	15:N:113:SER:OG	2.16	0.45
16:O:38:ARG:NH1	38:O:7674:HOH:O	2.46	0.45
24:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.45
26:Y:144:ARG:NH1	38:Y:8776:HOH:O	2.49	0.45
26:Y:184:GLU:OE2	26:Y:204:ARG:HD2	2.17	0.45
1:0:1202:A:H2'	1:0:1203:G:C5'	2.46	0.45
1:0:1299:G:H5'	38:0:4067:HOH:O	2.15	0.45
1:0:1375:A:C2'	1:0:1376:G:H5'	2.46	0.45
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.45
1:0:1842:A:C4	1:0:1979:G:C6	3.04	0.45
1:0:2245:C:H6	1:0:2245:C:O5'	1.99	0.45
1:0:2379:G:H4'	1:0:2380:A:H5'	1.98	0.45
1:0:2656:G:O2'	1:0:2657:G:H5'	2.16	0.45
1:0:2668:G:H2'	1:0:2669:U:C6	2.52	0.45
1:0:2909:G:H2'	1:0:2910:A:C8	2.51	0.45
1:0:423:A:C5	1:0:424:C:C5	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:790:A:H1'	1:0:1710:A:O2'	2.16	0.45
2:9:3027:C:N3	38:9:3445:HOH:O	2.35	0.45
2:9:3061:C:H2'	2:9:3062:A:C8	2.46	0.45
4:B:16:ARG:HB3	4:B:217:ARG:NH2	2.31	0.45
1:0:1168:C:H5''	31:I:88:GLY:H	1.82	0.45
12:K:113:ILE:HD12	12:K:128:ALA:HB2	1.98	0.45
1:0:1185:U:H2'	1:0:1186:C:H6	1.81	0.45
1:0:1377:C:C5'	1:0:1377:C:H6	2.28	0.45
1:0:1434:A:H2'	1:0:1436:C:C5	2.51	0.45
1:0:1588:G:C5	1:0:1589:G:C6	3.05	0.45
1:0:187:A:H3'	1:0:188:C:H6	1.82	0.45
1:0:2630:G:O6	3:A:206:ARG:NH2	2.50	0.45
1:0:2717:C:H5'	4:B:302:PRO:HA	1.98	0.45
1:0:2785:C:H4'	1:0:2786:G:OP2	2.17	0.45
1:0:2872:U:H2'	1:0:2873:C:H6	1.81	0.45
1:0:553:G:C2'	1:0:554:G:H5'	2.46	0.45
2:9:3034:A:O5'	2:9:3034:A:H8	1.99	0.45
2:9:3081:C:O2'	2:9:3082:U:H5'	2.17	0.45
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.99	0.45
17:P:131:PHE:CD1	17:P:137:LEU:HD13	2.51	0.45
1:0:1406:A:H4'	1:0:1407:A:H5''	1.99	0.45
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.45
1:0:1634:G:C6	1:0:1635:U:C4	3.04	0.45
1:0:1667:A:H2'	1:0:1668:U:H6	1.80	0.45
1:0:2382:A:OP1	30:3:80:ARG:HG2	2.16	0.45
1:0:2444:U:C2	1:0:2445:U:C6	3.04	0.45
1:0:539:G:H2'	1:0:540:A:C8	2.51	0.45
38:0:9348:HOH:O	28:1:1:THR:HA	2.17	0.45
4:B:55:ASN:HB3	4:B:64:GLY:H	1.81	0.45
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.86	0.45
10:H:76:GLU:C	10:H:77:LEU:HD23	2.37	0.45
21:T:79:LEU:HG	21:T:89:ARG:HB2	1.99	0.45
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.98	0.45
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.45
1:0:1665:G:H2'	1:0:1666:C:H6	1.82	0.45
1:0:1744:G:C2'	1:0:1745:G:H5'	2.47	0.45
1:0:204:A:C2'	1:0:205:U:H5'	2.47	0.45
1:0:2248:C:C5	1:0:2249:G:N7	2.84	0.45
1:0:2312:G:C2'	1:0:2313:C:H5'	2.47	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.15	0.45
1:0:2820:A:H2'	1:0:2821:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2885:A:H2'	1:0:2886:C:H6	1.82	0.45
30:3:18:GLN:OE1	30:3:73:GLU:HB2	2.17	0.45
3:A:199:HIS:CD2	3:A:201:PHE:H	2.33	0.45
11:J:19:MET:HE2	11:J:79:PHE:HA	1.98	0.45
1:0:1236:A:C8	11:J:63:ILE:HD11	2.52	0.45
13:L:67:ARG:O	13:L:71:GLU:HG3	2.17	0.45
1:0:1490:G:H4'	1:0:1533:A:OP1	2.16	0.45
1:0:229:G:O2'	1:0:230:C:H5'	2.16	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45
1:0:1684:A:C1'	29:2:43:ARG:HH22	2.22	0.45
6:D:146:LYS:HG2	15:N:106:LEU:HB2	1.99	0.45
6:D:153:THR:HA	6:D:156:ARG:HG3	1.98	0.45
14:M:46:LEU:HG	38:M:8812:HOH:O	2.17	0.45
1:0:185:G:C4'	1:0:186:A:H4'	2.45	0.45
1:0:2898:G:H4'	4:B:288:GLY:HA2	1.99	0.45
1:0:559:U:C5'	1:0:559:U:H6	2.27	0.45
1:0:69:A:C2'	1:0:70:A:OP2	2.65	0.45
2:9:3001:U:O3'	2:9:3003:A:C5'	2.65	0.45
2:9:3107:C:C5	38:9:3167:HOH:O	2.56	0.45
3:A:105:VAL:HG13	3:A:155:THR:O	2.17	0.45
4:B:145:HIS:HD2	4:B:146:THR:O	2.00	0.45
1:0:1118:A:H8	1:0:1119:G:H5''	1.81	0.44
1:0:1619:G:H2'	1:0:1620:C:O4'	2.16	0.44
1:0:1679:C:H5'	38:0:9314:HOH:O	2.16	0.44
1:0:1733:A:C6	1:0:1734:C:C2	3.05	0.44
1:0:2002:C:C2'	1:0:2003:U:H5'	2.47	0.44
1:0:249:G:H2'	1:0:250:C:C6	2.53	0.44
1:0:2856:A:OP1	25:X:15:ARG:NH2	2.50	0.44
1:0:941:G:C5	1:0:942:U:C4	3.05	0.44
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.84	0.44
7:E:81:GLU:O	7:E:172:PRO:HD3	2.17	0.44
14:M:59:GLY:C	14:M:141:ILE:HD11	2.37	0.44
14:M:139:PRO:HA	14:M:142:GLN:HB2	1.98	0.44
15:N:23:ARG:O	15:N:27:LEU:HG	2.17	0.44
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.47	0.44
21:T:24:ARG:HH21	21:T:39:ASN:ND2	2.15	0.44
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.15	0.44
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.44
1:0:154:C:H2'	1:0:155:C:H6	1.82	0.44
1:0:1789:G:C2'	1:0:1790:C:O5'	2.65	0.44
1:0:1882:C:H2'	1:0:1883:U:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1902:G:N2	1:0:1936:C:C2	2.85	0.44
1:0:2248:C:C2	1:0:2254:G:C2	3.05	0.44
1:0:2378:U:H3'	30:3:8:ASN:O	2.17	0.44
1:0:2664:A:OP1	1:0:2664:A:H8	2.00	0.44
1:0:697:G:H4'	1:0:730:G:O3'	2.17	0.44
1:0:794:U:H2'	1:0:795:G:H5'	1.99	0.44
4:B:81:ALA:HB1	4:B:142:LEU:HD13	1.98	0.44
5:C:228:ALA:HA	5:C:229:PRO:HD3	1.87	0.44
7:E:6:GLU:HA	7:E:46:THR:HG22	1.99	0.44
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.99	0.44
8:F:52:GLU:HG3	8:F:77:VAL:O	2.18	0.44
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.47	0.44
1:0:2890:A:C1'	22:U:56:ARG:NH2	2.76	0.44
1:0:2834:G:OP1	25:X:39:LYS:HE2	2.17	0.44
1:0:1202:A:H2'	1:0:1203:G:H5'	1.99	0.44
1:0:1798:C:H1'	17:P:66:GLN:OE1	2.17	0.44
1:0:1851:G:O2'	1:0:1852:A:H5'	2.17	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.52	0.44
1:0:2375:G:H2'	1:0:2376:C:C6	2.53	0.44
1:0:2598:U:O2	1:0:2600:A:C8	2.70	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
1:0:306:A:H2'	1:0:341:C:O2'	2.17	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.57	0.44
2:9:3018:U:OP2	6:D:154:LYS:HE2	2.17	0.44
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.44
8:F:27:GLY:HA3	8:F:101:ALA:O	2.17	0.44
10:H:138:CYS:HB2	38:H:8543:HOH:O	2.17	0.44
16:O:44:ASN:OD1	16:O:65:LEU:HB2	2.16	0.44
24:W:69:ARG:HD2	24:W:117:ARG:O	2.17	0.44
1:0:138:U:C5	1:0:140:G:O6	2.71	0.44
1:0:1925:G:H5'	30:3:29:ARG:NH1	2.32	0.44
1:0:2255:A:C2'	1:0:2256:G:H5'	2.48	0.44
1:0:2314:G:H2'	1:0:2315:C:H5'	2.00	0.44
1:0:2355:G:H5''	1:0:2356:A:OP2	2.18	0.44
1:0:883:U:H2'	1:0:883:U:O2	2.16	0.44
29:2:35:ARG:HH11	29:2:37:HIS:CD2	2.36	0.44
38:0:4225:HOH:O	29:2:38:LYS:HE3	2.17	0.44
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.47	0.44
26:Y:107:PRO:HB3	26:Y:182:PHE:CE2	2.53	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.17	0.44
1:0:1165:G:O2'	1:0:1174:A:C1'	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1520:G:C6	1:0:1521:C:C4	3.05	0.44
1:0:1557:G:C2'	1:0:1558:C:H5'	2.47	0.44
1:0:1537:C:C2	1:0:1649:G:C2	3.06	0.44
1:0:1768:C:H2'	1:0:1769:C:C5'	2.47	0.44
1:0:2004:U:H2'	1:0:2005:G:OP1	2.18	0.44
1:0:2073:G:C6	1:0:2489:G:H4'	2.52	0.44
1:0:2506:A:H1'	38:0:3742:HOH:O	2.16	0.44
1:0:255:A:H2'	1:0:256:C:C6	2.52	0.44
1:0:2853:U:C4	1:0:2906:A:N6	2.86	0.44
1:0:382:U:C5	1:0:406:G:N2	2.85	0.44
1:0:818:A:O2'	27:Z:13:ARG:HD3	2.18	0.44
1:0:907:A:H4'	1:0:1328:A:C2	2.53	0.44
38:0:3012:HOH:O	28:1:46:ARG:HA	2.17	0.44
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.99	0.44
8:F:34:ASN:HA	14:M:4:ALA:HB2	2.00	0.44
38:0:3230:HOH:O	31:I:92:PRO:HD3	2.17	0.44
15:N:119:GLN:O	15:N:123:ILE:HG13	2.18	0.44
17:P:59:ARG:HH22	17:P:66:GLN:NE2	2.14	0.44
38:0:3980:HOH:O	21:T:82:THR:HA	2.17	0.44
1:0:1894:C:C2	1:0:1939:U:C4	3.05	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.52	0.44
1:0:216:A:O2'	1:0:217:C:H5'	2.18	0.44
1:0:2401:A:H5'	38:0:9485:HOH:O	2.18	0.44
5:C:131:PHE:CD2	5:C:131:PHE:N	2.85	0.44
15:N:179:LEU:HD23	15:N:184:ILE:CD1	2.48	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
1:0:1383:U:H5''	38:X:6177:HOH:O	2.18	0.44
1:0:1453:G:H2'	1:0:1454:U:O4'	2.18	0.44
1:0:151:A:C2	1:0:442:A:C8	3.06	0.44
1:0:1805:G:O2'	1:0:1806:G:H5'	2.18	0.44
1:0:2337:G:O3'	6:D:97:GLN:HA	2.17	0.44
1:0:731:U:H2'	1:0:732:C:H6	1.82	0.44
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.29	0.44
6:D:10:PHE:CG	6:D:11:HIS:N	2.86	0.44
10:H:23:ILE:HA	10:H:120:ILE:HG21	1.99	0.44
10:H:162:ARG:HD3	38:H:8582:HOH:O	2.16	0.44
15:N:163:PHE:HZ	15:N:171:HIS:HD1	1.66	0.44
15:N:58:LEU:HD12	15:N:58:LEU:N	2.33	0.44
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.47	0.44
1:0:21:G:H5''	19:R:2:ILE:HA	1.95	0.44
21:T:9:LYS:HE3	21:T:13:ARG:HH11	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:144:ARG:HH11	26:Y:144:ARG:CG	2.31	0.44
1:O:1185:U:OP1	31:I:126:LYS:HD3	2.17	0.44
1:O:1181:A:N1	1:O:1192:A:O2'	2.50	0.44
1:O:1446:U:H2'	20:S:55:GLN:NE2	2.33	0.44
1:O:1520:G:N1	1:O:1667:A:C6	2.86	0.44
1:O:1538:C:O2'	1:O:1539:U:H5'	2.18	0.44
1:O:1644:C:N3	1:O:1645:U:C5	2.86	0.44
1:O:1850:U:H2'	1:O:1851:G:C8	2.52	0.44
1:O:1928:C:C2'	1:O:1929:G:H5'	2.48	0.44
1:O:2092:G:H2'	1:O:2613:G:OP1	2.18	0.44
1:O:241:A:N1	1:O:378:A:H4'	2.33	0.44
