



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:25 pm BST

PDB ID : 1XNQ  
Title : Structure of an Inosine-Adenine Wobble Base Pair Complex in the Context of the Decoding Center  
Authors : Murphy, F.V.; Ramakrishnan, V.  
Deposited on : 2004-10-05  
Resolution : 3.05 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

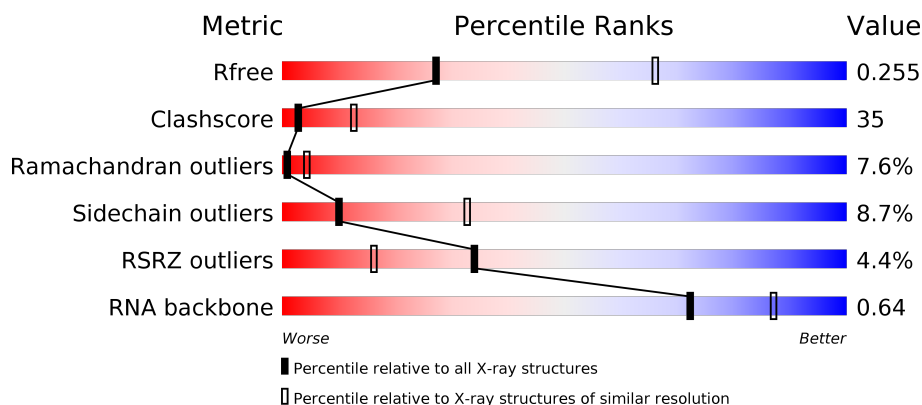
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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.



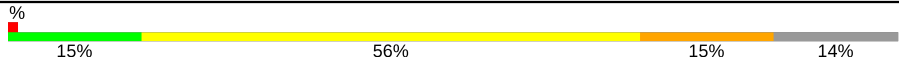
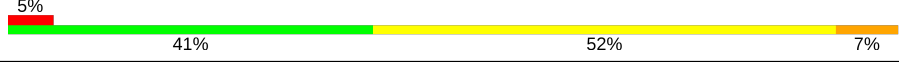
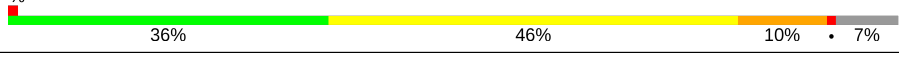
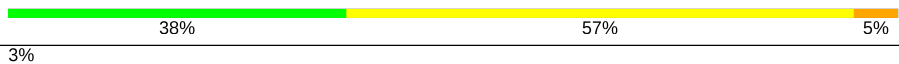
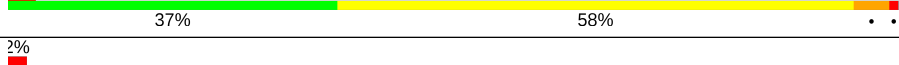
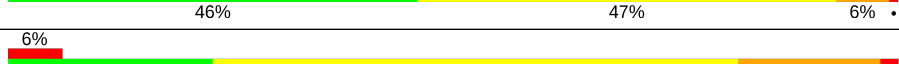
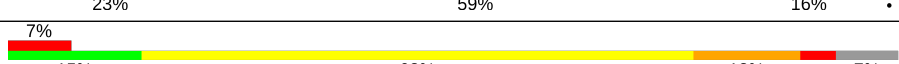
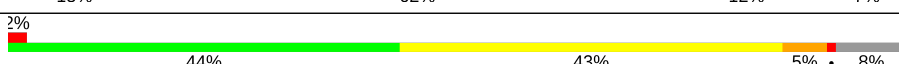
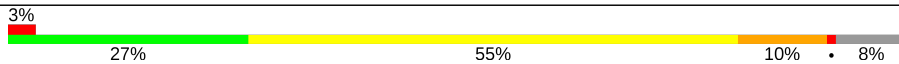
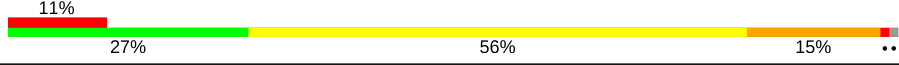
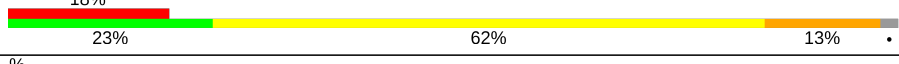
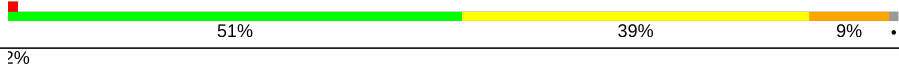
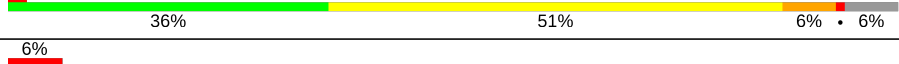

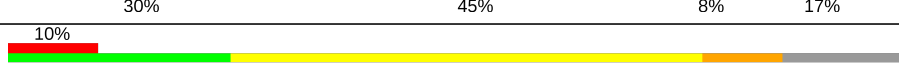
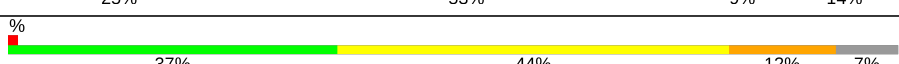
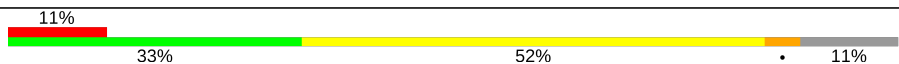

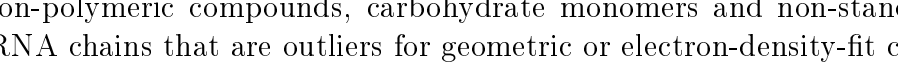
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>5%</div> <div>32%</div> <div>53%</div> <div>12%</div> <div>..</div> </div>
2	X	11	<div> <div>64%</div> <div>36%</div> </div>
3	W	4	<div> <div>75%</div> <div>25%</div> </div>
4	B	256	<div> <div>2%</div> <div>21%</div> <div>55%</div> <div>13%</div> <div>•</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

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
25	MG	A	1575	-	-	-	X
25	MG	A	1594	-	-	-	X
25	MG	A	467	-	-	-	X
25	MG	X	502	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52076 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called Anticodon tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	11	Total	C	N	O	P	0	0	0
			232	105	43	74	10			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	4	Total	C	N	O	P	0	0	0
			84	39	18	24	3			

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called Ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called Ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 12 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

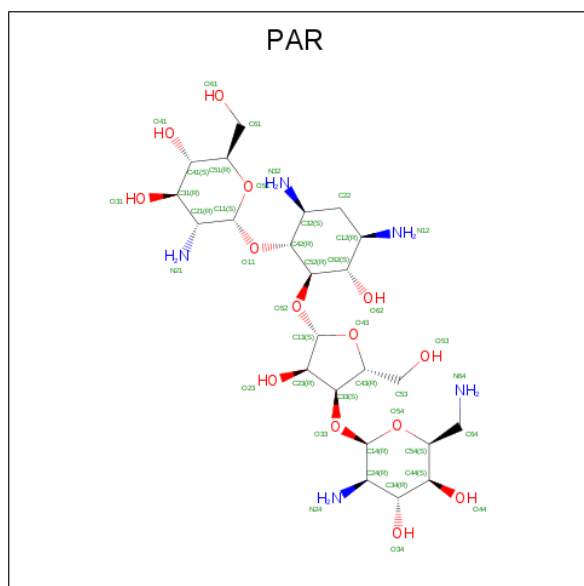
- Molecule 22 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called Ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	1	Total 1	Mg 1	0	0
25	A	104	Total 104	Mg 104	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

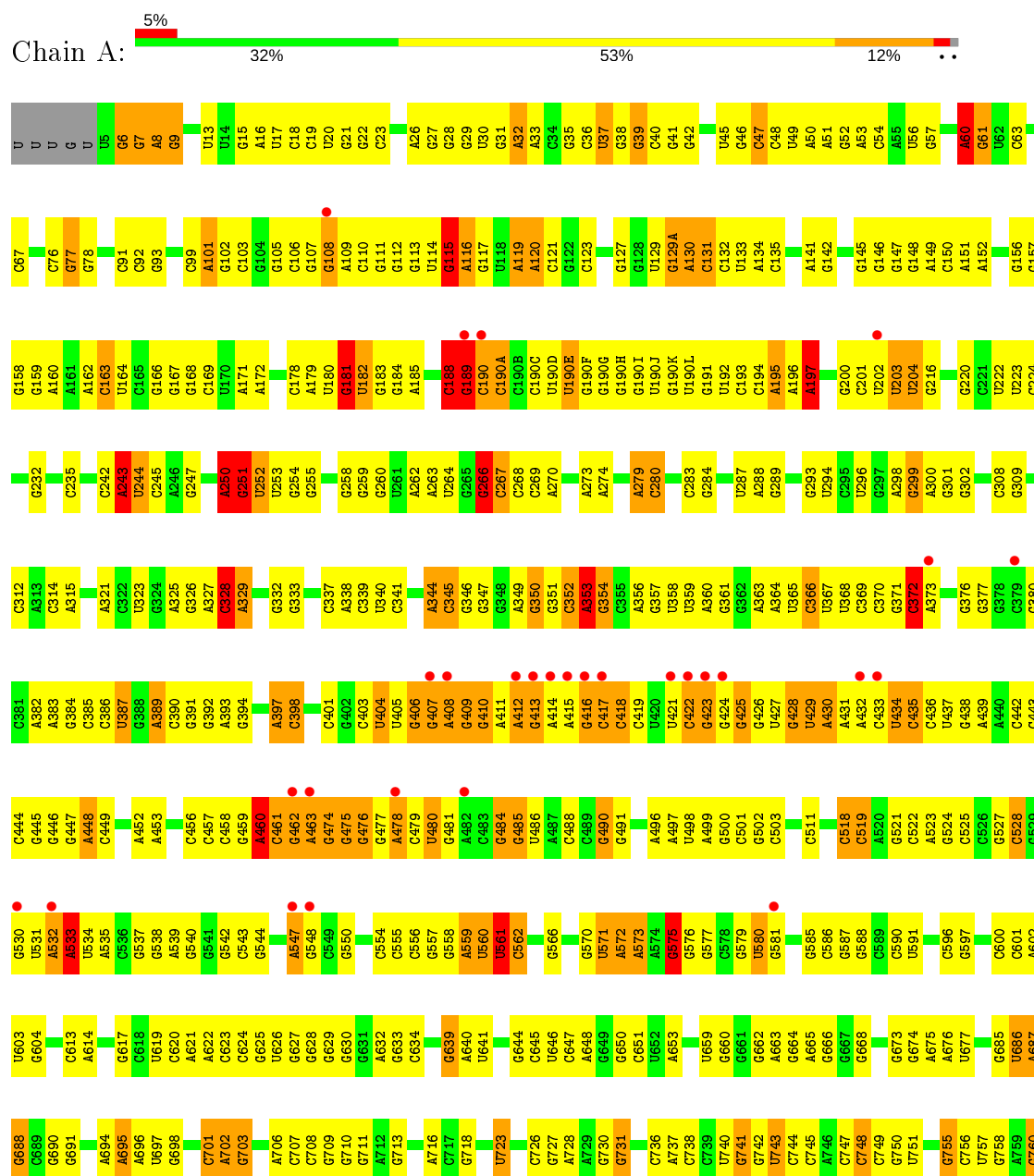
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

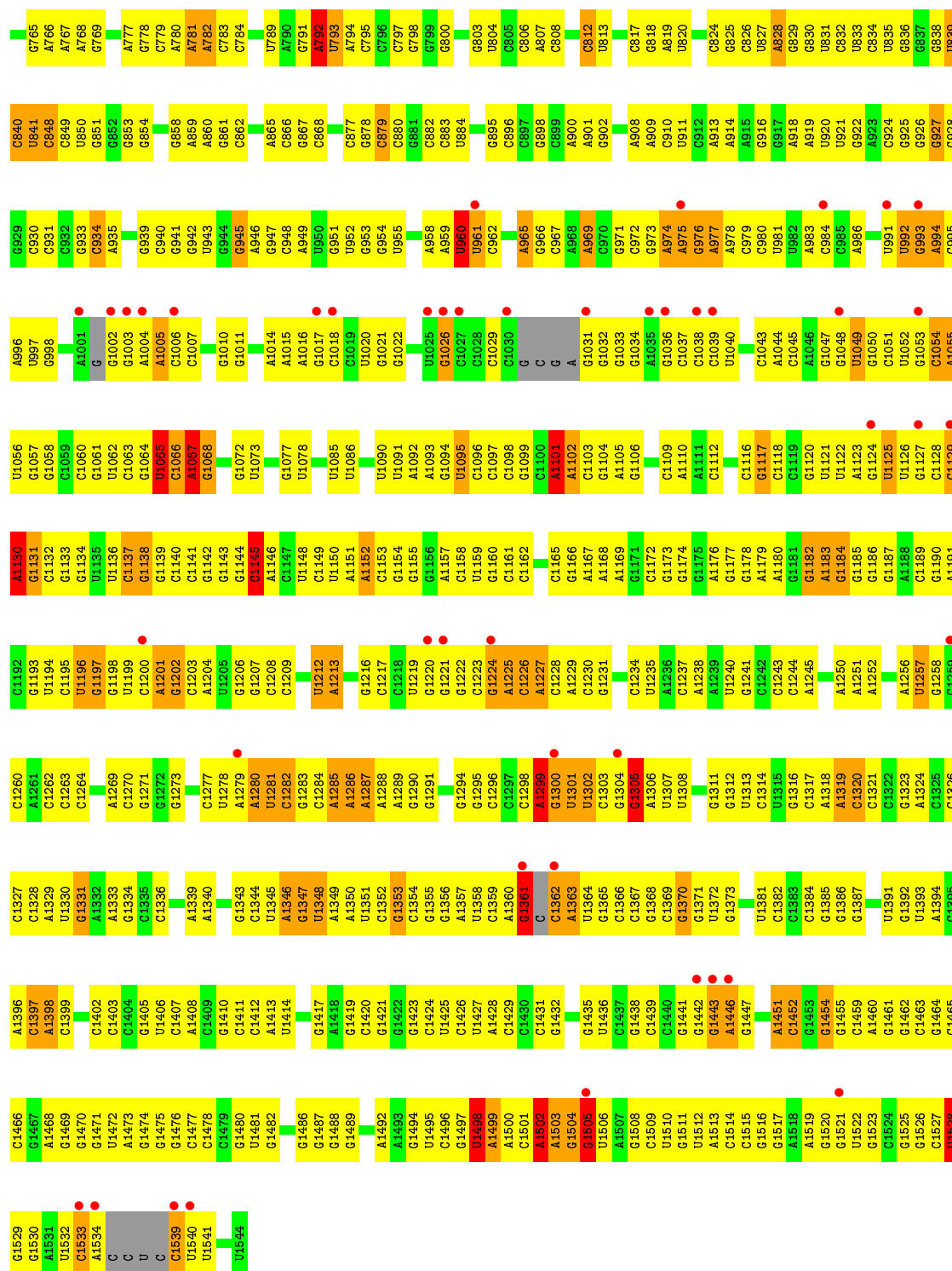


### 3 Residue-property plots

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: 16S ribosomal RNA



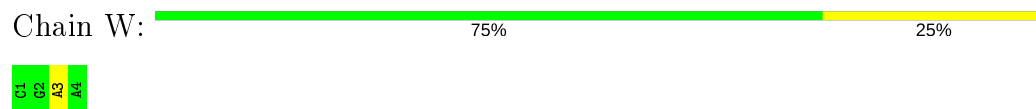


### • Molecule 2: Anticodon tRNA

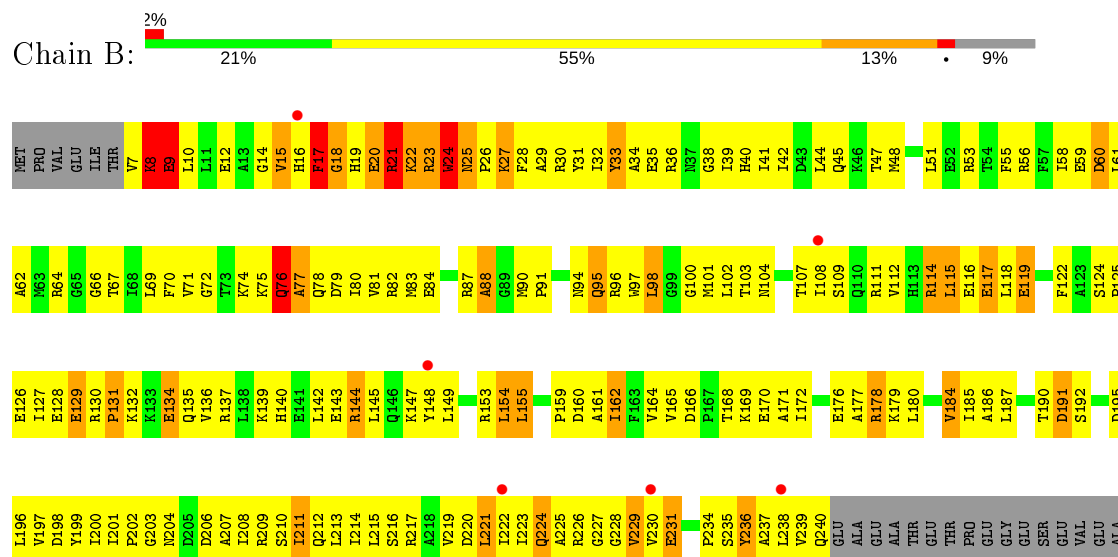
Chain X:



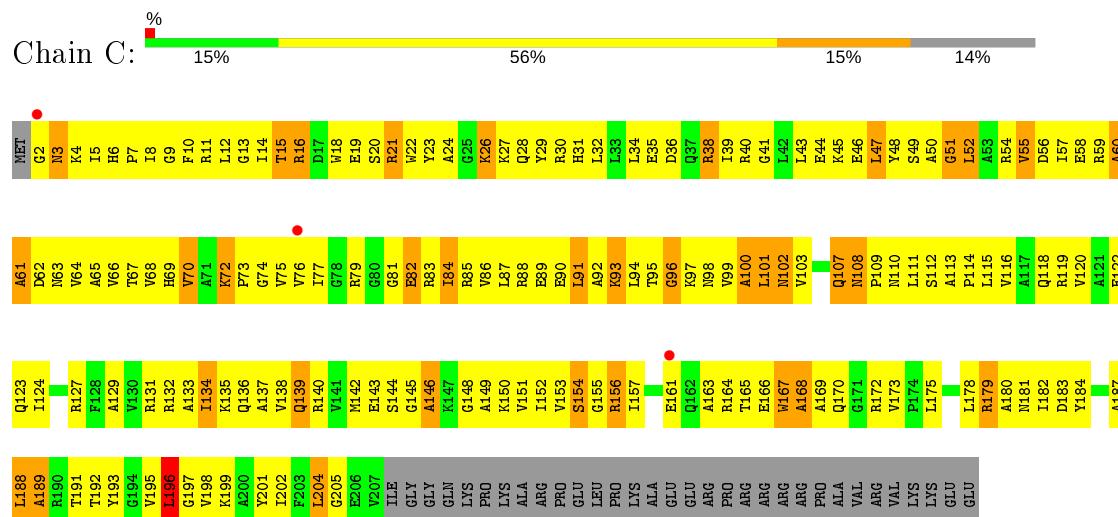
- Molecule 3: mRNA



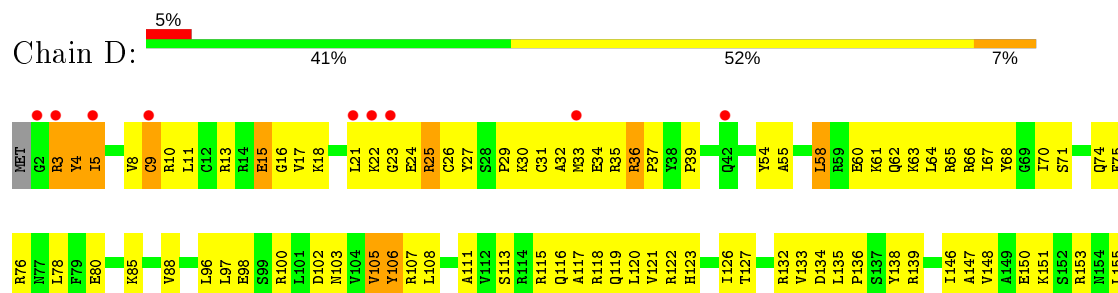
- Molecule 4: Ribosomal protein S2



- Molecule 5: Ribosomal protein S3

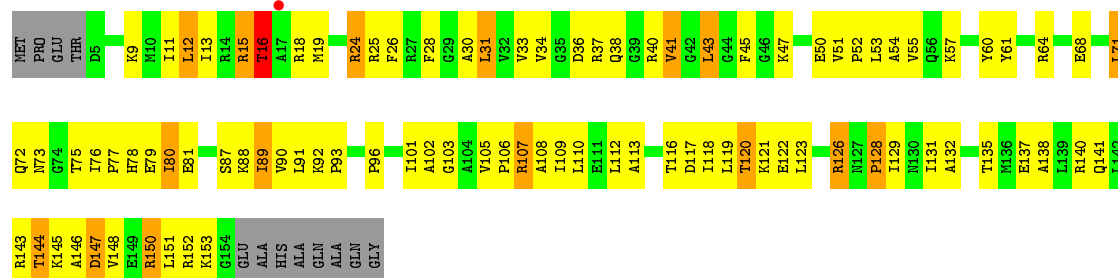


- Molecule 6: Ribosomal protein S4

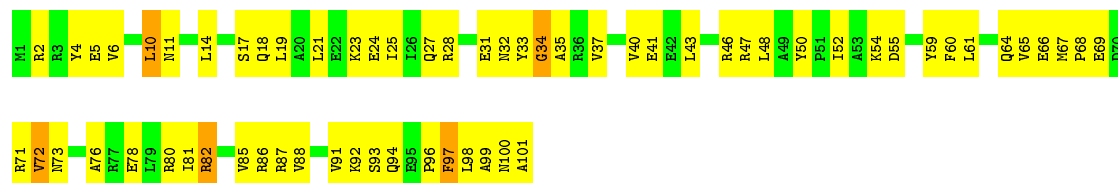




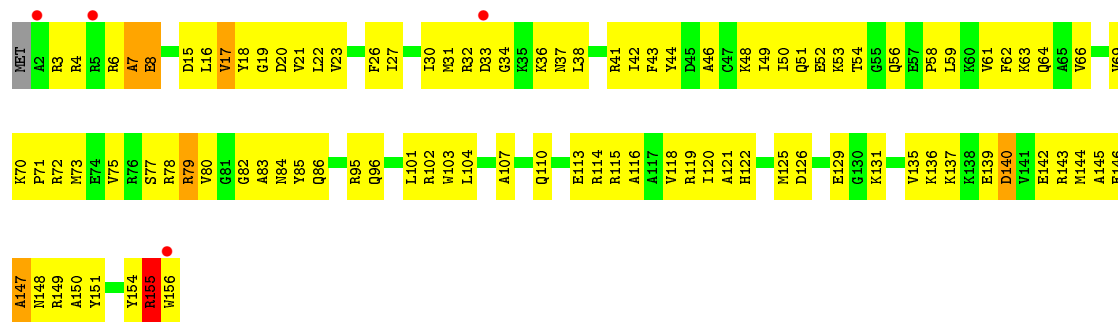
• Molecule 7: Ribosomal protein S5



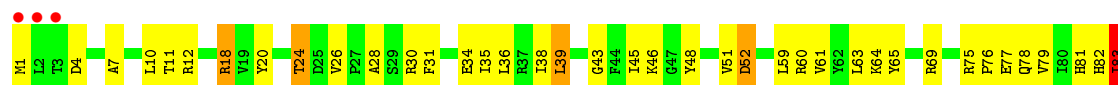
• Molecule 8: Ribosomal protein S6

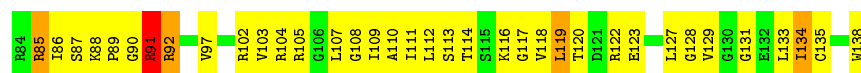


• Molecule 9: Ribosomal protein S7



• Molecule 10: Ribosomal protein S8

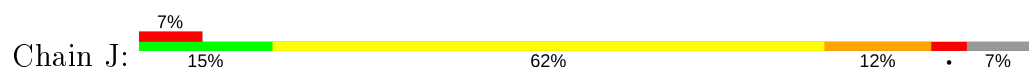




• Molecule 11: Ribosomal protein S9



• Molecule 12: Ribosomal protein S10



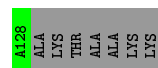
• Molecule 13: Ribosomal protein S11

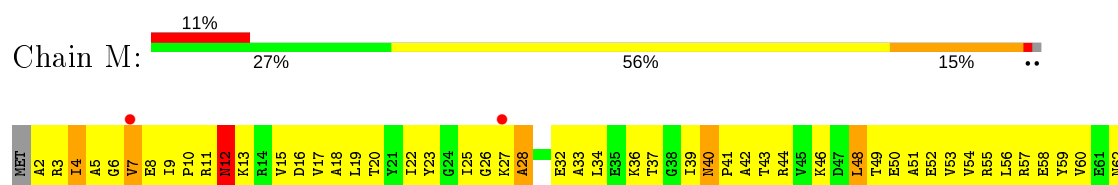


• Molecule 14: Ribosomal protein S12

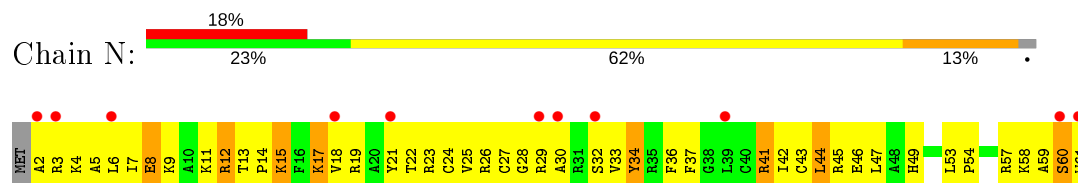


• Molecule 15: Ribosomal protein S13

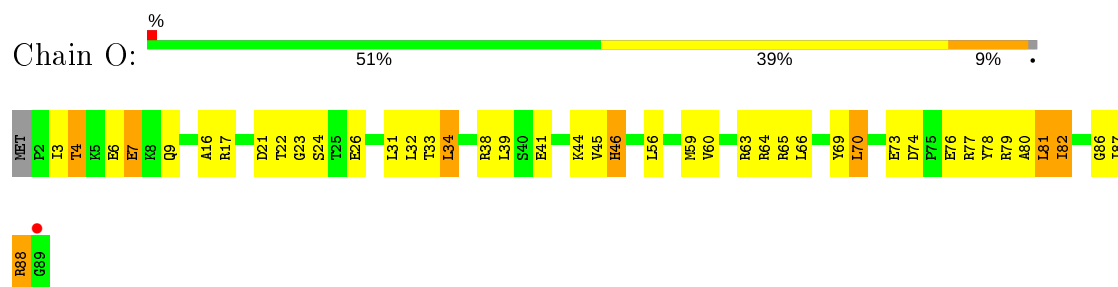




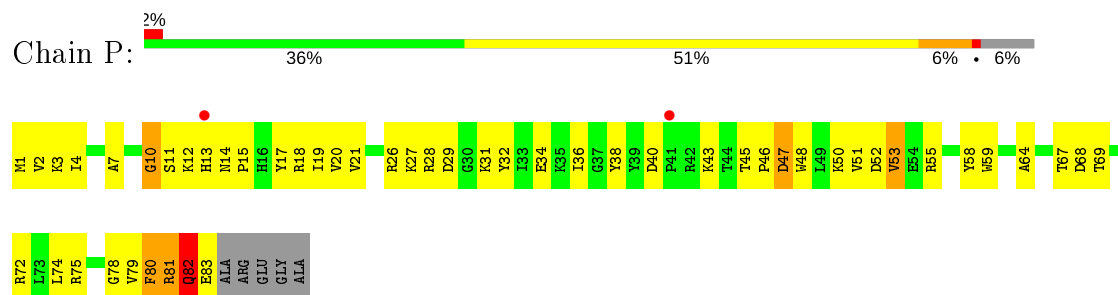
- Molecule 16: Ribosomal protein S14



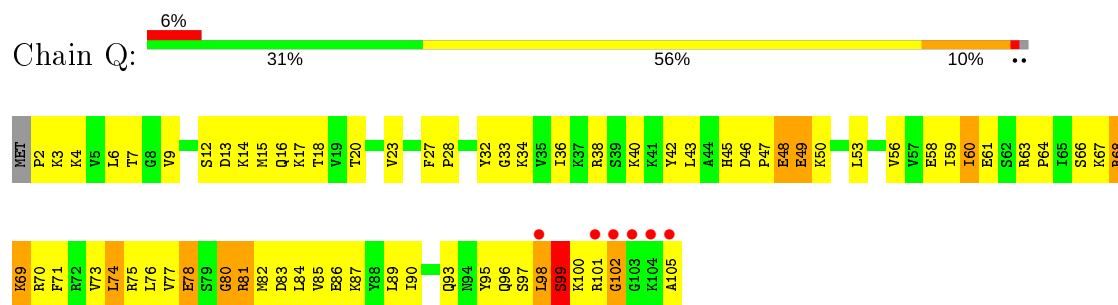
- Molecule 17: Ribosomal protein S15



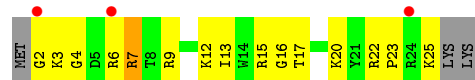
- Molecule 18: Ribosomal protein S16



- Molecule 19: Ribosomal protein S17



- Molecule 20: Ribosomal protein S18



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.13Å 401.13Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.05 283.65 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.6 (99.00-3.05) 88.7 (283.65-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.85 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.270 0.214 , 0.255	Depositor DCC
$R_{free}$ test set	13849 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 82.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	52076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	2/36244 (0.0%)	0.75	37/56567 (0.1%)
2	X	0.54	0/258	0.83	0/398
3	W	0.39	0/94	0.71	0/145
4	B	0.33	0/1935	0.62	0/2609
5	C	0.37	0/1636	0.64	1/2205 (0.0%)
6	D	0.37	0/1733	0.65	0/2318
7	E	0.44	0/1162	0.73	0/1564
8	F	0.32	0/856	0.60	0/1154
9	G	0.35	0/1276	0.62	1/1709 (0.1%)
10	H	0.42	0/1136	0.75	0/1527
11	I	0.35	0/1029	0.63	0/1378
12	J	0.36	0/805	0.68	1/1082 (0.1%)
13	K	0.40	0/900	0.63	0/1213
14	L	0.42	0/986	0.74	0/1320
15	M	0.34	0/1008	0.65	0/1347
16	N	0.42	0/501	0.70	0/664
17	O	0.35	0/745	0.57	0/992
18	P	0.45	0/716	0.76	0/963
19	Q	0.45	0/870	0.75	0/1159
20	R	0.33	0/603	0.61	0/799
21	S	0.30	0/661	0.61	0/890
22	T	0.40	0/764	0.68	0/1006
23	V	0.42	0/212	0.65	0/277
All	All	0.48	2/56130 (0.0%)	0.72	40/83286 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.55	1.50	1.42
1	A	1361	G	O3'-P	5.09	1.67	1.61

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	10.20	131.94	109.50
1	A	115	G	C2'-C3'-O3'	9.68	130.79	109.50
1	A	243	A	C2'-C3'-O3'	9.25	129.85	109.50
1	A	559	A	C2'-C3'-O3'	8.95	129.20	109.50
1	A	575	G	C2'-C3'-O3'	8.79	128.84	109.50
1	A	366	C	C2'-C3'-O3'	8.54	128.28	109.50
1	A	181	G	C2'-C3'-O3'	8.43	128.03	109.50
1	A	1503	A	C2'-C3'-O3'	8.38	127.94	109.50
1	A	1528	U	C2'-C3'-O3'	8.38	127.93	109.50