1:O:282:C:O2'	1:O:283:U:C4'	2.66	0.44
1:O:1787:C:C4'	1:O:2883:A:O4'	2.65	0.44
1:O:678:G:H3'	38:O:4438:HOH:O	2.18	0.44
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.16	0.44
38:O:5074:HOH:O	4:B:216:LYS:HA	2.17	0.44
10:H:46:GLN:NE2	10:H:137:TYR:HE2	2.15	0.44
11:J:45:VAL:HG11	11:J:121:LEU:CD2	2.48	0.44
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.99	0.44
14:M:164:THR:HG23	14:M:165:GLY:N	2.32	0.44
15:N:43:VAL:CG1	15:N:118:ILE:HD11	2.48	0.44
1:O:1167:G:H4'	31:I:135:LEU:CD2	2.45	0.44
1:O:1209:C:H2'	1:O:1210:G:C8	2.53	0.44
1:O:1659:A:H2'	1:O:1660:G:O4'	2.18	0.44
1:O:2524:G:H21	1:O:2526:C:H41	1.61	0.44
1:O:243:A:H61	1:O:269:G:H1'	1.83	0.44
1:O:958:G:H2'	1:O:959:C:C6	2.53	0.44
2:9:3045:A:C8	2:9:3046:C:C5	3.06	0.44
3:A:113:GLY:HA2	3:A:153:ARG:NH2	2.33	0.44
4:B:14:GLY:HA2	4:B:15:PRO:C	2.37	0.44
5:C:34:ALA:HB3	5:C:220:THR:HG21	2.00	0.44
6:D:172:VAL:HG12	6:D:173:GLU:N	2.32	0.44
11:J:93:ARG:HB3	11:J:93:ARG:HH11	1.83	0.44
15:N:37:ARG:NH2	38:N:8731:HOH:O	2.51	0.44
15:N:82:TYR:CD2	15:N:82:TYR:C	2.92	0.44
17:P:103:THR:HA	17:P:106:ARG:NH1	2.33	0.44
21:T:48:VAL:CG1	21:T:49:GLU:N	2.81	0.44
1:O:968:G:C2	1:O:1001:U:O2	2.71	0.43
1:O:1183:C:H42	1:O:1184:C:N4	2.15	0.43
1:O:1215:A:O3'	1:O:1216:G:C4'	2.66	0.43
1:O:1279:U:H5''	1:O:1280:A:OP2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1450:C:O2'	1:0:1493:A:H2'	2.17	0.43
1:0:1780:G:O2'	1:0:1781:G:H5'	2.17	0.43
1:0:226:A:H1'	1:0:393:G:C5	2.53	0.43
1:0:2403:C:H2'	1:0:2404:G:O5'	2.18	0.43
1:0:2672:C:O2'	1:0:2673:U:H5'	2.18	0.43
1:0:288:A:H2'	1:0:289:G:C8	2.52	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.43
1:0:629:A:C2	1:0:2074:A:C2	3.06	0.43
5:C:214:THR:HG23	38:C:8633:HOH:O	2.17	0.43
31:I:113:HIS:N	31:I:114:PRO:HD2	2.33	0.43
1:0:700:A:C2	13:L:71:GLU:HG2	2.52	0.43
14:M:37:VAL:HG21	14:M:108:THR:OG1	2.17	0.43
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.43
1:0:145:A:H4'	14:M:137:ASN:ND2	2.33	0.43
1:0:1662:C:H2'	1:0:1663:G:O4'	2.17	0.43
1:0:1973:A:H2'	1:0:1974:G:O4'	2.18	0.43
1:0:2249:G:N1	1:0:2253:G:C6	2.86	0.43
1:0:2729:C:H1'	1:0:2864:U:O2'	2.18	0.43
1:0:276:C:O5'	1:0:276:C:H6	2.00	0.43
1:0:2667:G:N3	1:0:2827:A:C2	2.85	0.43
1:0:764:C:H2'	1:0:765:G:O4'	2.18	0.43
1:0:814:G:N2	1:0:815:U:H1'	2.33	0.43
3:A:88:ILE:HG22	3:A:88:ILE:O	2.18	0.43
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.47	0.43
4:B:75:GLU:C	4:B:77:PRO:HD3	2.38	0.43
5:C:154:VAL:O	5:C:158:GLU:HG3	2.18	0.43
7:E:101:GLU:HB2	7:E:116:THR:O	2.18	0.43
7:E:40:VAL:HA	7:E:48:VAL:O	2.18	0.43
14:M:28:GLN:O	14:M:32:ARG:HG3	2.18	0.43
19:R:119:VAL:HG12	19:R:119:VAL:O	2.18	0.43
24:W:21:LEU:HD22	24:W:26:ILE:HD13	1.98	0.43
1:0:1167:G:H3'	38:0:7466:HOH:O	2.18	0.43
1:0:1644:C:O2'	1:0:1645:U:H5'	2.18	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.36	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2444:U:C4	1:0:2445:U:C5	3.06	0.43
1:0:289:G:N2	1:0:363:A:C2	2.66	0.43
1:0:454:U:C2	38:0:9027:HOH:O	2.56	0.43
1:0:947:U:O2'	1:0:948:G:H5'	2.18	0.43
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.83	0.43
12:K:18:ILE:HG22	12:K:93:ASN:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:67:VAL:HB	14:M:97:ILE:HG23	1.99	0.43
20:S:37:VAL:O	20:S:41:VAL:HG23	2.17	0.43
38:O:3751:HOH:O	21:T:9:LYS:HD3	2.17	0.43
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.54	0.43
1:O:1592:G:C5	1:O:1593:C:C4	3.07	0.43
1:O:1785:G:H1'	1:O:1812:G:N3	2.33	0.43
1:O:2511:A:H2'	1:O:2512:U:O4'	2.19	0.43
1:O:2624:A:O2'	1:O:2625:C:H5'	2.18	0.43
1:O:37:A:C2	1:O:446:G:C2	3.07	0.43
3:A:217:ARG:HG3	3:A:217:ARG:HH11	1.82	0.43
1:O:2443:C:H5'	13:L:57:VAL:HG21	1.99	0.43
16:O:88:LYS:HD3	38:O:7061:HOH:O	2.17	0.43
18:Q:30:VAL:HG12	18:Q:30:VAL:O	2.18	0.43
1:O:488:U:O2'	21:T:82:THR:HG21	2.19	0.43
23:V:1:THR:HG23	23:V:2:VAL:N	2.32	0.43
1:O:1055:G:OP2	10:H:96:ARG:NH1	2.52	0.43
1:O:1520:G:C6	1:O:1521:C:N4	2.87	0.43
1:O:1556:G:O2'	1:O:1557:G:H5'	2.19	0.43
1:O:160:A:C4	1:O:177:A:C2	3.06	0.43
1:O:2028:U:H2'	1:O:2029:C:C6	2.53	0.43
1:O:2105:C:H2'	1:O:2106:C:C6	2.54	0.43
1:O:2455:A:H2'	1:O:2456:A:O4'	2.17	0.43
1:O:2607:U:H4'	38:O:9432:HOH:O	2.17	0.43
1:O:2834:G:C4	1:O:2847:G:N2	2.86	0.43
1:O:34:C:C4	1:O:35:U:C4	3.07	0.43
1:O:559:U:H2'	1:O:560:C:C5'	2.49	0.43
18:Q:43:ILE:HG13	18:Q:52:PHE:CZ	2.54	0.43
24:W:65:VAL:CG1	24:W:116:LEU:HD13	2.47	0.43
1:O:1400:C:H2'	1:O:1401:G:C5'	2.48	0.43
1:O:1513:C:O2'	1:O:1514:C:H5'	2.18	0.43
1:O:1581:A:C5	1:O:1582:C:C5	3.07	0.43
1:O:1644:C:C4	1:O:1645:U:C5	3.06	0.43
1:O:1878:G:C1'	38:O:6112:HOH:O	2.56	0.43
1:O:2761:A:C4	1:O:2763:G:C8	3.06	0.43
1:O:2911:C:O2'	1:O:2912:C:H5'	2.19	0.43
1:O:440:C:H2'	1:O:441:A:C8	2.54	0.43
1:O:510:U:H6	38:O:7411:HOH:O	1.99	0.43
1:O:559:U:O2'	1:O:560:C:H5'	2.18	0.43
28:1:25:LYS:HD2	29:2:48:ASP:HA	1.99	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.43
1:0:1204:C:H1'	38:0:4743:HOH:O	2.18	0.43
1:0:1215:A:O3'	1:0:1216:G:H4'	2.18	0.43
1:0:1649:G:O2'	1:0:1650:C:H5'	2.19	0.43
1:0:1669:A:H2'	1:0:1670:G:C8	2.54	0.43
1:0:195:C:H5''	38:M:8796:HOH:O	2.17	0.43
1:0:2072:G:N2	38:0:6848:HOH:O	2.41	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
1:0:2897:C:H2'	1:0:2898:G:C8	2.53	0.43
1:0:2912:C:H2'	1:0:2913:A:C8	2.53	0.43
1:0:372:A:H2'	1:0:373:G:H8	1.83	0.43
30:3:48:ASN:ND2	30:3:50:GLY:H	2.16	0.43
2:9:3039:U:O2'	2:9:3042:C:H5	2.00	0.43
2:9:3065:A:C2'	2:9:3066:G:OP2	2.66	0.43
11:J:90:LYS:HB2	36:J:8702:CL:CL	2.55	0.43
16:O:47:ARG:HG3	16:O:47:ARG:HH11	1.84	0.43
24:W:108:ARG:HG3	24:W:114:PRO:HG3	2.00	0.43
1:0:1829:A:H61	27:Z:18:TYR:HA	1.82	0.43
1:0:1052:G:N3	1:0:1052:G:H2'	2.34	0.43
1:0:1462:C:H2'	1:0:1463:A:H8	1.79	0.43
1:0:1592:G:H2'	1:0:1593:C:C6	2.54	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.43
1:0:2252:A:H2'	1:0:2253:G:C5'	2.48	0.43
1:0:301:G:O2'	1:0:302:A:H5'	2.19	0.43
1:0:432:G:H2'	1:0:433:C:H6	1.84	0.43
1:0:69:A:C8	1:0:69:A:C5'	2.97	0.43
30:3:22:VAL:HG12	30:3:67:LEU:HD22	2.01	0.43
4:B:307:ARG:HG2	4:B:308:LEU:N	2.33	0.43
4:B:79:MET:HE3	4:B:79:MET:HB2	1.90	0.43
1:0:2338:G:H1'	6:D:105:SER:OG	2.19	0.43
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.77	0.43
15:N:22:GLN:HA	15:N:25:ARG:CZ	2.49	0.43
19:R:106:GLY:HA2	19:R:109:MET:HE3	2.00	0.43
24:W:126:ASP:HB3	24:W:135:GLY:O	2.19	0.43
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.52	0.43
1:0:1298:U:H2'	1:0:1299:G:C8	2.54	0.43
1:0:1463:A:H8	1:0:1463:A:O5'	2.01	0.43
1:0:1573:A:H2'	1:0:1574:C:H5'	2.00	0.43
1:0:527:U:H2'	1:0:528:G:C8	2.54	0.43
38:0:7425:HOH:O	4:B:211:THR:HG21	2.18	0.43
6:D:86:THR:O	6:D:90:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1500:U:P	17:P:41:ARG:HH22	2.42	0.43
1:0:20:G:H21	19:R:117:HIS:HD2	1.66	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.54	0.43
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.43
1:0:1717:A:H5''	17:P:54:LYS:HB2	2.01	0.43
1:0:1730:G:H5''	1:0:1731:C:C6	2.52	0.43
1:0:17:G:H2'	1:0:18:C:C6	2.54	0.43
1:0:2119:C:O2'	1:0:2120:U:H5'	2.19	0.43
1:0:2487:C:H5	38:0:4883:HOH:O	2.01	0.43
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.43
1:0:298:C:N3	1:0:299:U:C5	2.87	0.43
1:0:311:C:H2'	1:0:312:U:C6	2.54	0.43
1:0:321:A:H1'	38:0:7016:HOH:O	2.19	0.43
1:0:595:U:O2'	1:0:596:C:H5'	2.19	0.43
1:0:932:U:H2'	1:0:933:C:C6	2.54	0.43
2:9:3096:C:O2'	2:9:3097:U:H5'	2.19	0.43
3:A:167:LYS:CE	27:Z:26:VAL:HG22	2.49	0.43
3:A:69:LEU:HB3	38:A:8775:HOH:O	2.18	0.43
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.49	0.43
15:N:154:LEU:HD11	38:N:8723:HOH:O	2.19	0.43
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.99	0.43
21:T:41:ARG:NH1	21:T:42:VAL:O	2.52	0.43
1:0:1285:U:H4'	24:W:74:GLU:OE1	2.19	0.43
27:Z:24:ARG:HG2	27:Z:28:GLU:OE2	2.19	0.43
1:0:1175:G:H1'	1:0:1193:A:C2'	2.46	0.42
1:0:1421:C:O2'	1:0:1422:U:H5'	2.19	0.42
1:0:1568:G:C5	1:0:1569:U:C5	3.07	0.42
1:0:1713:G:H1'	38:0:5065:HOH:O	2.19	0.42
1:0:797:A:N6	1:0:816:G:H1'	2.34	0.42
1:0:825:U:H5''	1:0:826:U:OP1	2.19	0.42
1:0:876:A:N3	1:0:876:A:C2'	2.82	0.42
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.30	0.42
5:C:33:LYS:HE2	38:C:8558:HOH:O	2.19	0.42
10:H:166:SER:CB	10:H:167:PRO:CD	2.92	0.42
1:0:2132:C:H1'	14:M:124:GLY:HA3	2.01	0.42
25:X:76:ARG:HH11	25:X:76:ARG:CG	2.21	0.42
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.42
1:0:2531:U:O2'	1:0:2532:A:H5'	2.19	0.42
1:0:36:C:C2	1:0:447:A:C2	3.07	0.42
1:0:40:C:H4'	38:0:6982:HOH:O	2.18	0.42
1:0:432:G:O2'	1:0:433:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.42
1:0:666:A:H2'	1:0:667:C:H5'	1.99	0.42
1:0:789:C:H1'	1:0:827:A:C2	2.53	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.42
4:B:82:VAL:HG12	4:B:82:VAL:O	2.18	0.42
38:0:6279:HOH:O	6:D:99:ASP:HA	2.19	0.42
10:H:47:ILE:HD12	10:H:146:VAL:HG11	2.00	0.42
15:N:73:ALA:HB1	15:N:74:PRO:HD2	2.00	0.42
38:0:7398:HOH:O	21:T:9:LYS:HD2	2.18	0.42
27:Z:49:ARG:HB2	27:Z:55:TRP:CZ3	2.54	0.42
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.19	0.42
1:0:1159:G:H1	1:0:1208:C:N4	2.15	0.42
1:0:1202:A:C2'	1:0:1203:G:H5'	2.49	0.42
1:0:1246:A:H8	1:0:1246:A:H5'	1.85	0.42
1:0:1822:A:O2'	1:0:1823:G:H5'	2.19	0.42
1:0:2467:A:H2'	38:0:5453:HOH:O	2.19	0.42
1:0:2577:A:H5'	38:0:7721:HOH:O	2.18	0.42
1:0:364:C:H2'	1:0:365:G:C8	2.54	0.42
1:0:152:A:H1'	1:0:440:C:O2'	2.19	0.42
1:0:670:G:H2'	1:0:671:A:O4'	2.19	0.42
1:0:800:G:H2'	1:0:801:U:C6	2.54	0.42
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.50	0.42
38:0:6782:HOH:O	4:B:282:GLY:HA2	2.19	0.42
1:0:450:C:H4'	5:C:46:TYR:CE1	2.54	0.42
1:0:1164:U:OP1	31:I:74:PRO:HA	2.19	0.42
14:M:42:ARG:HA	14:M:43:PRO:HD3	1.85	0.42
15:N:175:LEU:HD12	15:N:175:LEU:HA	1.79	0.42
38:0:5628:HOH:O	17:P:58:SER:HB3	2.19	0.42
25:X:76:ARG:NH1	25:X:76:ARG:CG	2.81	0.42
1:0:1501:A:C6	1:0:1502:A:C6	3.07	0.42
1:0:2504:A:H2'	1:0:2505:G:O4'	2.19	0.42
1:0:2509:A:OP2	1:0:2510:C:C5	2.68	0.42
1:0:2635:A:C2'	1:0:2636:C:H5'	2.48	0.42
1:0:285:A:C2	1:0:368:C:H4'	2.54	0.42
1:0:461:C:H6	38:0:5831:HOH:O	2.03	0.42
1:0:856:G:H2'	38:0:5424:HOH:O	2.19	0.42
2:9:3003:A:C8	2:9:3003:A:O5'	2.72	0.42
11:J:131:THR:HB	11:J:134:GLU:HG3	2.00	0.42
13:L:41:HIS:H	13:L:41:HIS:CD2	2.38	0.42
1:0:645:U:OP2	13:L:4:LYS:HE2	2.19	0.42
19:R:119:VAL:HG21	19:R:142:ASP:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2044:G:OP1	25:X:23:HIS:HE1	2.01	0.42
1:0:1205:U:O2'	1:0:1206:U:H5''	2.19	0.42
1:0:1661:A:O2'	1:0:1662:C:H5'	2.20	0.42
1:0:2377:U:O5'	1:0:2377:U:H6	2.02	0.42
1:0:2863:G:C2	1:0:2894:C:O2	2.72	0.42
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.42
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.42
20:S:58:MET:SD	29:2:8:LYS:HE3	2.59	0.42
2:9:3001:U:C5'	2:9:3003:A:OP1	2.66	0.42
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.86	0.42
5:C:218:VAL:HG12	38:C:8621:HOH:O	2.19	0.42
31:I:93:GLN:HA	31:I:96:PHE:CE2	2.55	0.42
13:L:114:VAL:HG11	38:L:8770:HOH:O	2.19	0.42
20:S:33:SER:OG	20:S:36:GLU:HG3	2.18	0.42
21:T:53:GLY:HA3	38:T:6384:HOH:O	2.18	0.42
26:Y:219:GLU:HG3	26:Y:220:GLU:N	2.34	0.42
1:0:1176:C:H1'	38:0:3922:HOH:O	2.19	0.42
1:0:1189:A:H3'	38:0:7650:HOH:O	2.18	0.42
1:0:240:C:O2	1:0:240:C:H2'	2.20	0.42
3:A:217:ARG:NH1	3:A:217:ARG:CG	2.83	0.42
1:0:750:A:O3'	5:C:101:ASP:HB2	2.20	0.42
31:I:92:PRO:C	31:I:94:GLU:H	2.23	0.42
15:N:69:TYR:CD2	15:N:184:ILE:HD11	2.54	0.42
23:V:12:THR:HG23	23:V:14:ALA:H	1.85	0.42
27:Z:39:CYS:SG	27:Z:41:ASN:N	2.93	0.42
27:Z:39:CYS:SG	27:Z:57:CYS:HB2	2.60	0.42
1:0:1407:A:O2'	1:0:1408:U:H3'	2.19	0.42
1:0:1553:C:H2'	1:0:1554:U:H6	1.85	0.42
1:0:1626:A:H2'	1:0:1627:G:C5'	2.49	0.42
1:0:1773:G:H2'	1:0:1774:G:H5'	2.02	0.42
1:0:2064:U:H2'	1:0:2065:C:C6	2.55	0.42
1:0:298:C:C2	1:0:299:U:C6	3.07	0.42
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.42
1:0:794:U:C2'	1:0:795:G:H5'	2.49	0.42
2:9:3094:G:O2'	2:9:3095:C:H5'	2.20	0.42
38:0:7388:HOH:O	31:I:90:GLY:HA2	2.19	0.42
14:M:109:PHE:HB3	14:M:112:LEU:HG	2.02	0.42
15:N:143:ARG:HA	15:N:172:PHE:CD2	2.55	0.42
38:0:9656:HOH:O	16:O:112:ARG:HD2	2.19	0.42
24:W:73:LEU:HA	24:W:73:LEU:HD12	1.75	0.42
1:0:1156:C:O2'	1:0:1157:C:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:634:G:O2'	1:0:1358:A:OP1	2.34	0.42
1:0:1947:G:O2'	1:0:1948:G:H5'	2.19	0.42
1:0:1972:U:C2'	1:0:1973:A:H5''	2.49	0.42
1:0:2488:A:N6	1:0:2534:C:H42	2.10	0.42
1:0:275:G:C2	1:0:376:C:C2	3.07	0.42
1:0:506:G:H22	1:0:509:A:H5''	1.82	0.42
1:0:24:G:N2	1:0:518:G:H1'	2.34	0.42
3:A:35:GLY:O	3:A:36:ASP:CB	2.68	0.42
4:B:149:ASP:HA	38:B:8861:HOH:O	2.19	0.42
8:F:91:VAL:CG1	8:F:92:GLY:N	2.81	0.42
12:K:98:VAL:HG13	12:K:102:GLU:HA	2.00	0.42
12:K:34:VAL:HG22	12:K:47:ALA:HB2	2.01	0.42
26:Y:189:ASN:HD22	26:Y:192:ASP:H	1.67	0.42
1:0:1183:C:N3	1:0:1184:C:C5	2.87	0.42
1:0:1597:A:O4'	17:P:95:GLU:HG2	2.20	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.34	0.42
1:0:283:U:C6	1:0:284:C:N3	2.88	0.42
1:0:2871:G:H2'	1:0:2872:U:C6	2.55	0.42
1:0:53:C:H2'	1:0:54:G:O4'	2.20	0.42
1:0:807:A:H2'	1:0:808:A:C8	2.54	0.42
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.02	0.42
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.42
12:K:72:VAL:HG11	12:K:121:PHE:CD1	2.54	0.42
15:N:108:SER:HA	15:N:109:PRO:HD3	1.78	0.42
16:O:96:VAL:CG1	16:O:100:GLN:HB2	2.49	0.42
18:Q:40:HIS:CE1	18:Q:94:GLN:HG3	2.55	0.42
1:0:2444:U:N3	1:0:2445:U:C5	2.88	0.42
1:0:2073:G:OP2	1:0:2490:A:H5'	2.20	0.42
1:0:2769:C:C2'	1:0:2770:G:C5'	2.87	0.42
1:0:2815:G:N7	11:J:80:LYS:NZ	2.63	0.42
1:0:2836:G:H1'	38:0:6818:HOH:O	2.19	0.42
1:0:2853:U:C5	1:0:2906:A:N6	2.88	0.42
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.42
30:3:11:CYS:HB2	30:3:20:HIS:HE1	1.85	0.42
5:C:194:PHE:CE2	5:C:234:VAL:HG11	2.55	0.42
1:0:2283:G:C6	10:H:113:MET:HB3	2.55	0.42
10:H:143:ALA:O	10:H:147:LYS:HG3	2.20	0.42
15:N:42:HIS:CB	15:N:62:HIS:HE1	2.33	0.42
15:N:37:ARG:HD3	36:N:8707:CL:CL	2.57	0.42
21:T:48:VAL:HG12	21:T:49:GLU:N	2.35	0.42
38:0:6235:HOH:O	22:U:56:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1543:G:N1	1:0:1641:A:OP2	2.38	0.41
1:0:1836:A:H1'	28:1:1:THR:O	2.20	0.41
1:0:2414:A:H1'	38:0:4703:HOH:O	2.19	0.41
1:0:484:A:C6	1:0:486:A:C6	3.08	0.41
1:0:61:G:C2	1:0:62:C:C2	3.08	0.41
1:0:635:A:H2	38:0:9207:HOH:O	2.02	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.08	0.41
1:0:2272:G:OP1	3:A:223:ARG:HD2	2.20	0.41
9:G:64:ASN:N	9:G:64:ASN:ND2	2.66	0.41
17:P:109:ARG:NH1	17:P:119:TYR:CE2	2.88	0.41
1:0:1188:A:C5	1:0:1189:A:N1	2.88	0.41
1:0:1352:A:H5''	1:0:1353:C:OP2	2.19	0.41
1:0:138:U:OP2	1:0:139:C:C5	2.73	0.41
1:0:1444:G:O2'	1:0:1445:G:H5'	2.19	0.41
1:0:1494:A:H1'	1:0:1495:C:C6	2.55	0.41
1:0:154:C:H2'	1:0:155:C:C6	2.55	0.41
1:0:392:U:C5'	14:M:193:LYS:HB3	2.50	0.41
1:0:843:A:C2	1:0:846:A:C8	3.08	0.41
8:F:99:THR:HG23	8:F:99:THR:O	2.20	0.41
15:N:87:LEU:HG	15:N:91:ARG:NH1	2.34	0.41
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.55	0.41
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.41
1:0:1425:G:O2'	1:0:1426:C:H5'	2.19	0.41
1:0:1433:G:O2'	1:0:1434:A:H5'	2.20	0.41
1:0:1915:U:O2'	1:0:1916:C:H5'	2.20	0.41
1:0:1928:C:H2'	1:0:1929:G:H5'	2.02	0.41
1:0:216:A:N6	1:0:225:G:C2	2.88	0.41
1:0:2250:G:C6	1:0:2251:G:C2	3.08	0.41
1:0:2255:A:N1	1:0:2256:G:C4	2.88	0.41
1:0:2374:A:H2'	1:0:2375:G:C8	2.55	0.41
1:0:353:G:C6	1:0:354:A:C6	3.08	0.41
1:0:581:G:H4'	1:0:1254:C:O2'	2.19	0.41
1:0:812:A:H2'	1:0:813:C:H6	1.85	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
2:9:3039:U:H2'	2:9:3040:C:OP1	2.21	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.91	0.41
21:T:18:GLU:O	21:T:21:LYS:HE2	2.20	0.41
1:0:1262:C:H1'	24:W:120:PRO:HG3	2.02	0.41
26:Y:122:ARG:NH2	38:Y:8735:HOH:O	2.53	0.41
1:0:622:G:P	26:Y:148:GLY:HA3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2345:A:N6	38:0:9272:HOH:O	2.53	0.41
1:0:2335:C:C2	1:0:2350:G:C2	3.09	0.41
1:0:2582:G:H4'	38:K:4440:HOH:O	2.20	0.41
1:0:331:A:C6	1:0:332:G:C4	3.08	0.41
1:0:813:C:H3'	38:0:7188:HOH:O	2.20	0.41
1:0:821:U:H4'	38:Z:8631:HOH:O	2.20	0.41
1:0:89:G:H4'	38:0:4762:HOH:O	2.20	0.41
1:0:99:A:C8	1:0:100:C:C5	3.09	0.41
4:B:43:GLY:O	4:B:308:LEU:HD12	2.20	0.41
5:C:19:PRO:CD	5:C:240:LEU:HD22	2.50	0.41
6:D:35:ALA:N	38:D:5576:HOH:O	2.53	0.41
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.34	0.41
17:P:126:ALA:C	17:P:128:GLY:H	2.23	0.41
26:Y:151:SER:HB3	26:Y:154:ARG:HB3	2.03	0.41
1:0:1102:C:H5	38:0:3488:HOH:O	2.04	0.41
1:0:1180:U:H2'	1:0:1181:A:C8	2.56	0.41
1:0:1117:A:C2	1:0:1244:U:C2	3.09	0.41
1:0:912:A:C4	1:0:1294:A:C2	3.08	0.41
1:0:1427:A:H61	1:0:1440:U:C1'	2.33	0.41
1:0:1447:U:H3'	1:0:1506:U:O2	2.20	0.41
1:0:1773:G:C2'	1:0:1774:G:H5'	2.51	0.41
1:0:184:G:O2'	1:0:185:G:H5'	2.20	0.41
1:0:2368:A:H8	38:N:8730:HOH:O	2.04	0.41
1:0:2407:G:O2'	1:0:2408:A:H5'	2.19	0.41
1:0:2473:U:O3'	1:0:2474:A:H3'	2.20	0.41
1:0:254:C:N4	1:0:255:A:C6	2.89	0.41
1:0:2768:A:C2'	1:0:2769:C:O4'	2.63	0.41
1:0:451:C:C2'	1:0:452:G:H5'	2.51	0.41
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.41
17:P:114:LEU:HA	17:P:118:GLN:NE2	2.35	0.41
26:Y:144:ARG:HG3	26:Y:144:ARG:HH11	1.85	0.41
1:0:1196:C:H2'	1:0:1197:G:H5'	2.02	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
1:0:1882:C:H2'	1:0:1883:U:C6	2.55	0.41
1:0:834:G:H3'	1:0:835:U:H4'	2.02	0.41
2:9:3054:A:C5'	38:D:3359:HOH:O	2.69	0.41