1	A	965	A	C2'-C3'-O3'	7.83	126.73	109.50
1	A	189	G	N9-C1'-C2'	-7.77	103.46	112.00
1	A	533	A	C2'-C3'-O3'	7.54	126.10	109.50
1	A	792	A	C2'-C3'-O3'	7.54	126.08	109.50
1	A	188	C	C2'-C3'-O3'	7.52	126.05	109.50
1	A	60	A	C2'-C3'-O3'	7.48	125.95	109.50
1	A	1505	G	C2'-C3'-O3'	7.30	125.57	109.50
1	A	1299	A	N9-C1'-C2'	6.99	123.09	114.00
1	A	760	G	N9-C1'-C2'	-6.83	104.49	112.00
1	A	812	C	C2'-C3'-O3'	6.69	124.41	113.70
5	C	196	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	266	G	C2'-C3'-O3'	6.52	124.14	113.70
1	A	960	U	C2'-C3'-O3'	6.36	123.88	113.70
9	G	147	ALA	N-CA-C	-6.31	93.95	111.00
1	A	686	U	N1-C1'-C2'	6.11	121.94	114.00
1	A	1502	A	N9-C1'-C2'	5.87	121.62	114.00
1	A	372	C	C2'-C3'-O3'	5.86	123.08	113.70
1	A	1528	U	C4'-C3'-O3'	5.83	124.65	113.00
1	A	353	A	C5'-C4'-O4'	-5.81	102.13	109.10
1	A	328	C	C2'-C3'-O3'	5.76	122.92	113.70
1	A	1346	A	C2'-C3'-O3'	5.73	122.86	113.70
1	A	484	G	C2'-C3'-O3'	5.70	122.83	113.70
1	A	1101	A	C2'-C3'-O3'	5.62	122.69	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	U	C1'-O4'-C4'	-5.50	105.50	109.90
1	A	1067	A	C2'-C3'-O3'	5.46	122.44	113.70
12	J	60	ARG	N-CA-C	5.42	125.63	111.00
1	A	266	G	N9-C1'-C2'	5.22	120.78	114.00
1	A	1305	G	N9-C1'-C2'	5.17	120.73	114.00
1	A	203	U	N1-C1'-C2'	5.13	120.67	114.00
1	A	63	C	C5'-C4'-C3'	-5.13	107.79	116.00
1	A	389	A	C5'-C4'-C3'	5.10	124.17	116.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	1498	U	C3'
1	A	1528	U	C3'

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1077	G	Sidechain
1	A	108	G	Sidechain
1	A	1130	A	Sidechain
1	A	1145	C	Sidechain
1	A	1299	A	Sidechain
1	A	1331	G	Sidechain
1	A	1361	G	Sidechain
1	A	1370	G	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	1498	U	Sidechain
1	A	1502	A	Sidechain
1	A	1519	A	Sidechain
1	A	189	G	Sidechain
1	A	197	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	299	G	Sidechain
1	A	323	U	Sidechain
1	A	37	U	Sidechain
1	A	380	G	Sidechain
1	A	387	U	Sidechain
1	A	404	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	460	A	Sidechain
1	A	490	G	Sidechain
1	A	528	C	Sidechain
1	A	554	C	Sidechain
1	A	561	U	Sidechain
1	A	571	U	Sidechain
1	A	572	A	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	580	U	Sidechain
1	A	587	G	Sidechain
1	A	639	G	Sidechain
1	A	727	G	Sidechain
1	A	741	G	Sidechain
1	A	743	U	Sidechain
1	A	77	G	Sidechain
1	A	879	C	Sidechain
1	A	880	C	Sidechain
1	A	898	G	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	1153	0
2	X	232	0	120	4	0
3	W	84	0	46	1	0
4	B	1900	0	1951	274	0
5	C	1612	0	1677	274	0
6	D	1703	0	1764	153	0
7	E	1146	0	1207	118	0
8	F	843	0	857	68	0
9	G	1257	0	1296	110	0
10	H	1116	0	1177	112	0
11	I	1011	0	1043	124	0
12	J	792	0	835	151	1
13	K	885	0	904	77	0
14	L	970	0	1057	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	997	0	1072	124	0
16	N	492	0	529	66	0
17	O	734	0	771	54	0
18	P	700	0	720	66	0
19	Q	857	0	930	84	0
20	R	597	0	668	68	0
21	S	647	0	673	88	0
22	T	762	0	856	72	0
23	V	208	0	221	16	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	J	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52076	0	36765	3117	1

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 35.