3:A:179:MET:HG2	3:A:186:TRP:CG	2.55	0.41
4:B:260:HIS:HE1	38:B:8783:HOH:O	2.02	0.41
14:M:48:LYS:HE3	14:M:52:GLN:NE2	2.36	0.41
4:B:329:TYR:HE2	22:U:15:PRO:HG2	1.81	0.41
24:W:149:LEU:HG	24:W:153:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:111:C:H2'	1:0:112:G:C5'	2.51	0.41
1:0:1191:A:H2'	1:0:1193:A:H5'	2.03	0.41
1:0:1747:A:C8	12:K:44:LEU:HD13	2.56	0.41
1:0:1964:U:O2	1:0:1964:U:H2'	2.20	0.41
1:0:365:G:C5	1:0:366:U:C5	3.09	0.41
1:0:731:U:C2	1:0:732:C:C5	3.09	0.41
3:A:135:VAL:HG22	3:A:136:ALA:N	2.36	0.41
4:B:80:ARG:HA	4:B:186:GLY:O	2.21	0.41
4:B:60:SER:HA	4:B:61:PRO:HD3	1.88	0.41
1:0:189:A:OP1	14:M:171:ARG:NH2	2.53	0.41
14:M:75:ARG:HB3	14:M:75:ARG:HE	1.76	0.41
16:O:7:LEU:O	16:O:11:ILE:HG13	2.21	0.41
17:P:20:ARG:HH12	17:P:54:LYS:HD3	1.84	0.41
19:R:149:GLU:HA	19:R:150:PRO:HD3	1.86	0.41
20:S:52:VAL:HG22	20:S:66:VAL:HG13	2.02	0.41
22:U:14:GLU:HA	22:U:15:PRO:HD2	1.94	0.41
23:V:31:ARG:NE	38:V:2682:HOH:O	2.53	0.41
24:W:3:ALA:O	24:W:54:PHE:HA	2.19	0.41
26:Y:115:ARG:NE	38:Y:8755:HOH:O	2.53	0.41
1:0:1162:G:C6	1:0:1163:G:C6	3.09	0.41
1:0:1195:G:C2	1:0:1205:U:C2	3.08	0.41
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.41
1:0:2102:G:C2	1:0:2104:C:C4	3.09	0.41
1:0:2110:G:H5''	38:0:6390:HOH:O	2.20	0.41
1:0:2524:G:N2	1:0:2526:C:H41	2.18	0.41
1:0:2599:A:C6	1:0:2600:A:N1	2.89	0.41
1:0:2615:U:C5	1:0:2616:G:C6	3.09	0.41
1:0:263:U:O4'	8:F:59:ILE:HD13	2.21	0.41
1:0:333:G:O2'	1:0:334:G:H5'	2.21	0.41
1:0:77:G:O2'	1:0:78:G:H5'	2.21	0.41
2:9:3076:G:H3'	2:9:3077:A:C5'	2.33	0.41
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.20	0.41
4:B:198:GLU:HA	38:B:8858:HOH:O	2.21	0.41
16:O:49:GLU:HG2	38:O:5191:HOH:O	2.21	0.41
16:O:53:GLN:HG2	16:O:56:GLU:OE1	2.20	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2437:A:H2'	1:0:2438:G:C8	2.55	0.41
1:0:2526:C:H5''	38:0:7578:HOH:O	2.20	0.41
31:I:133:THR:N	38:I:5371:HOH:O	2.54	0.41
15:N:12:ARG:HH11	15:N:18:THR:HG1	1.67	0.41
15:N:42:HIS:HB3	15:N:62:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:59:PHE:O	19:R:63:ASN:HB3	2.20	0.41
19:R:84:ALA:O	19:R:88:PHE:HD1	2.04	0.41
1:0:1236:A:C8	11:J:63:ILE:CD1	3.04	0.41
1:0:1746:A:O4'	1:0:1747:A:C2	2.73	0.41
1:0:1945:G:C2'	1:0:1946:C:H5'	2.51	0.41
1:0:2241:C:H2'	1:0:2242:U:C6	2.55	0.41
1:0:2247:C:O2'	1:0:2248:C:H5'	2.20	0.41
1:0:2296:C:H2'	1:0:2297:U:C6	2.56	0.41
1:0:2504:A:H4'	10:H:71:ARG:HH11	1.85	0.41
1:0:2503:A:H2	1:0:2517:A:N7	2.18	0.41
1:0:466:A:H2'	1:0:467:G:O4'	2.21	0.41
1:0:665:A:C6	1:0:666:A:C6	3.09	0.41
1:0:731:U:O2'	1:0:732:C:H5'	2.21	0.41
1:0:960:G:C2'	1:0:961:A:OP2	2.69	0.41
2:9:3065:A:O2'	2:9:3066:G:P	2.79	0.41
3:A:126:ALA:HB1	3:A:138:VAL:HG12	2.03	0.41
3:A:48:ASP:HA	3:A:49:PRO:HD3	1.88	0.41
2:9:3041:C:O4'	6:D:50:VAL:HG22	2.21	0.41
13:L:143:THR:HG21	38:L:8738:HOH:O	2.21	0.41
24:W:149:LEU:HG	24:W:153:MET:HE1	2.02	0.41
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	2.03	0.41
27:Z:47:VAL:HA	27:Z:56:GLN:O	2.21	0.41
1:0:154:C:C2	1:0:155:C:C5	3.09	0.41
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.54	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
1:0:66:G:H4'	1:0:69:A:O4'	2.20	0.41
1:0:803:C:O2'	1:0:804:C:H5'	2.21	0.41
30:3:3:MET:O	30:3:90:PHE:HA	2.21	0.41
2:9:3037:C:O2'	2:9:3038:A:H5'	2.21	0.41
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.36	0.41
6:D:55:LYS:O	6:D:56:ARG:HB2	2.21	0.41
12:K:98:VAL:HG11	12:K:102:GLU:HA	2.03	0.41
1:0:962:C:C1'	15:N:5:ARG:NH1	2.84	0.41
17:P:59:ARG:NH2	17:P:66:GLN:NE2	2.62	0.41
25:X:43:VAL:HG22	25:X:76:ARG:NH1	2.36	0.41
1:0:1024:G:C6	1:0:1025:C:N3	2.90	0.40
1:0:1081:A:H5''	38:0:3145:HOH:O	2.20	0.40
1:0:1586:G:H2'	1:0:1587:U:H6	1.86	0.40
1:0:1857:A:H5''	38:0:6684:HOH:O	2.21	0.40
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2686:C:H1'	38:0:7593:HOH:O	2.22	0.40
1:0:307:G:C2	1:0:309:C:C4	3.09	0.40
1:0:696:C:C2'	1:0:697:G:H5'	2.51	0.40
1:0:724:G:O2'	1:0:725:C:H5'	2.21	0.40
3:A:144:GLU:HG2	3:A:145:MET:N	2.36	0.40
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.50	0.40
6:D:67:ASP:HA	6:D:68:PRO:HD3	1.98	0.40
11:J:132:LEU:HA	11:J:132:LEU:HD23	1.88	0.40
17:P:13:VAL:HG11	17:P:40:VAL:HG11	2.03	0.40
38:0:6510:HOH:O	18:Q:3:SER:HB3	2.20	0.40
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.57	0.40
1:0:1587:U:O2'	1:0:1588:G:H5'	2.21	0.40
1:0:2659:U:H4'	19:R:76:ASP:HB3	2.03	0.40
1:0:2716:G:H5'	4:B:262:ARG:HG3	2.02	0.40
1:0:2780:C:H2'	1:0:2781:U:C6	2.57	0.40
1:0:503:G:H2'	1:0:504:G:H8	1.86	0.40
1:0:626:U:C4	1:0:627:G:C6	3.09	0.40
1:0:800:G:H4'	38:0:7041:HOH:O	2.21	0.40
2:9:3042:C:C5'	2:9:3043:G:OP2	2.68	0.40
2:9:3065:A:C5	2:9:3113:C:C5	3.09	0.40
1:0:1735:C:OP2	4:B:234:ARG:HG3	2.20	0.40
1:0:2582:G:H5''	4:B:3:PRO:HB3	2.02	0.40
5:C:193:LEU:HD13	5:C:222:ASP:HB2	2.04	0.40
7:E:108:LEU:HA	7:E:108:LEU:HD12	1.94	0.40
31:I:101:SER:O	31:I:105:VAL:HG23	2.21	0.40
11:J:74:ARG:NH1	11:J:105:LEU:HD11	2.35	0.40
1:0:2842:G:H5'	19:R:68:HIS:O	2.21	0.40
3:A:167:LYS:HE3	27:Z:26:VAL:HA	2.03	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.56	0.40
1:0:1207:A:C8	1:0:1208:C:C5	3.10	0.40
1:0:1393:A:H2'	1:0:1394:C:C6	2.56	0.40
1:0:1416:G:C2'	1:0:1417:G:H5'	2.51	0.40
1:0:2599:A:C6	1:0:2600:A:C6	3.09	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.22	0.40
1:0:461:C:H2'	38:0:5831:HOH:O	2.21	0.40
1:0:682:A:H2'	1:0:683:G:O4'	2.21	0.40
1:0:805:G:N2	1:0:807:A:H3'	2.36	0.40
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.22	0.40
10:H:154:TYR:CD1	10:H:154:TYR:C	2.94	0.40
12:K:59:LYS:HA	38:K:5358:HOH:O	2.20	0.40
38:0:4065:HOH:O	14:M:97:ILE:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:103:THR:HA	17:P:106:ARG:CZ	2.52	0.40
25:X:21:PRO:HG2	25:X:24:LYS:HD3	2.02	0.40
1:0:1684:A:H1'	29:2:43:ARG:NH2	2.22	0.40
1:0:1976:G:H1'	1:0:2005:G:N2	2.36	0.40
1:0:2372:A:H2'	1:0:2373:U:C6	2.56	0.40
1:0:2589:U:H2'	1:0:2590:U:C6	2.57	0.40
1:0:541:C:C2'	1:0:542:A:C5'	2.83	0.40
1:0:599:G:H2'	1:0:600:G:H8	1.87	0.40
1:0:68:U:O2'	1:0:69:A:H5''	2.21	0.40
1:0:820:G:H5'	1:0:821:U:C5'	2.50	0.40
2:9:3057:A:N6	38:9:3535:HOH:O	2.46	0.40
4:B:243:ASN:HA	4:B:244:PRO:C	2.41	0.40
4:B:26:PHE:HE1	38:B:8848:HOH:O	2.04	0.40
4:B:41:PHE:HB3	4:B:190:MET:CE	2.51	0.40
7:E:69:ILE:HA	7:E:72:MET:CE	2.51	0.40
15:N:163:PHE:O	15:N:164:ASP:O	2.40	0.40
21:T:89:ARG:O	21:T:89:ARG:HG3	2.22	0.40
1:0:588:G:O6	24:W:154:ARG:NH1	2.54	0.40
27:Z:42:CYS:O	27:Z:44:GLU:N	2.53	0.40
3:A:76:VAL:HG23	27:Z:63:LYS:HB3	2.04	0.40
1:0:1139:U:H2'	1:0:1140:C:C6	2.57	0.40
1:0:1195:G:N2	1:0:1205:U:C2	2.89	0.40
1:0:1460:G:OP1	3:A:17:ARG:NH1	2.54	0.40
1:0:1592:G:O2'	1:0:1593:C:O5'	2.37	0.40
1:0:1634:G:C5	1:0:1635:U:C5	3.09	0.40
1:0:1795:G:H2'	1:0:1796:A:O4'	2.21	0.40
1:0:1972:U:C2'	1:0:1973:A:C5'	3.00	0.40
1:0:1889:C:O2	1:0:2010:A:H2	2.05	0.40
1:0:2415:A:N3	15:N:26:LEU:HD13	2.37	0.40
1:0:366:U:H2'	1:0:367:G:O4'	2.21	0.40
1:0:484:A:N6	1:0:486:A:C6	2.89	0.40
1:0:921:G:H4'	1:0:924:G:N1	2.36	0.40
2:9:3056:A:C3'	2:9:3057:A:H5''	2.50	0.40
11:J:6:PHE:HB3	11:J:109:TYR:OH	2.21	0.40
12:K:78:LYS:HA	12:K:79:PRO:HD3	1.95	0.40
8:F:57:GLU:HB2	14:M:23:LEU:HD11	2.04	0.40
15:N:169:PRO:O	15:N:172:PHE:HB3	2.21	0.40
12:K:130:MET:SD	22:U:25:ASP:O	2.80	0.40
27:Z:33:MET:HG3	27:Z:69:TYR:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/239 (98%)	209 (89%)	23 (10%)	3 (1%)	14	35
4	B	335/337 (99%)	305 (91%)	24 (7%)	6 (2%)	10	25
5	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	38	66
6	D	134/177 (76%)	107 (80%)	23 (17%)	4 (3%)	5	12
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	20	46
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	143 (92%)	9 (6%)	4 (3%)	6	15
11	J	140/145 (97%)	128 (91%)	11 (8%)	1 (1%)	25	53
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	32	60
15	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	11	28
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	13	33
18	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	17	40
19	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	25	53
20	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	14	35
21	T	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
22	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
23	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	11	28
24	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	14	35
25	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	6	17
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	58 (82%)	9 (13%)	4 (6%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
31	I	68/162 (42%)	65 (96%)	3 (4%)	0	100	100
All	All	3705/4418 (84%)	3435 (93%)	232 (6%)	38 (1%)	18	43

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	137	PRO
6	D	173	GLU
8	F	101	ALA
10	H	166	SER
10	H	168	ALA
15	N	154	LEU
15	N	164	ASP
24	W	77	ALA
25	X	87	ALA
27	Z	81	ARG
3	A	34	ASP
3	A	36	ASP
6	D	27	ILE
10	H	16	ARG
10	H	140	VAL
11	J	5	GLU
15	N	139	TRP
17	P	117	SER
4	B	185	GLY
17	P	116	SER
3	A	27	LEU
4	B	138	GLY
4	B	169	GLY
4	B	206	THR
5	C	201	SER
24	W	76	ASP
27	Z	42	CYS
4	B	2	GLN
4	B	34	GLY
20	S	58	MET
27	Z	36	ASP
27	Z	43	GLY

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Mol	Chain	Res	Type
14	M	88	VAL
18	Q	18	PRO
6	D	28	GLY
19	R	81	PRO
23	V	43	PRO
25	X	70	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	169 (94%)	10 (6%)	25	51
4	B	282/282 (100%)	264 (94%)	18 (6%)	20	45
5	C	193/193 (100%)	177 (92%)	16 (8%)	13	30
6	D	117/148 (79%)	113 (97%)	4 (3%)	42	73
7	E	152/156 (97%)	149 (98%)	3 (2%)	60	86
8	F	93/94 (99%)	92 (99%)	1 (1%)	78	93
9	G	27/283 (10%)	26 (96%)	1 (4%)	39	70
10	H	132/138 (96%)	125 (95%)	7 (5%)	26	54
11	J	118/121 (98%)	110 (93%)	8 (7%)	18	41
12	K	106/106 (100%)	105 (99%)	1 (1%)	82	94
13	L	113/127 (89%)	107 (95%)	6 (5%)	26	54
14	M	158/158 (100%)	150 (95%)	8 (5%)	28	56
15	N	149/150 (99%)	145 (97%)	4 (3%)	50	80
16	O	93/94 (99%)	89 (96%)	4 (4%)	33	64
17	P	113/117 (97%)	108 (96%)	5 (4%)	33	63
18	Q	79/80 (99%)	77 (98%)	2 (2%)	53	82
19	R	117/122 (96%)	112 (96%)	5 (4%)	33	64
20	S	71/74 (96%)	69 (97%)	2 (3%)	49	79
21	T	105/106 (99%)	100 (95%)	5 (5%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/52 (85%)	43 (98%)	1 (2%)	56	84
23	V	51/57 (90%)	49 (96%)	2 (4%)	37	68
24	W	130/130 (100%)	124 (95%)	6 (5%)	31	61
25	X	66/74 (89%)	62 (94%)	4 (6%)	22	47
26	Y	120/196 (61%)	114 (95%)	6 (5%)	28	57
27	Z	60/60 (100%)	58 (97%)	2 (3%)	43	73
28	1	46/47 (98%)	46 (100%)	0	100	100
29	2	42/46 (91%)	40 (95%)	2 (5%)	30	59
30	3	79/79 (100%)	77 (98%)	2 (2%)	53	82
31	I	58/130 (45%)	57 (98%)	1 (2%)	66	88
All	All	3093/3601 (86%)	2957 (96%)	136 (4%)	33	63