All (3117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:A:H4'	1:A:244:U:H5'	1.30	1.13
12:J:45:ARG:HH11	12:J:45:ARG:HB3	0.99	1.13
14:L:47:LYS:HB3	14:L:48:PRO:HD3	1.32	1.12
6:D:151:LYS:H	6:D:151:LYS:HD2	1.08	1.11
6:D:36:ARG:H	6:D:37:PRO:HD3	1.14	1.10
1:A:972:C:H4'	12:J:57:LYS:HG2	1.31	1.09
1:A:349:A:H2'	1:A:350:G:H5''	1.29	1.09
1:A:1053:G:H4'	1:A:1054:C:H5'	1.32	1.06
1:A:1250:A:H4'	11:I:68:GLY:H	1.15	1.06
14:L:126:LYS:HD2	14:L:126:LYS:H	1.16	1.06
12:J:4:ILE:HD11	12:J:74:ILE:HD12	1.38	1.06
1:A:462:G:N2	18:P:82:GLN:HB3	1.70	1.05
5:C:79:ARG:HG2	5:C:82:GLU:HB2	1.37	1.05
14:L:67:THR:HG22	14:L:96:VAL:HG13	1.37	1.04
4:B:91:PRO:HG3	4:B:154:LEU:HB2	1.40	1.03
1:A:1314:C:OP2	21:S:6:LYS:HG2	1.59	1.02
1:A:839:U:H5'	1:A:840:C:H5	1.20	1.02
13:K:106:LYS:HE2	13:K:106:LYS:HA	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:35:GLU:HA	5:C:38:ARG:HH12	1.24	1.02
4:B:84:GLU:HB3	4:B:219:VAL:HG21	1.42	1.01
7:E:126:ARG:HG3	7:E:126:ARG:HH11	1.20	1.01
21:S:33:THR:HG22	21:S:35:SER:H	1.26	1.01
5:C:19:GLU:HG2	5:C:54:ARG:HE	1.25	1.00
5:C:38:ARG:HH11	5:C:38:ARG:HB2	1.20	1.00
9:G:146:GLU:HG3	9:G:149:ARG:HH21	1.25	1.00
5:C:14:ILE:HG22	5:C:15:THR:H	1.28	0.99
1:A:478:A:O2'	1:A:479:C:H5'	1.62	0.99
1:A:189:G:H2'	1:A:190(K):G:N2	1.78	0.97
7:E:50:GLU:HB3	7:E:53:LEU:HD13	1.47	0.97
15:M:10:PRO:HB2	15:M:18:ALA:HB1	1.46	0.97
7:E:33:VAL:HG11	7:E:109:ILE:HG12	1.43	0.96
1:A:1057:G:H5''	5:C:154:SER:HB2	1.45	0.96
12:J:29:ARG:HH11	12:J:29:ARG:N	1.62	0.96
4:B:19:HIS:HE2	4:B:206:ASP:HB3	1.30	0.95
1:A:349:A:C2'	1:A:350:G:H5''	1.96	0.95
5:C:21:ARG:HD2	5:C:21:ARG:H	1.30	0.95
1:A:1116:C:H2'	1:A:1117:G:H5''	1.46	0.95
6:D:36:ARG:H	6:D:37:PRO:CD	1.80	0.95
1:A:664:G:H22	1:A:741:G:H1	1.11	0.95
5:C:188:LEU:HD13	5:C:189:ALA:H	1.31	0.95
15:M:37:THR:HG23	15:M:55:ARG:HD2	1.49	0.95
1:A:1305:G:HO2'	1:A:1306:A:H8	0.96	0.94
6:D:176:LEU:HA	6:D:183:GLY:HA2	1.48	0.94
12:J:45:ARG:NH1	12:J:45:ARG:HB3	1.82	0.94
1:A:1054:C:C5	2:X:34:I:H1'	2.02	0.94
1:A:839:U:H5'	1:A:840:C:C5	2.01	0.94
1:A:189:G:H2'	1:A:190:C:H5'	1.47	0.93
8:F:33:TYR:HA	8:F:71:ARG:HH21	1.33	0.93
1:A:188:C:H2'	1:A:189:G:H4'	1.50	0.93
6:D:22:LYS:HB2	6:D:26:CYS:SG	2.09	0.93
13:K:40:ILE:HG22	13:K:41:THR:HG23	1.48	0.93
1:A:967:C:H4'	11:I:128:ARG:HH21	1.32	0.92
7:E:80:ILE:HD11	7:E:91:LEU:HB2	1.49	0.92
20:R:53:ARG:HH11	20:R:59:SER:HA	1.35	0.92
4:B:132:LYS:HA	4:B:135:GLN:HB2	1.49	0.92
1:A:462:G:H21	18:P:82:GLN:NE2	1.66	0.92
1:A:1086:U:H3	1:A:1099:G:H22	1.13	0.92
4:B:21:ARG:HH11	4:B:23:ARG:HD2	1.33	0.92
5:C:83:ARG:HH21	5:C:87:LEU:HD21	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:47:LYS:HB3	14:L:48:PRO:CD	2.00	0.92
11:I:16:ARG:HD3	11:I:64:THR:HB	1.53	0.91
1:A:408:A:H4'	1:A:429:U:O2	1.71	0.90
4:B:178:ARG:HG3	4:B:178:ARG:HH11	1.35	0.90
5:C:3:ASN:HD22	5:C:3:ASN:H	0.93	0.90
9:G:50:ILE:O	9:G:54:THR:HB	1.71	0.90
19:Q:68:ARG:HG3	19:Q:68:ARG:O	1.72	0.90
1:A:1356:G:H2'	1:A:1357:A:C8	2.06	0.90
11:I:43:ALA:HA	11:I:74:ILE:HD13	1.52	0.90
6:D:170:VAL:HG21	6:D:176:LEU:HD22	1.54	0.89
12:J:29:ARG:HH12	12:J:84:GLN:HE22	1.20	0.89
15:M:34:LEU:HD13	15:M:41:PRO:HA	1.51	0.89
15:M:117:VAL:HG12	15:M:118:ALA:H	1.37	0.89
1:A:1502:A:H2	1:A:1505:G:H1	1.16	0.89
13:K:84:VAL:HG23	13:K:110:ASP:HA	1.53	0.89
1:A:579:G:H5'	1:A:728:A:H1'	1.55	0.89
5:C:3:ASN:ND2	5:C:3:ASN:H	1.71	0.89
1:A:190:C:C5'	1:A:190(K):G:H21	1.85	0.88
1:A:1250:A:H4'	11:I:68:GLY:N	1.87	0.88
7:E:80:ILE:CD1	7:E:91:LEU:HB2	2.03	0.88
9:G:155:ARG:HA	9:G:155:ARG:NH1	1.88	0.88
17:O:56:LEU:HA	17:O:59:MET:HE2	1.54	0.88
12:J:10:GLY:H	12:J:16:LEU:HD11	1.39	0.88
12:J:29:ARG:NH1	12:J:29:ARG:H	1.71	0.88
21:S:28:LYS:HG2	21:S:29:ARG:H	1.36	0.88
12:J:29:ARG:HH11	12:J:29:ARG:H	0.93	0.88
19:Q:14:LYS:HD2	19:Q:14:LYS:H	1.38	0.87
1:A:838:G:H2'	1:A:839:U:H5''	1.55	0.87
7:E:50:GLU:HG3	7:E:52:PRO:HD2	1.57	0.87
1:A:250:A:H4'	1:A:251:G:O5'	1.72	0.87
6:D:36:ARG:N	6:D:37:PRO:HD3	1.89	0.87
6:D:151:LYS:N	6:D:151:LYS:HD2	1.90	0.87
4:B:97:TRP:HZ2	4:B:102:LEU:HD13	1.39	0.87
4:B:61:LEU:HD23	4:B:64:ARG:HD2	1.54	0.86
1:A:266:G:H5''	1:A:268:C:H41	1.38	0.86
1:A:189:G:N2	1:A:190(J):U:H3	1.74	0.85
9:G:146:GLU:HG3	9:G:149:ARG:NH2	1.91	0.85
15:M:23:TYR:HB3	15:M:67:GLU:HA	1.58	0.85
7:E:15:ARG:HD3	7:E:26:PHE:CD2	2.10	0.85
19:Q:14:LYS:HD2	19:Q:14:LYS:N	1.92	0.85
5:C:64:VAL:HG12	5:C:66:VAL:HG23	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:C:C2'	1:A:1117:G:H5''	2.06	0.85
1:A:969:A:H61	15:M:126:LYS:HG3	1.39	0.85
14:L:47:LYS:CB	14:L:48:PRO:HD3	2.07	0.85
1:A:1126:U:H3	1:A:1127:G:N2	1.74	0.84
1:A:1226:C:H4'	1:A:1227:A:OP1	1.77	0.84
4:B:15:VAL:HG12	4:B:16:HIS:H	1.42	0.84
11:I:6:GLY:N	11:I:84:ALA:HB2	1.92	0.84
4:B:139:LYS:O	4:B:139:LYS:HD3	1.78	0.84
5:C:191:THR:HG21	5:C:193:TYR:CZ	2.13	0.84
6:D:151:LYS:H	6:D:151:LYS:CD	1.90	0.84
7:E:51:VAL:HB	7:E:52:PRO:HD3	1.60	0.84
6:D:3:ARG:HD2	6:D:3:ARG:N	1.92	0.83
4:B:88:ALA:HB3	4:B:90:MET:HG2	1.58	0.83
4:B:101:MET:HA	4:B:108:ILE:HG13	1.61	0.83
7:E:81:GLU:HG2	7:E:90:VAL:HG22	1.58	0.83
1:A:1281:U:H5'	1:A:1282:C:H5	1.40	0.83
4:B:124:SER:HB2	4:B:125:PRO:HD2	1.59	0.83
7:E:53:LEU:H	7:E:53:LEU:HD12	1.44	0.83
5:C:6:HIS:HD2	5:C:8:ILE:HB	1.44	0.83
10:H:51:VAL:HG21	10:H:60:ARG:NH1	1.94	0.83
1:A:243:A:C4'	1:A:244:U:H5'	2.06	0.83
12:J:45:ARG:HH11	12:J:45:ARG:CB	1.88	0.83
14:L:126:LYS:HD2	14:L:126:LYS:N	1.94	0.83
20:R:47:THR:HG22	20:R:48:GLY:H	1.43	0.83
11:I:111:ARG:HH11	11:I:111:ARG:HB3	1.43	0.82
12:J:46:ARG:HG2	12:J:46:ARG:HH11	1.43	0.82
12:J:60:ARG:N	12:J:60:ARG:HD2	1.93	0.82
1:A:406:G:H1	1:A:436:C:H42	1.28	0.82
5:C:91:LEU:HD23	5:C:92:ALA:N	1.95	0.82
4:B:69:LEU:HD12	4:B:155:LEU:HD11	1.62	0.82
4:B:23:ARG:NH1	4:B:24:TRP:HA	1.95	0.82
5:C:3:ASN:N	5:C:3:ASN:HD22	1.70	0.82
1:A:1152:A:H5''	12:J:13:HIS:CD2	2.14	0.82
17:O:87:ILE:HG22	17:O:88:ARG:HE	1.45	0.81
5:C:28:GLN:HA	5:C:31:HIS:HD2	1.45	0.81
4:B:18:GLY:H	4:B:42:ILE:H	1.29	0.81
1:A:1208:C:H2'	1:A:1209:C:C6	2.15	0.80
1:A:1006:C:H2'	1:A:1007:C:H6	1.47	0.80
13:K:33:THR:HG22	13:K:39:PRO:HA	1.63	0.80
1:A:1251:A:H2'	1:A:1252:A:C8	2.17	0.80
1:A:302:G:H5''	14:L:17:LYS:NZ	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:41:ARG:HG2	14:L:42:THR:H	1.47	0.80
21:S:55:LYS:HG2	21:S:56:GLN:HE21	1.47	0.80
1:A:190:C:O2	1:A:190:C:H2'	1.82	0.80
4:B:19:HIS:NE2	4:B:206:ASP:HB3	1.96	0.80
1:A:706:A:O2'	13:K:29:ILE:HD11	1.81	0.80
1:A:1053:G:C4'	1:A:1054:C:H5'	2.09	0.79
12:J:49:VAL:HG23	16:N:41:ARG:HB2	1.63	0.79
1:A:1305:G:O2'	1:A:1306:A:H8	1.65	0.79
21:S:22:LEU:HD21	21:S:28:LYS:HD2	1.64	0.79
1:A:1190:G:H3'	5:C:3:ASN:OD1	1.82	0.79
1:A:189:G:H22	1:A:190(J):U:H3	1.31	0.79
11:I:9:ARG:HG2	11:I:14:VAL:HG22	1.64	0.79
1:A:954:G:H21	1:A:1227:A:H62	1.27	0.79
1:A:1057:G:H5''	5:C:154:SER:CB	2.12	0.79
12:J:34:VAL:HG22	12:J:74:ILE:HG23	1.65	0.79
1:A:972:C:H4'	12:J:57:LYS:CG	2.12	0.79
1:A:1208:C:H2'	1:A:1209:C:H6	1.47	0.78
4:B:25:ASN:C	4:B:25:ASN:HD22	1.86	0.78
1:A:189:G:H1	1:A:190(I):G:H1	0.82	0.78
4:B:18:GLY:HA2	4:B:41:ILE:HA	1.65	0.78
1:A:694:A:H3'	1:A:695:A:H5''	1.64	0.78
4:B:71:VAL:O	4:B:165:VAL:HG23	1.83	0.78
14:L:27:LEU:O	14:L:29:GLY:N	2.16	0.78
15:M:3:ARG:HB2	15:M:3:ARG:HH11	1.48	0.78
1:A:1142:G:H2'	1:A:1143:G:O4'	1.83	0.78
7:E:79:GLU:HG3	7:E:93:PRO:HD2	1.64	0.78
12:J:32:ALA:HB2	12:J:75:ILE:HB	1.66	0.78
15:M:54:VAL:O	15:M:58:GLU:HG2	1.83	0.78
11:I:51:ARG:HG2	11:I:56:LEU:HD12	1.66	0.78
1:A:371:G:O2'	1:A:372:C:H5'	1.83	0.78
17:O:17:ARG:HH11	17:O:17:ARG:HG3	1.48	0.78
5:C:150:LYS:HG3	5:C:169:ALA:HB2	1.64	0.77
22:T:21:LYS:NZ	22:T:21:LYS:HB2	1.99	0.77
1:A:243:A:H4'	1:A:244:U:C5'	2.11	0.77
4:B:97:TRP:CZ2	4:B:102:LEU:HD13	2.18	0.77
4:B:178:ARG:HH21	4:B:196:LEU:HA	1.48	0.77
1:A:1223:C:P	21:S:78:ARG:HH12	2.07	0.77
4:B:80:ILE:HD11	4:B:208:ILE:HG23	1.65	0.77
10:H:92:ARG:HH11	10:H:92:ARG:HG2	1.49	0.77
1:A:412:A:H5'	1:A:417:C:C4	2.20	0.77
21:S:41:VAL:H	21:S:44:MET:HE3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:81:ARG:HA	18:P:81:ARG:NE	2.00	0.77
1:A:1216:G:H5''	16:N:5:ALA:HB2	1.67	0.77
5:C:75:VAL:O	5:C:83:ARG:HD3	1.84	0.77
12:J:75:ILE:H	12:J:75:ILE:HD12	1.48	0.77
14:L:59:ARG:HD3	14:L:65:GLU:HG3	1.65	0.77
4:B:197:VAL:HB	4:B:200:ILE:HG12	1.65	0.77
15:M:49:THR:HG22	15:M:51:ALA:H	1.48	0.77
17:O:6:GLU:CD	17:O:6:GLU:H	1.86	0.77
21:S:6:LYS:HD2	21:S:6:LYS:N	2.00	0.77
1:A:328:C:O2	1:A:328:C:H2'	1.82	0.77
1:A:1086:U:H3	1:A:1099:G:N2	1.83	0.76
1:A:409:G:H5'	1:A:430:A:N6	2.00	0.76
5:C:191:THR:HG22	5:C:192:THR:N	2.00	0.76
20:R:36:ASN:ND2	20:R:38:GLU:HG2	2.00	0.76
1:A:133:U:OP1	22:T:74:LYS:HE2	1.85	0.76
1:A:462:G:N2	18:P:82:GLN:HE21	1.83	0.76
1:A:99:C:H2'	1:A:101:A:C8	2.21	0.76
1:A:738:C:H5''	8:F:69:GLU:HB3	1.67	0.76
1:A:430:A:H2'	1:A:431:A:H5''	1.67	0.76
5:C:21:ARG:HD2	5:C:21:ARG:N	2.00	0.76
5:C:64:VAL:HG23	5:C:99:VAL:HG11	1.67	0.76
15:M:12:ASN:HB2	15:M:46:LYS:HB3	1.67	0.76
6:D:3:ARG:H	6:D:3:ARG:HH11	1.32	0.76
6:D:78:LEU:HD22	6:D:96:LEU:HB3	1.68	0.76
9:G:26:PHE:CE2	9:G:30:ILE:HD11	2.21	0.76
1:A:112:G:H21	1:A:354:G:H5'	1.50	0.75
1:A:1425:U:H2'	1:A:1426:C:H6	1.50	0.75
4:B:88:ALA:CB	4:B:90:MET:HG2	2.16	0.75
15:M:40:ASN:HD22	15:M:41:PRO:N	1.82	0.75
1:A:1201:A:H4'	1:A:1202:G:O5'	1.86	0.75
1:A:939:G:H5''	9:G:102:ARG:NH2	2.02	0.75
13:K:84:VAL:HG11	13:K:95:ILE:HD11	1.69	0.75
5:C:107:GLN:NE2	5:C:107:GLN:H	1.85	0.75
11:I:65:VAL:HG21	11:I:73:GLN:HB3	1.67	0.75
1:A:35:G:H2'	1:A:36:C:C6	2.20	0.75
8:F:10:LEU:CD1	8:F:59:TYR:HB3	2.16	0.74
5:C:38:ARG:HH11	5:C:38:ARG:CB	1.99	0.74
11:I:4:TYR:CD2	11:I:88:TYR:HA	2.22	0.74
16:N:9:LYS:HE3	16:N:21:TYR:O	1.87	0.74
1:A:1391:U:H2'	1:A:1392:G:C8	2.22	0.74