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	GLU
3	A	36	ASP
3	A	64	ASP
3	A	66	ARG
3	A	69	LEU
3	A	94	LEU
3	A	131	HIS
3	A	179	MET
3	A	206	ARG
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	49	THR
4	B	51	VAL
4	B	53	LEU
4	B	56	ASP
4	B	97	LEU
4	B	98	THR
4	B	162	MET
4	B	171	VAL
4	B	175	LEU

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Mol	Chain	Res	Type
4	B	190	MET
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	257	THR
5	C	2	GLN
5	C	27	ARG
5	C	76	ARG
5	C	78	ARG
5	C	131	PHE
5	C	135	GLU
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	237	GLU
5	C	240	LEU
6	D	24	HIS
6	D	61	PHE
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	16	ASP
7	E	86	VAL
8	F	12	LEU
9	G	64	ASN
10	H	1	LYS
10	H	30	GLN
10	H	59	HIS
10	H	62	LEU
10	H	84	LYS
10	H	88	ARG
10	H	154	TYR
11	J	7	ASP
11	J	32	ASP
11	J	39	VAL
11	J	46	ILE
11	J	52	GLN

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Mol	Chain	Res	Type
11	J	79	PHE
11	J	107	ASN
11	J	131	THR
12	K	10	GLN
13	L	30	ARG
13	L	32	ASP
13	L	35	ARG
13	L	99	GLU
13	L	101	ASP
13	L	104	ASP
14	M	23	LEU
14	M	46	LEU
14	M	68	ARG
14	M	81	ARG
14	M	93	ARG
14	M	99	ARG
14	M	120	VAL
14	M	164	THR
15	N	26	LEU
15	N	49	THR
15	N	50	LEU
15	N	53	ASN
16	O	3	THR
16	O	43	VAL
16	O	67	SER
16	O	98	LEU
17	P	16	VAL
17	P	91	LYS
17	P	98	ILE
17	P	110	ASP
17	P	120	ARG
18	Q	16	ASN
18	Q	95	GLU
19	R	39	THR
19	R	55	GLN
19	R	82	GLU
19	R	132	ARG
19	R	143	VAL
20	S	10	VAL
20	S	71	ASP
21	T	26	THR
21	T	39	ASN

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Mol	Chain	Res	Type
21	T	73	HIS
21	T	89	ARG
21	T	112	LEU
22	U	52	THR
23	V	12	THR
23	V	22	ASP
24	W	26	ILE
24	W	52	VAL
24	W	73	LEU
24	W	142	ASP
24	W	146	ILE
24	W	154	ARG
25	X	27	ASP
25	X	49	ARG
25	X	72	VAL
25	X	82	GLU
26	Y	144	ARG
26	Y	154	ARG
26	Y	163	THR
26	Y	189	ASN
26	Y	203	VAL
26	Y	204	ARG
27	Z	36	ASP
27	Z	60	CYS
29	2	18	ASN
29	2	31	ARG
30	3	3	MET
30	3	14	CYS
31	I	113	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	125	ASN
3	A	127	GLN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN

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Mol	Chain	Res	Type
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	85	GLN
6	D	103	ASN
6	D	133	ASN
7	E	143	GLN
9	G	64	ASN
10	H	31	HIS
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	170	ASN
11	J	52	GLN
11	J	107	ASN
11	J	126	ASN
12	K	10	GLN
12	K	67	GLN
13	L	18	HIS
13	L	41	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	53	ASN
15	N	93	GLN
15	N	107	ASN
15	N	119	GLN
17	P	50	GLN
17	P	66	GLN
17	P	88	GLN
17	P	118	GLN
18	Q	16	ASN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	113	HIS
19	R	117	HIS
19	R	123	GLN

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Mol	Chain	Res	Type
20	S	53	ASN
21	T	39	ASN
22	U	39	ASN
23	V	4	HIS
23	V	60	GLN
24	W	12	ASN
24	W	28	HIS
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
25	X	36	HIS
26	Y	133	HIS
26	Y	134	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	37	HIS
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	15	ASN
30	3	30	GLN
30	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	235 (8%)	35 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	253 (8%)	36 (1%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A

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Mol	Chain	Res	Type
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G

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Mol	Chain	Res	Type
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	630	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	699	C
1	0	701	U
1	0	705	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G

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Mol	Chain	Res	Type
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1419	U
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1507	C
1	0	1524	U

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Mol	Chain	Res	Type
1	0	1525	G
1	0	1526	A
1	0	1562	C
1	0	1592	G
1	0	1605	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G

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Mol	Chain	Res	Type
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2346	C
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G

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Mol	Chain	Res	Type
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3034	A
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	169	A
1	0	284	C
1	0	603	A
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1120	U
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1667	A
1	0	1685	A
1	0	1730	G
1	0	1856	C
1	0	1878	G
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2850	C
2	9	3065	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	OMU	0	2587	1	14,22,23	0.90	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1	18,26,27	1.05	2 (11%)	22,38,41	2.45	4 (18%)
1	UR3	0	2619	1	14,22,23	0.67	0	16,32,35	0.74	0
1	PSU	0	2621	1	16,21,22	1.71	3 (18%)	20,30,33	6.11	5 (25%)
1	1MA	0	628	1,35	16,25,26	1.05	1 (6%)	13,37,40	1.14	1 (7%)

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
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.16	1.47	1.52
1	0	2588	OMG	C8-N7	-2.02	1.30	1.34
1	0	2587	OMU	C4-N3	2.17	1.37	1.33
1	0	2621	PSU	C4-N3	2.63	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38
1	0	628	1MA	C6-N6	2.81	1.33	1.27
1	0	2588	OMG	C6-N1	3.50	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.44	114.42	128.40
1	0	2621	PSU	C5-C4-N3	-12.53	115.15	125.43
1	0	2588	OMG	C5-C6-N1	-8.30	111.67	123.48
1	0	628	1MA	C2-N3-C4	-3.63	110.84	116.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2587	OMU	C5-C4-N3	-3.56	114.62	123.12
1	0	2588	OMG	C2-N3-C4	-2.82	111.86	115.16
1	0	2621	PSU	C5-C1'-C2'	-2.62	111.02	115.55
1	0	2588	OMG	N3-C2-N1	-2.40	123.95	127.46
1	0	2621	PSU	C6-N1-C2	2.83	119.88	115.36
1	0	2588	OMG	C6-N1-C2	6.26	125.06	116.06
1	0	2621	PSU	C4-N3-C2	13.57	127.03	115.16
1	0	2587	OMU	C4-N3-C2	15.15	127.15	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 230 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	$\# Z  > 2$
32	GIR	0	9000	-	9,12,12	0.76	0	5,16,16	0.71	0

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
32	GIR	0	9000	-	-	0/4/10/10	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	0	2749/2922 (94%)	-0.34	40 (1%) 74 75	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.33	4 (3%) 47 46	38, 64, 91, 149	0
3	A	237/239 (99%)	0.62	28 (11%) 5 4	30, 58, 99, 119	0
4	B	337/337 (100%)	0.15	3 (0%) 84 85	28, 56, 84, 95	0
5	C	246/246 (100%)	0.22	1 (0%) 92 93	25, 49, 74, 80	0
6	D	140/177 (79%)	2.12	62 (44%) 0 0	61, 105, 127, 136	0
7	E	172/178 (96%)	0.45	6 (3%) 44 44	46, 68, 87, 93	0
8	F	119/120 (99%)	0.95	20 (16%) 2 1	53, 78, 99, 117	0
9	G	29/348 (8%)	1.99	11 (37%) 0 0	77, 94, 105, 107	0
10	H	160/171 (93%)	0.41	6 (3%) 41 39	40, 58, 92, 100	0
11	J	142/145 (97%)	-0.02	0 100 100	35, 50, 74, 90	0
12	K	132/132 (100%)	0.09	1 (0%) 86 86	36, 54, 77, 87	0
13	L	145/165 (87%)	0.87	21 (14%) 3 2	29, 71, 118, 130	0
14	M	194/194 (100%)	0.01	1 (0%) 90 92	35, 47, 63, 73	0
15	N	186/187 (99%)	0.97	33 (17%) 2 1	41, 68, 115, 120	0
16	O	115/116 (99%)	0.26	2 (1%) 70 72	41, 57, 75, 80	0
17	P	143/149 (95%)	0.26	3 (2%) 64 65	43, 59, 78, 83	0
18	Q	95/96 (98%)	0.00	0 100 100	37, 48, 62, 78	0
19	R	150/155 (96%)	-0.03	0 100 100	33, 47, 66, 74	0
20	S	81/85 (95%)	0.84	9 (11%) 6 5	47, 67, 87, 94	0
21	T	119/120 (99%)	0.54	8 (6%) 19 16	41, 61, 88, 108	0
22	U	53/66 (80%)	0.41	1 (1%) 67 68	44, 61, 77, 83	0
23	V	65/71 (91%)	1.96	25 (38%) 0 0	60, 84, 118, 121	0
24	W	154/154 (100%)	0.05	1 (0%) 89 90	34, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/92 (89%)	0.42	7 (8%) 11 9	45, 61, 87, 102	0
26	Y	142/241 (58%)	0.17	6 (4%) 37 35	28, 47, 71, 92	0
27	Z	73/73 (100%)	2.91	36 (49%) 0 0	61, 98, 111, 115	0
28	1	56/57 (98%)	-0.00	0 100 100	29, 37, 43, 50	0
29	2	46/50 (92%)	0.61	7 (15%) 2 2	39, 68, 101, 114	0
30	3	92/92 (100%)	0.48	2 (2%) 62 63	40, 62, 75, 83	0
31	I	70/162 (43%)	3.94	61 (87%) 0 0	105, 124, 141, 141	0
All	All	6646/7462 (89%)	0.18	405 (6%) 22 20	24, 55, 105, 153	0

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	12.9
27	Z	26	VAL	12.8
27	Z	20	ARG	11.1
27	Z	11	SER	9.8
27	Z	34	ASN	9.3
27	Z	21	VAL	9.0
31	I	137	VAL	8.5
31	I	133	THR	8.1
6	D	63	ILE	8.0
6	D	10	PHE	7.8
6	D	69	ILE	7.8
31	I	102	VAL	7.6
31	I	79	ILE	7.4
31	I	93	GLN	7.4
31	I	96	PHE	7.3
9	G	27	ILE	7.1
3	A	37	VAL	7.0
27	Z	14	PHE	7.0
27	Z	31	SER	7.0
27	Z	22	SER	6.9
27	Z	25	ARG	6.9
31	I	88	GLY	6.8
15	N	147	ILE	6.7
27	Z	18	TYR	6.7
27	Z	37	HIS	6.4
31	I	84	GLY	6.2
31	I	117	LEU	6.2
2	9	3001	U	6.1

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Mol	Chain	Res	Type	RSRZ
31	I	85	PHE	6.1
23	V	40	PRO	6.1
31	I	97	VAL	6.0
23	V	39	ALA	6.0
23	V	43	PRO	5.9
13	L	80	ASP	5.9
6	D	66	GLY	5.9
31	I	109	ALA	5.9
31	I	139	ILE	5.9
27	Z	30	GLU	5.9
31	I	71	GLY	5.8
27	Z	33	MET	5.7
31	I	111	GLN	5.6
27	Z	16	ALA	5.5
6	D	26	GLY	5.5
27	Z	28	GLU	5.5
31	I	105	VAL	5.5
27	Z	35	GLU	5.5
27	Z	29	ILE	5.5
1	0	1173	A	5.4
6	D	18	ILE	5.3
6	D	27	ILE	5.3
31	I	98	ALA	5.3
6	D	64	ARG	5.3
27	Z	32	GLU	5.2
31	I	113	HIS	5.2
1	0	1198	U	5.1
6	D	128	LEU	5.1
1	0	1177	A	5.0
31	I	121	LEU	5.0
15	N	166	ALA	4.9
6	D	75	LEU	4.9
31	I	81	ASP	4.9
27	Z	12	GLY	4.9
27	Z	23	ARG	4.9
27	Z	24	ARG	4.9
6	D	171	ASP	4.8
3	A	237	GLY	4.8
1	0	1172	G	4.8
31	I	91	GLU	4.7
15	N	183	ASP	4.7
27	Z	44	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
3	A	38	ILE	4.6
31	I	83	ALA	4.6
31	I	135	LEU	4.5
1	0	735	C	4.5
1	0	1199	A	4.5
6	D	85	GLN	4.5
27	Z	45	ASP	4.5
6	D	11	HIS	4.4
31	I	107	GLN	4.4
31	I	77	GLU	4.4
8	F	119	ARG	4.4
6	D	25	MET	4.3
15	N	145	ALA	4.3
31	I	116	LEU	4.3
27	Z	19	GLY	4.3
27	Z	59	TYR	4.3
6	D	61	PHE	4.2
27	Z	36	ASP	4.2
6	D	170	TYR	4.2
6	D	62	ASP	4.2
31	I	103	ASP	4.1
20	S	81	ILE	4.1
26	Y	235	GLU	4.1
1	0	1951	G	4.1
6	D	88	LEU	4.1
6	D	57	THR	4.1
13	L	89	PHE	4.1
31	I	104	GLN	4.0
25	X	88	GLU	4.0
6	D	90	LEU	4.0
6	D	166	ILE	4.0
1	0	1175	G	4.0
6	D	58	VAL	3.9
6	D	93	LEU	3.9
31	I	87	THR	3.9
6	D	17	ARG	3.9
1	0	1171	A	3.9
3	A	82	VAL	3.9
13	L	60	GLU	3.9
27	Z	15	GLY	3.9
6	D	89	PRO	3.9
27	Z	10	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	1169	U	3.8
1	0	2237	G	3.8
31	I	114	PRO	3.8
23	V	8	ILE	3.8
31	I	76	ALA	3.8
10	H	45	VAL	3.7
3	A	60	PHE	3.7
31	I	75	THR	3.7
31	I	73	PRO	3.7
27	Z	46	ARG	3.6
15	N	115	VAL	3.6
9	G	23	ILE	3.6
15	N	179	LEU	3.6
2	9	3002	U	3.6
31	I	136	GLY	3.6
31	I	106	LYS	3.6
15	N	161	GLY	3.5
15	N	162	ASP	3.5
15	N	172	PHE	3.5
6	D	23	VAL	3.5
13	L	81	VAL	3.5
23	V	31	ARG	3.5
6	D	141	VAL	3.4
31	I	128	VAL	3.4
9	G	24	VAL	3.4
6	D	84	LEU	3.4
31	I	110	GLU	3.4
6	D	172	VAL	3.4
8	F	47	LEU	3.4
23	V	3	LEU	3.4
26	Y	234	VAL	3.4
15	N	150	TYR	3.4
31	I	126	LYS	3.4
1	0	1170	U	3.4
20	S	2	TRP	3.4
2	9	3024	U	3.4
31	I	124	ALA	3.4
6	D	68	PRO	3.4
6	D	134	LEU	3.4
21	T	119	ALA	3.3
27	Z	17	ARG	3.3
31	I	78	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
31	I	118	SER	3.3
23	V	52	ALA	3.3
13	L	106	VAL	3.3
15	N	148	ALA	3.2
13	L	105	TYR	3.2
31	I	132	CYS	3.2
1	0	970	U	3.2
3	A	31	LYS	3.2
13	L	91	VAL	3.2
23	V	41	GLU	3.2
1	0	1200	A	3.2
23	V	37	GLY	3.2
31	I	115	ASP	3.1
1	0	1202	A	3.1
1	0	282	C	3.1
14	M	194	ALA	3.1
4	B	128	ILE	3.1
23	V	38	GLY	3.1
29	2	35	ARG	3.1
26	Y	98	GLN	3.1
6	D	106	PHE	3.1
21	T	112	LEU	3.1
6	D	44	ILE	3.1
15	N	75	THR	3.0
31	I	92	PRO	3.0
21	T	116	ASP	3.0
23	V	49	LEU	3.0
31	I	100	LEU	3.0
6	D	13	MET	3.0
9	G	21	ASP	3.0
13	L	150	GLN	3.0
1	0	1168	C	3.0
8	F	20	LEU	3.0
21	T	115	GLU	3.0
27	Z	13	ARG	3.0
13	L	99	GLU	3.0
15	N	159	TYR	2.9
13	L	120	LEU	2.9
6	D	47	GLN	2.9
6	D	24	HIS	2.9
9	G	63	ARG	2.9
6	D	130	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
8	F	29	VAL	2.9
6	D	22	VAL	2.9
31	I	72	VAL	2.9
6	D	43	GLU	2.9
7	E	10	ASP	2.9
27	Z	47	VAL	2.9
3	A	133	ARG	2.9
8	F	75	ILE	2.9
4	B	181	ILE	2.9
8	F	91	VAL	2.9
30	3	1	MET	2.8
15	N	185	GLU	2.8
8	F	49	PHE	2.8
6	D	73	VAL	2.8
23	V	32	ALA	2.8
6	D	51	ARG	2.8
10	H	74	ILE	2.8
3	A	36	ASP	2.8
3	A	88	ILE	2.8
31	I	80	LYS	2.8
15	N	80	SER	2.8
13	L	75	LEU	2.8
23	V	59	ILE	2.8
9	G	71	LEU	2.8
1	0	1192	A	2.7
31	I	86	GLU	2.7
13	L	140	VAL	2.7
30	3	76	LYS	2.7
29	2	39	ARG	2.7
31	I	99	ASP	2.7
6	D	72	LYS	2.7
3	A	85	SER	2.7
1	0	960	G	2.7
8	F	99	THR	2.7
23	V	5	VAL	2.7
3	A	35	GLY	2.7
8	F	17	LEU	2.7
1	0	1178	G	2.7
1	0	2344	G	2.7
13	L	104	ASP	2.7
23	V	7	GLU	2.7
27	Z	27	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	1181	A	2.7
23	V	44	GLY	2.7
31	I	129	VAL	2.7
29	2	49	GLU	2.6
21	T	117	ASP	2.6
21	T	82	THR	2.6
3	A	103	VAL	2.6
3	A	96	LEU	2.6
6	D	56	ARG	2.6
6	D	71	ALA	2.6
1	0	285	A	2.6
6	D	45	THR	2.6
10	H	137	TYR	2.6
26	Y	97	LEU	2.6
6	D	98	PHE	2.6
25	X	80	GLU	2.6
15	N	160	SER	2.6
31	I	122	THR	2.6
3	A	135	VAL	2.6
15	N	152	GLU	2.6
1	0	1174	A	2.6
1	0	1180	U	2.5
1	0	1163	G	2.5
4	B	119	HIS	2.5
9	G	73	ASP	2.5
13	L	133	VAL	2.5
15	N	119	GLN	2.5
3	A	97	ALA	2.5
23	V	35	ALA	2.5
1	0	1167	G	2.5
13	L	118	LEU	2.5
9	G	65	THR	2.5
25	X	77	PHE	2.5
31	I	89	SER	2.5
16	O	48	ILE	2.5
8	F	98	VAL	2.5
31	I	123	ASN	2.5
31	I	108	ILE	2.5
17	P	67	LYS	2.5
1	0	1950	G	2.5
25	X	74	ALA	2.4
8	F	44	SER	2.4