1:A:190:C:H5''	1:A:190(K):G:H21	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:C:O2'	1:A:557:G:H5'	1.87	0.74
9:G:23:VAL:O	9:G:27:ILE:HG13	1.87	0.74
1:A:189:G:H2'	1:A:190(K):G:H22	1.53	0.74
11:I:53:VAL:HG21	11:I:85:LEU:HD21	1.70	0.74
1:A:1190:G:OP1	5:C:4:LYS:HA	1.87	0.74
1:A:462:G:H22	18:P:82:GLN:HB3	1.52	0.74
6:D:146:ILE:HD12	6:D:146:ILE:N	2.02	0.74
12:J:84:GLN:O	12:J:88:LEU:HD12	1.86	0.74
13:K:57:THR:HG23	13:K:60:ALA:H	1.52	0.74
1:A:413:G:N3	1:A:416:G:H5'	2.03	0.74
5:C:34:LEU:HD22	5:C:38:ARG:CZ	2.18	0.74
7:E:126:ARG:CG	7:E:126:ARG:HH11	1.98	0.74
8:F:78:GLU:O	8:F:81:ILE:HG22	1.87	0.74
16:N:27:CYS:SG	16:N:29:ARG:HB2	2.28	0.73
5:C:58:GLU:HB3	12:J:92:THR:HG21	1.70	0.73
7:E:76:ILE:HG23	7:E:77:PRO:HD2	1.68	0.73
7:E:78:HIS:HD2	10:H:107:LEU:HD12	1.53	0.73
20:R:33:ASP:OD2	20:R:36:ASN:HB2	1.88	0.73
9:G:18:TYR:CD2	9:G:59:LEU:HB2	2.23	0.73
11:I:48:GLU:N	11:I:49:PRO:HD2	2.03	0.73
1:A:838:G:C2'	1:A:839:U:H5''	2.18	0.73
6:D:35:ARG:O	6:D:36:ARG:HB2	1.89	0.73
20:R:86:VAL:HG12	20:R:87:ARG:H	1.53	0.73
1:A:1224:G:H1	1:A:1362:C:H42	1.34	0.73
5:C:14:ILE:O	5:C:16:ARG:N	2.22	0.73
6:D:3:ARG:HH11	6:D:3:ARG:N	1.87	0.73
20:R:88:LYS:HG2	20:R:88:LYS:OXT	1.87	0.73
1:A:1168:A:H2'	1:A:1169:A:C8	2.22	0.73
12:J:38:ILE:HB	12:J:71:LEU:HB2	1.71	0.73
15:M:3:ARG:HA	15:M:8:GLU:O	1.89	0.73
1:A:190:C:H5'	1:A:190(K):G:H21	1.52	0.73
12:J:90:LEU:H	12:J:91:PRO:CD	2.02	0.73
1:A:928:G:H4'	1:A:1533:C:H5'	1.70	0.73
4:B:91:PRO:HG2	4:B:155:LEU:HG	1.70	0.73
7:E:24:ARG:HH11	7:E:24:ARG:HB3	1.54	0.73
16:N:26:ARG:NH1	16:N:47:LEU:HG	2.04	0.73
18:P:28:ARG:HH11	18:P:28:ARG:HG2	1.53	0.73
1:A:1057:G:O2'	1:A:1058:G:H5'	1.89	0.72
18:P:81:ARG:HA	18:P:81:ARG:HE	1.54	0.72
20:R:53:ARG:NH1	20:R:59:SER:HA	2.04	0.72
11:I:118:LYS:O	11:I:119:ALA:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:G:H2'	1:A:1033:G:O4'	1.89	0.72
1:A:839:U:C5'	1:A:840:C:H5	2.02	0.72
4:B:95:GLN:O	4:B:96:ARG:HD2	1.88	0.72
1:A:1250:A:C4'	11:I:68:GLY:H	1.97	0.72
22:T:57:ARG:HH11	22:T:57:ARG:HB2	1.54	0.72
1:A:1152:A:H2'	1:A:1153:C:C6	2.25	0.72
4:B:137:ARG:HA	4:B:140:HIS:HD2	1.53	0.72
5:C:123:GLN:HE22	5:C:140:ARG:HH22	1.36	0.72
19:Q:59:ILE:HG22	19:Q:71:PHE:CD1	2.24	0.72
1:A:112:G:N2	1:A:354:G:H5'	2.04	0.72
1:A:677:U:H3	1:A:713:G:H22	1.37	0.72
1:A:840:C:H5''	1:A:841:U:OP1	1.90	0.72
6:D:150:GLU:O	6:D:153:ARG:HG2	1.90	0.72
14:L:43:VAL:HG12	14:L:44:THR:H	1.55	0.72
1:A:556:C:OP2	14:L:20:LYS:HE3	1.89	0.72
11:I:97:LYS:HB3	11:I:98:PRO:HD3	1.72	0.72
1:A:462:G:N2	18:P:82:GLN:NE2	2.38	0.72
4:B:137:ARG:HA	4:B:140:HIS:CD2	2.25	0.71
15:M:8:GLU:C	15:M:9:ILE:HD12	2.09	0.71
1:A:1360:A:H2'	1:A:1361:G:C8	2.24	0.71
15:M:73:GLU:O	15:M:76:ALA:HB3	1.90	0.71
5:C:64:VAL:CG2	5:C:99:VAL:HG11	2.20	0.71
9:G:113:GLU:HG2	9:G:119:ARG:HG2	1.71	0.71
20:R:86:VAL:HG12	20:R:87:ARG:N	2.05	0.71
5:C:123:GLN:NE2	5:C:140:ARG:HH22	1.88	0.71
5:C:156:ARG:H	5:C:163:ALA:HA	1.55	0.71
12:J:82:ILE:HG22	12:J:86:MET:SD	2.29	0.71
8:F:97:PHE:HB2	20:R:32:ARG:HH21	1.54	0.71
1:A:860:A:H2'	1:A:861:G:O4'	1.90	0.71
7:E:122:GLU:O	7:E:123:LEU:HD23	1.91	0.71
15:M:79:LYS:HG2	15:M:83:ASP:OD2	1.89	0.71
18:P:74:LEU:O	18:P:79:VAL:HG23	1.91	0.71
1:A:1502:A:H2	1:A:1505:G:N1	1.88	0.71
1:A:462:G:H21	18:P:82:GLN:HE21	1.37	0.71
9:G:79:ARG:HD3	9:G:80:VAL:N	2.04	0.71
14:L:45:PRO:HD3	14:L:51:ALA:O	1.91	0.71
17:O:78:TYR:CZ	17:O:82:ILE:HD11	2.25	0.71
18:P:34:GLU:OE2	18:P:55:ARG:HD3	1.90	0.71
1:A:1369:C:H2'	1:A:1370:G:C8	2.25	0.71
1:A:413:G:H4'	1:A:416:G:H21	1.54	0.71
1:A:463:A:H4'	1:A:474:G:OP2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:24:ARG:HB3	7:E:24:ARG:NH1	2.05	0.71
21:S:20:LEU:HD12	21:S:21:GLU:N	2.06	0.71
1:A:1263:C:H2'	1:A:1264:C:C6	2.25	0.71
1:A:977:A:H2'	1:A:978:A:H5''	1.72	0.71
5:C:83:ARG:HA	5:C:86:VAL:HG23	1.73	0.71
7:E:137:GLU:O	7:E:141:GLN:HG3	1.90	0.71
11:I:111:ARG:HH11	11:I:111:ARG:CB	2.04	0.71
15:M:5:ALA:HB3	15:M:8:GLU:HG3	1.72	0.71
1:A:1189:C:P	12:J:51:ARG:HH22	2.14	0.70
1:A:204:U:O2	1:A:204:U:H2'	1.90	0.70
1:A:1285:A:H4'	1:A:1286:A:O5'	1.91	0.70
1:A:1238:A:H5'	1:A:1336:C:H41	1.55	0.70
1:A:1343:G:H2'	1:A:1344:C:C6	2.25	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.27	0.70
1:A:353:A:H5'	1:A:353:A:H8	1.56	0.70
6:D:162:LEU:HD13	6:D:181:MET:SD	2.31	0.70
11:I:127:LYS:HE3	11:I:127:LYS:H	1.57	0.70
12:J:89:ASP:OD2	12:J:91:PRO:HD2	1.90	0.70
7:E:11:ILE:HG22	7:E:12:LEU:HD12	1.73	0.70
1:A:141:A:H1'	1:A:182:U:O2	1.92	0.70
7:E:11:ILE:HB	7:E:31:LEU:HB3	1.73	0.70
5:C:191:THR:HG21	5:C:193:TYR:CE2	2.25	0.70
12:J:8:LEU:HD22	12:J:20:ALA:HB2	1.72	0.70
19:Q:18:THR:HG23	19:Q:69:LYS:HE3	1.71	0.70
1:A:1281:U:H5'	1:A:1282:C:C5	2.26	0.70
1:A:17:U:H2'	1:A:18:C:C6	2.25	0.70
5:C:6:HIS:CD2	5:C:8:ILE:HB	2.26	0.70
6:D:126:ILE:HG22	6:D:127:THR:N	2.06	0.70