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Mol	Chain	Res	Type	RSRZ
13	L	147	GLU	2.4
25	X	7	GLU	2.4
17	P	71	TYR	2.4
29	2	36	ASN	2.4
2	9	3023	U	2.4
15	N	127	LEU	2.4
20	S	68	LEU	2.4
7	E	170	ARG	2.4
15	N	158	LEU	2.4
23	V	42	ASN	2.4
23	V	23	LEU	2.4
8	F	39	SER	2.4
1	0	1279	U	2.4
6	D	92	GLU	2.4
15	N	149	GLU	2.4
3	A	89	ALA	2.4
27	Z	58	SER	2.4
3	A	236	GLY	2.4
3	A	94	LEU	2.4
6	D	41	LEU	2.4
20	S	1	SER	2.4
1	0	1195	G	2.4
20	S	67	ARG	2.4
13	L	100	ALA	2.3
15	N	83	LEU	2.3
21	T	118	SER	2.3
31	I	125	ALA	2.3
23	V	33	VAL	2.3
9	G	72	ASP	2.3
15	N	143	ARG	2.3
1	0	2884	G	2.3
6	D	136	ARG	2.3
13	L	97	VAL	2.3
27	Z	79	VAL	2.3
9	G	26	MET	2.3
10	H	83	TYR	2.3
13	L	96	VAL	2.3
6	D	65	GLU	2.3
6	D	81	GLU	2.3
3	A	34	ASP	2.3
7	E	45	ASP	2.3
6	D	104	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
15	N	138	ASP	2.3
15	N	167	ASP	2.3
1	0	1204	C	2.3
23	V	2	VAL	2.3
31	I	90	GLY	2.2
15	N	64	SER	2.2
8	F	28	ALA	2.2
1	0	1193	A	2.2
10	H	71	ARG	2.2
20	S	45	TYR	2.2
6	D	83	PHE	2.2
15	N	180	LEU	2.2
29	2	42	TRP	2.2
31	I	74	PRO	2.2
8	F	106	ALA	2.2
31	I	120	ASP	2.2
7	E	87	PHE	2.2
3	A	58	VAL	2.2
20	S	49	VAL	2.2
1	0	284	C	2.2
1	0	2004	U	2.2
6	D	162	ALA	2.2
31	I	95	ASP	2.2
6	D	70	GLY	2.2
3	A	99	ILE	2.2
20	S	77	VAL	2.2
26	Y	108	ASP	2.2
6	D	165	PHE	2.2
22	U	47	ARG	2.2
23	V	46	ILE	2.2
27	Z	80	ARG	2.2
8	F	90	GLU	2.2
15	N	139	TRP	2.2
3	A	41	THR	2.2
15	N	178	THR	2.2
31	I	138	THR	2.2
25	X	71	ARG	2.2
6	D	40	ILE	2.1
6	D	135	VAL	2.1
6	D	28	GLY	2.1
6	D	129	ASP	2.1
31	I	140	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	D	137	PRO	2.1
7	E	108	LEU	2.1
15	N	175	LEU	2.1
13	L	130	ARG	2.1
15	N	137	ALA	2.1
1	0	370	G	2.1
3	A	64	ASP	2.1
3	A	83	GLY	2.1
26	Y	216	ARG	2.1
3	A	59	GLU	2.1
13	L	125	PHE	2.1
1	0	2238	A	2.1
6	D	76	ARG	2.1
15	N	118	ILE	2.1
9	G	28	GLU	2.1
10	H	73	LEU	2.1
16	O	89	ILE	2.1
25	X	85	VAL	2.1
1	0	2345	A	2.1
15	N	155	GLU	2.1
1	0	138	U	2.1
8	F	16	ALA	2.1
3	A	158	VAL	2.1
20	S	24	LEU	2.1
3	A	80	LEU	2.1
7	E	5	LEU	2.1
23	V	45	ARG	2.0
21	T	85	GLU	2.0
8	F	11	ASP	2.0
8	F	14	ASP	2.0
23	V	28	LEU	2.0
12	K	132	VAL	2.0
5	C	135	GLU	2.0
29	2	24	TRP	2.0
24	W	93	ILE	2.0
1	0	1197	G	2.0
3	A	62	ASP	2.0
8	F	15	ASP	2.0
8	F	117	GLU	2.0
17	P	120	ARG	2.0
29	2	27	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.99	0.18	-	28,32,33,35	0
1	OMU	0	2587	21/22	0.98	0.13	-	34,36,37,39	0
1	UR3	0	2619	21/22	0.98	0.16	-	36,39,42,48	0
1	PSU	0	2621	20/21	0.99	0.14	-	28,30,33,34	0
1	OMG	0	2588	24/25	0.98	0.15	-	33,36,38,39	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8574	1/1	0.82	0.54	31.81	66,66,66,66	0
35	NA	0	8529	1/1	0.55	0.45	20.44	77,77,77,77	0
35	NA	R	8586	1/1	0.48	0.79	20.05	95,95,95,95	0
35	NA	0	8503	1/1	0.90	0.36	18.55	47,47,47,47	0
35	NA	0	8571	1/1	0.78	0.42	15.79	65,65,65,65	0
35	NA	9	8583	1/1	0.86	0.43	15.38	65,65,65,65	0
35	NA	0	8577	1/1	0.80	0.38	13.98	71,71,71,71	0
35	NA	0	8526	1/1	0.89	0.64	13.85	58,58,58,58	0
35	NA	0	8532	1/1	0.90	0.30	13.35	49,49,49,49	0
35	NA	0	8566	1/1	0.87	0.29	11.53	66,66,66,66	0
35	NA	0	8569	1/1	0.90	0.37	10.70	74,74,74,74	0
36	CL	0	8715	1/1	0.93	0.24	9.67	86,86,86,86	0
35	NA	0	8502	1/1	0.97	0.21	8.71	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8572	1/1	0.95	0.28	8.43	54,54,54,54	0
35	NA	0	8573	1/1	0.93	0.29	8.41	69,69,69,69	0
35	NA	0	8550	1/1	0.93	0.26	8.16	45,45,45,45	0
35	NA	0	8514	1/1	0.96	0.27	8.07	38,38,38,38	0
35	NA	0	8564	1/1	0.93	0.29	7.64	53,53,53,53	0
35	NA	0	8578	1/1	0.97	0.28	7.06	51,51,51,51	0
35	NA	0	8521	1/1	0.94	0.28	5.98	61,61,61,61	0
35	NA	0	8582	1/1	0.78	0.21	5.33	79,79,79,79	0
35	NA	0	8561	1/1	0.92	0.23	5.12	56,56,56,56	0
35	NA	L	8580	1/1	0.97	0.28	5.12	57,57,57,57	0
35	NA	0	8576	1/1	0.98	0.24	4.85	46,46,46,46	0
35	NA	0	8555	1/1	0.97	0.34	4.50	57,57,57,57	0
33	MG	0	8060	1/1	0.99	0.27	4.33	40,40,40,40	0
36	CL	0	8705	1/1	0.89	0.20	4.23	67,67,67,67	0
35	NA	0	8568	1/1	0.69	0.18	3.24	71,71,71,71	0
35	NA	R	8537	1/1	0.89	0.25	2.82	48,48,48,48	0
35	NA	0	8535	1/1	0.95	0.22	2.55	56,56,56,56	0
35	NA	0	8556	1/1	0.92	0.20	2.46	49,49,49,49	0
35	NA	0	8565	1/1	0.93	0.38	2.24	40,40,40,40	0
35	NA	0	8562	1/1	0.92	0.20	2.12	60,60,60,60	0
33	MG	0	8080	1/1	0.97	0.20	1.92	45,45,45,45	0
35	NA	0	8527	1/1	0.92	0.17	1.91	44,44,44,44	0
35	NA	C	8504	1/1	0.83	0.27	1.81	49,49,49,49	0
35	NA	0	8579	1/1	0.97	0.19	1.21	64,64,64,64	0
35	NA	0	8524	1/1	0.95	0.19	1.18	62,62,62,62	0
32	GIR	0	9000	12/12	0.91	0.21	1.17	23,40,50,53	0
34	K	0	8401	1/1	0.96	0.18	1.09	85,85,85,85	0
35	NA	M	8547	1/1	0.94	0.18	1.03	34,34,34,34	0
35	NA	0	8543	1/1	0.96	0.19	0.74	39,39,39,39	0
36	CL	O	8708	1/1	0.91	0.21	0.59	73,73,73,73	0
33	MG	0	8057	1/1	0.97	0.18	0.48	45,45,45,45	0
35	NA	0	8505	1/1	0.95	0.18	0.12	33,33,33,33	0
33	MG	0	8054	1/1	0.97	0.17	-0.57	37,37,37,37	0
35	NA	A	8545	1/1	0.96	0.16	-0.70	62,62,62,62	0
33	MG	0	8010	1/1	1.00	0.17	-0.91	33,33,33,33	0
37	CD	Z	8603	1/1	0.97	0.09	-1.02	98,98,98,98	0
36	CL	M	8718	1/1	0.99	0.13	-1.19	47,47,47,47	0
33	MG	0	8008	1/1	0.97	0.14	-1.24	37,37,37,37	0
35	NA	0	8533	1/1	0.85	0.14	-1.27	39,39,39,39	0
35	NA	0	8531	1/1	0.97	0.15	-1.28	50,50,50,50	0
35	NA	0	8523	1/1	0.95	0.17	-1.30	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8018	1/1	0.98	0.14	-1.38	50,50,50,50	0
33	MG	0	8076	1/1	0.98	0.12	-1.39	55,55,55,55	0
36	CL	3	8704	1/1	0.93	0.16	-1.43	71,71,71,71	0
35	NA	J	8546	1/1	0.93	0.13	-1.46	53,53,53,53	0
33	MG	0	8017	1/1	0.98	0.13	-1.53	26,26,26,26	0
35	NA	0	8544	1/1	0.97	0.10	-1.55	28,28,28,28	0
37	CD	3	8604	1/1	0.99	0.08	-1.59	68,68,68,68	0
33	MG	0	8053	1/1	0.94	0.16	-1.65	45,45,45,45	0
33	MG	0	8014	1/1	0.96	0.16	-1.68	32,32,32,32	0
33	MG	0	8038	1/1	0.99	0.13	-1.70	34,34,34,34	0
36	CL	0	8716	1/1	0.96	0.10	-1.81	56,56,56,56	0
35	NA	0	8510	1/1	0.92	0.12	-1.95	36,36,36,36	0
37	CD	U	8601	1/1	1.00	0.09	-1.99	62,62,62,62	0
33	MG	0	8012	1/1	0.97	0.10	-2.02	39,39,39,39	0
35	NA	0	8525	1/1	0.96	0.15	-2.05	56,56,56,56	0
36	CL	J	8721	1/1	0.98	0.10	-2.16	58,58,58,58	0
35	NA	0	8539	1/1	0.96	0.15	-2.25	30,30,30,30	0
33	MG	T	8073	1/1	0.85	0.12	-2.32	71,71,71,71	0
35	NA	H	8509	1/1	0.95	0.10	-2.36	39,39,39,39	0
36	CL	0	8712	1/1	0.98	0.08	-2.46	49,49,49,49	0
33	MG	0	8015	1/1	0.97	0.14	-2.50	35,35,35,35	0
34	K	0	8402	1/1	0.99	0.14	-2.50	57,57,57,57	0
35	NA	R	8538	1/1	0.85	0.08	-2.58	60,60,60,60	0
35	NA	0	8517	1/1	0.93	0.06	-2.62	51,51,51,51	0
33	MG	0	8112	1/1	0.99	0.12	-2.63	42,42,42,42	0
33	MG	0	8021	1/1	0.98	0.12	-2.63	30,30,30,30	0
33	MG	0	8007	1/1	0.98	0.13	-2.68	22,22,22,22	0
33	MG	0	8058	1/1	0.97	0.06	-2.98	39,39,39,39	0
35	NA	Q	8548	1/1	0.95	0.06	-3.01	42,42,42,42	0
35	NA	0	8520	1/1	0.97	0.14	-3.02	34,34,34,34	0
33	MG	0	8074	1/1	0.98	0.05	-3.04	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.07	-3.05	36,36,36,36	0
33	MG	0	8004	1/1	0.98	0.09	-3.05	29,29,29,29	0
33	MG	0	8039	1/1	0.94	0.11	-3.06	52,52,52,52	0
33	MG	0	8067	1/1	0.97	0.12	-3.15	52,52,52,52	0
33	MG	0	8013	1/1	0.97	0.12	-3.23	38,38,38,38	0
33	MG	B	8055	1/1	0.94	0.05	-3.30	48,48,48,48	0
33	MG	0	8096	1/1	0.87	0.11	-3.41	52,52,52,52	0
33	MG	Y	8109	1/1	0.99	0.09	-3.42	37,37,37,37	0
33	MG	B	8056	1/1	0.98	0.05	-3.45	55,55,55,55	0
36	CL	0	8713	1/1	0.93	0.08	-3.49	65,65,65,65	0
36	CL	B	8719	1/1	0.98	0.12	-3.65	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CD	1	8602	1/1	0.99	0.10	-3.66	63,63,63,63	0
33	MG	0	8001	1/1	0.99	0.14	-3.86	36,36,36,36	0
33	MG	0	8032	1/1	0.97	0.06	-4.41	28,28,28,28	0
33	MG	0	8091	1/1	0.96	0.07	-4.76	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.14	-5.13	33,33,33,33	0
33	MG	3	8078	1/1	0.98	0.05	-5.22	43,43,43,43	0
33	MG	0	8108	1/1	0.99	0.09	-5.55	70,70,70,70	0
33	MG	0	8044	1/1	0.91	0.10	-5.58	46,46,46,46	0
33	MG	0	8110	1/1	0.97	0.11	-5.65	27,27,27,27	0
35	NA	0	8553	1/1	0.97	0.11	-5.89	30,30,30,30	0
33	MG	0	8052	1/1	0.98	0.07	-7.12	54,54,54,54	0
33	MG	A	8065	1/1	0.99	0.06	-7.63	41,41,41,41	0
33	MG	0	8019	1/1	0.98	0.06	-8.09	35,35,35,35	0
33	MG	0	8020	1/1	0.98	0.09	-8.52	33,33,33,33	0
33	MG	0	8022	1/1	0.98	0.10	-8.67	38,38,38,38	0
33	MG	0	8006	1/1	0.99	0.06	-9.02	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.05	-9.19	47,47,47,47	0
33	MG	0	8035	1/1	0.97	0.05	-9.96	46,46,46,46	0
33	MG	0	8033	1/1	0.97	0.09	-10.68	31,31,31,31	0
33	MG	0	8003	1/1	0.99	0.09	-11.24	35,35,35,35	0
33	MG	0	8064	1/1	0.97	0.07	-11.92	30,30,30,30	0
33	MG	0	8002	1/1	0.98	0.09	-16.72	34,34,34,34	0
35	NA	0	8536	1/1	0.95	0.10	-	55,55,55,55	0
33	MG	0	8011	1/1	0.98	0.18	-	27,27,27,27	0
33	MG	0	8036	1/1	0.98	0.06	-	33,33,33,33	0
33	MG	0	8090	1/1	0.68	0.75	-	69,69,69,69	0
33	MG	0	8075	1/1	0.95	0.06	-	44,44,44,44	0
33	MG	0	8027	1/1	0.97	0.04	-	44,44,44,44	0
35	NA	0	8575	1/1	0.96	0.27	-	61,61,61,61	0
33	MG	0	8115	1/1	0.98	0.08	-	52,52,52,52	0
35	NA	0	8563	1/1	0.85	0.46	-	57,57,57,57	0
33	MG	0	8059	1/1	0.99	0.06	-	43,43,43,43	0
33	MG	0	8063	1/1	0.97	0.21	-	60,60,60,60	0
36	CL	R	8706	1/1	0.96	0.15	-	46,46,46,46	0
33	MG	0	8079	1/1	0.98	0.17	-	37,37,37,37	0
33	MG	0	8106	1/1	0.98	0.09	-	65,65,65,65	0
35	NA	0	8567	1/1	0.89	0.29	-	59,59,59,59	0
33	MG	0	8046	1/1	0.92	0.09	-	53,53,53,53	0
33	MG	0	8116	1/1	0.88	0.07	-	58,58,58,58	0
33	MG	0	8083	1/1	0.99	0.12	-	43,43,43,43	0
36	CL	0	8717	1/1	0.91	0.11	-	65,65,65,65	0
33	MG	0	8072	1/1	0.97	0.07	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8031	1/1	0.96	0.12	-	34,34,34,34	0
35	NA	0	8518	1/1	0.97	0.19	-	42,42,42,42	0
33	MG	0	8048	1/1	0.98	0.12	-	54,54,54,54	0
35	NA	S	8512	1/1	0.87	0.09	-	43,43,43,43	0
33	MG	0	8093	1/1	0.97	0.09	-	56,56,56,56	0
33	MG	0	8111	1/1	0.98	0.09	-	42,42,42,42	0
36	CL	A	8709	1/1	0.93	0.24	-	77,77,77,77	0
36	CL	0	8714	1/1	0.96	0.14	-	54,54,54,54	0
35	NA	0	8515	1/1	0.97	0.20	-	42,42,42,42	0
33	MG	0	8034	1/1	0.99	0.09	-	33,33,33,33	0
33	MG	A	8066	1/1	0.91	0.04	-	72,72,72,72	0
33	MG	0	8088	1/1	0.97	0.14	-	38,38,38,38	0
36	CL	0	8703	1/1	0.98	0.08	-	58,58,58,58	0
35	NA	0	8540	1/1	0.78	0.21	-	58,58,58,58	0
33	MG	0	8098	1/1	0.98	0.08	-	40,40,40,40	0
33	MG	0	8117	1/1	0.98	0.06	-	32,32,32,32	0
36	CL	J	8701	1/1	0.94	0.22	-	66,66,66,66	0
33	MG	0	8041	1/1	0.91	0.19	-	56,56,56,56	0
36	CL	0	8722	1/1	0.87	0.37	-	81,81,81,81	0
35	NA	0	8584	1/1	0.88	0.14	-	62,62,62,62	0
33	MG	0	8045	1/1	0.98	0.07	-	53,53,53,53	0
33	MG	0	8026	1/1	0.98	0.17	-	26,26,26,26	0
33	MG	0	8042	1/1	0.96	0.10	-	38,38,38,38	0
35	NA	0	8552	1/1	0.78	0.21	-	62,62,62,62	0
33	MG	0	8089	1/1	0.97	0.14	-	74,74,74,74	0
33	MG	0	8087	1/1	0.88	0.12	-	66,66,66,66	0
35	NA	0	8528	1/1	0.98	0.32	-	42,42,42,42	0
35	NA	0	8511	1/1	0.90	0.15	-	50,50,50,50	0
33	MG	0	8101	1/1	0.93	0.19	-	69,69,69,69	0
33	MG	0	8071	1/1	0.96	0.04	-	69,69,69,69	0
35	NA	0	8558	1/1	0.95	0.35	-	82,82,82,82	0
33	MG	0	8103	1/1	0.93	0.18	-	82,82,82,82	0
35	NA	0	8541	1/1	0.94	0.10	-	50,50,50,50	0
33	MG	0	8099	1/1	0.96	0.16	-	45,45,45,45	0
33	MG	0	8092	1/1	0.79	0.13	-	89,89,89,89	0
33	MG	0	8016	1/1	0.98	0.09	-	40,40,40,40	0
33	MG	0	8062	1/1	0.98	0.09	-	54,54,54,54	0
33	MG	0	8081	1/1	0.94	0.10	-	49,49,49,49	0
33	MG	K	8069	1/1	0.97	0.05	-	58,58,58,58	0
33	MG	0	8086	1/1	0.95	0.07	-	52,52,52,52	0
35	NA	0	8559	1/1	0.94	0.24	-	49,49,49,49	0
33	MG	0	8050	1/1	0.90	0.08	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8114	1/1	0.86	0.65	-	67,67,67,67	0
35	NA	0	8516	1/1	0.92	0.25	-	54,54,54,54	0
35	NA	0	8542	1/1	0.90	0.39	-	47,47,47,47	0
36	CL	Q	8711	1/1	0.98	0.08	-	55,55,55,55	0
33	MG	0	8068	1/1	0.96	0.04	-	61,61,61,61	0
33	MG	9	8095	1/1	0.89	0.12	-	76,76,76,76	0
33	MG	0	8040	1/1	0.97	0.13	-	60,60,60,60	0
35	NA	0	8506	1/1	0.90	0.37	-	48,48,48,48	0
33	MG	0	8030	1/1	0.99	0.10	-	25,25,25,25	0
35	NA	0	8501	1/1	0.95	0.21	-	32,32,32,32	0
33	MG	0	8049	1/1	0.75	0.19	-	92,92,92,92	0
35	NA	0	8554	1/1	0.98	0.16	-	40,40,40,40	0
33	MG	0	8082	1/1	0.88	0.14	-	63,63,63,63	0
36	CL	N	8707	1/1	0.95	0.11	-	66,66,66,66	0
35	NA	0	8581	1/1	0.95	0.08	-	48,48,48,48	0
35	NA	0	8534	1/1	0.95	0.07	-	45,45,45,45	0
33	MG	0	8061	1/1	0.97	0.17	-	41,41,41,41	0
33	MG	0	8113	1/1	0.91	0.12	-	53,53,53,53	0
36	CL	Y	8720	1/1	0.98	0.13	-	46,46,46,46	0
33	MG	0	8051	1/1	0.97	0.05	-	59,59,59,59	0
33	MG	0	8028	1/1	0.97	0.05	-	38,38,38,38	0
37	CD	O	8605	1/1	0.96	0.08	-	93,93,93,93	0
33	MG	0	8009	1/1	0.99	0.17	-	35,35,35,35	0
33	MG	0	8085	1/1	0.94	0.12	-	54,54,54,54	0
36	CL	J	8702	1/1	0.97	0.10	-	57,57,57,57	0
36	CL	L	8710	1/1	0.95	0.19	-	60,60,60,60	0
35	NA	0	8513	1/1	0.90	0.09	-	62,62,62,62	0
35	NA	0	8570	1/1	0.95	0.34	-	69,69,69,69	0
35	NA	9	8551	1/1	0.71	0.19	-	50,50,50,50	0
35	NA	0	8549	1/1	0.96	0.18	-	51,51,51,51	0
33	MG	0	8097	1/1	0.94	0.10	-	34,34,34,34	0
33	MG	0	8043	1/1	0.96	0.08	-	48,48,48,48	0
35	NA	0	8557	1/1	0.92	0.12	-	61,61,61,61	0
33	MG	0	8094	1/1	0.97	0.07	-	77,77,77,77	0
33	MG	0	8029	1/1	0.98	0.07	-	35,35,35,35	0
33	MG	0	8102	1/1	0.91	0.29	-	73,73,73,73	0
35	NA	0	8507	1/1	0.94	0.32	-	59,59,59,59	0
33	MG	0	8104	1/1	0.91	0.23	-	65,65,65,65	0
33	MG	0	8100	1/1	0.91	0.18	-	66,66,66,66	0
35	NA	0	8560	1/1	0.95	0.30	-	51,51,51,51	0
33	MG	0	8024	1/1	0.98	0.13	-	21,21,21,21	0
33	MG	0	8070	1/1	0.97	0.16	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8037	1/1	0.98	0.09	-	43,43,43,43	0
35	NA	H	8522	1/1	0.83	0.33	-	67,67,67,67	0
35	NA	0	8530	1/1	0.97	0.15	-	50,50,50,50	0
33	MG	0	8047	1/1	0.93	0.13	-	74,74,74,74	0
35	NA	0	8585	1/1	0.86	0.26	-	51,51,51,51	0
33	MG	0	8005	1/1	0.99	0.16	-	33,33,33,33	0
33	MG	0	8023	1/1	0.97	0.27	-	41,41,41,41	0
33	MG	0	8025	1/1	0.97	0.09	-	37,37,37,37	0
35	NA	0	8508	1/1	0.92	0.15	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.