5:C:70:VAL:HG21	5:C:76:VAL:HG21	1.73	0.70
12:J:10:GLY:N	12:J:16:LEU:HD11	2.06	0.70
13:K:29:ILE:C	13:K:29:ILE:HD12	2.12	0.70
1:A:1366:C:H2'	1:A:1367:C:H6	1.57	0.70
1:A:524:G:H2'	1:A:525:C:C6	2.27	0.70
5:C:102:ASN:N	5:C:102:ASN:HD22	1.88	0.70
10:H:91:ARG:HG3	14:L:7:ILE:HG13	1.74	0.70
13:K:50:TYR:HB3	13:K:54:ARG:HB2	1.74	0.70
1:A:135:C:O2	18:P:1:MET:HB2	1.92	0.69
5:C:5:ILE:O	5:C:5:ILE:HD12	1.92	0.69
12:J:31:GLY:HA2	12:J:76:ASN:HD21	1.55	0.69
14:L:55:VAL:HG12	14:L:56:ALA:N	2.07	0.69
21:S:17:GLU:HA	21:S:20:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:98:LEU:H	4:B:98:LEU:HD23	1.56	0.69
12:J:50:ILE:HG12	12:J:60:ARG:HE	1.57	0.69
13:K:27:ASN:OD1	13:K:55:LYS:HB3	1.93	0.69
6:D:173:TRP:HB2	6:D:187:ARG:O	1.92	0.69
10:H:46:LYS:H	10:H:64:LYS:HG3	1.57	0.69
1:A:972:C:C4'	12:J:57:LYS:HG2	2.17	0.69
15:M:49:THR:CG2	15:M:51:ALA:H	2.05	0.69
6:D:9:CYS:SG	6:D:22:LYS:HG3	2.32	0.69
5:C:49:SER:O	5:C:72:LYS:HD2	1.92	0.69
21:S:33:THR:HG22	21:S:34:TRP:H	1.58	0.69
21:S:40:ILE:HG21	21:S:62:ILE:HD11	1.75	0.69
1:A:1392:G:H21	1:A:1502:A:H8	1.40	0.69
1:A:130:A:OP2	1:A:190(E):U:H2'	1.93	0.69
5:C:204:LEU:O	5:C:204:LEU:HD12	1.93	0.69
13:K:124:LYS:HE3	13:K:125:PHE:CE1	2.28	0.69
14:L:55:VAL:HG11	14:L:67:THR:HG23	1.74	0.69
7:E:15:ARG:HD3	7:E:26:PHE:HD2	1.55	0.69
4:B:18:GLY:CA	4:B:41:ILE:HA	2.23	0.69
6:D:3:ARG:HH11	6:D:3:ARG:CA	2.05	0.69
12:J:49:VAL:O	12:J:60:ARG:O	2.11	0.69
19:Q:101:ARG:NE	19:Q:101:ARG:HA	2.07	0.69
1:A:1137:C:H4'	1:A:1138:G:C2	2.28	0.69
10:H:20:TYR:CE2	10:H:75:ARG:HD2	2.28	0.69
11:I:10:ARG:HG2	11:I:75:ASP:HB2	1.75	0.69
11:I:8:GLY:HA2	11:I:79:LEU:HD13	1.75	0.69
5:C:154:SER:OG	5:C:155:GLY:N	2.24	0.68
9:G:54:THR:HG22	9:G:56:GLN:H	1.57	0.68
14:L:27:LEU:C	14:L:29:GLY:H	1.94	0.68
20:R:22:VAL:HG13	20:R:42:ARG:HD2	1.74	0.68
1:A:853:G:O2'	1:A:854:G:H5'	1.93	0.68
12:J:75:ILE:HD12	12:J:75:ILE:N	2.08	0.68
15:M:40:ASN:HD22	15:M:41:PRO:CD	2.06	0.68
1:A:1123:A:H4'	12:J:37:PRO:HD2	1.76	0.68
1:A:975:A:O5'	1:A:976:G:H5'	1.93	0.68
5:C:64:VAL:HB	5:C:99:VAL:HB	1.75	0.68
1:A:687:A:H4'	1:A:688:G:O5'	1.94	0.68
5:C:38:ARG:HB2	5:C:38:ARG:NH1	2.02	0.68
6:D:62:GLN:HE22	6:D:65:ARG:HH12	1.39	0.68
7:E:36:ASP:OD2	7:E:40:ARG:HB2	1.94	0.68
1:A:1065:U:H4'	1:A:1066:C:O5'	1.93	0.68
1:A:1193:G:O2'	1:A:1194:U:H5'	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H1	1:A:436:C:N4	1.91	0.68
4:B:35:GLU:HG2	4:B:40:HIS:HA	1.74	0.68
12:J:48:THR:HA	12:J:62:HIS:HD2	1.58	0.68
1:A:1128:C:O2'	1:A:1130:A:C8	2.47	0.68
4:B:178:ARG:HH21	4:B:196:LEU:CA	2.05	0.68
4:B:178:ARG:HH21	4:B:196:LEU:C	1.97	0.68
5:C:79:ARG:HB3	5:C:79:ARG:NH1	2.09	0.68
20:R:36:ASN:HD21	20:R:38:GLU:HG2	1.56	0.68
1:A:1356:G:H2'	1:A:1357:A:H8	1.56	0.68
1:A:1425:U:H2'	1:A:1426:C:C6	2.28	0.68
11:I:106:ALA:O	11:I:108:VAL:HG23	1.93	0.68
11:I:23:ASN:HB3	11:I:25:LYS:HG3	1.75	0.68
19:Q:97:SER:HB2	19:Q:98:LEU:HD12	1.75	0.68
1:A:353:A:H5'	1:A:353:A:C8	2.29	0.68
10:H:90:GLY:O	10:H:91:ARG:HB2	1.92	0.68
1:A:1367:C:H4'	12:J:48:THR:HG21	1.75	0.68
1:A:195:A:H4'	22:T:68:LYS:HE2	1.75	0.68
4:B:88:ALA:C	4:B:90:MET:H	1.97	0.68
22:T:10:LEU:O	22:T:13:LEU:HG	1.94	0.68
1:A:1015:A:H2'	1:A:1016:A:C8	2.30	0.67
5:C:20:SER:HB3	5:C:22:TRP:NE1	2.09	0.67
5:C:191:THR:HG22	5:C:193:TYR:H	1.60	0.67
5:C:35:GLU:HA	5:C:38:ARG:NH1	2.04	0.67
8:F:2:ARG:CZ	8:F:69:GLU:HG2	2.24	0.67
9:G:22:LEU:HD11	9:G:101:LEU:HD21	1.74	0.67
15:M:94:ARG:HG3	15:M:94:ARG:HH11	1.57	0.67
1:A:895:G:H2'	1:A:896:C:C6	2.29	0.67
5:C:139:GLN:HE21	5:C:139:GLN:HA	1.58	0.67
17:O:70:LEU:HD12	17:O:78:TYR:HB2	1.76	0.67
19:Q:12:SER:HA	19:Q:14:LYS:HZ3	1.59	0.67
21:S:13:ASP:HA	21:S:16:LEU:HB3	1.76	0.67
1:A:448:A:OP2	1:A:485:G:N2	2.28	0.67
5:C:13:GLY:HA3	16:N:57:ARG:NH2	2.08	0.67
1:A:113:G:H1'	1:A:354:G:H5'	1.76	0.67
4:B:29:ALA:HA	4:B:32:ILE:HD12	1.75	0.67
6:D:70:ILE:HD11	6:D:100:ARG:HD2	1.76	0.67
12:J:6:ILE:HA	12:J:98:ILE:HG22	1.74	0.67
13:K:51:LYS:HE2	13:K:52:GLY:H	1.58	0.67
14:L:89:ARG:NH1	14:L:97:ARG:HG2	2.09	0.67
1:A:1228:C:OP1	15:M:115:LYS:HE3	1.92	0.67
15:M:5:ALA:HB3	15:M:8:GLU:CG	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:A:H2'	1:A:326:G:N2	2.09	0.67
4:B:126:GLU:HA	4:B:129:GLU:OE2	1.94	0.67
5:C:23:TYR:CD2	5:C:24:ALA:N	2.62	0.67
6:D:153:ARG:NE	6:D:181:MET:HE3	2.10	0.67
1:A:1497:G:O2'	1:A:1498:U:H5'	1.94	0.67
1:A:287:U:O2'	1:A:288:A:H5'	1.93	0.67
1:A:423:G:H5''	1:A:424:G:N2	2.08	0.67
5:C:108:ASN:ND2	5:C:111:LEU:HG	2.09	0.67
12:J:60:ARG:O	12:J:61:GLU:O	2.13	0.67
14:L:38:THR:HG22	14:L:39:VAL:HG23	1.77	0.67
20:R:26:LEU:HD12	20:R:27:GLY:H	1.59	0.67
1:A:411:A:H1'	1:A:417:C:O2	1.94	0.67
1:A:939:G:H5''	9:G:102:ARG:HH22	1.58	0.67
1:A:189:G:C6	1:A:190:C:H3'	2.29	0.67
15:M:17:VAL:O	15:M:20:THR:HB	1.95	0.67
18:P:11:SER:HB3	18:P:14:ASN:HB3	1.77	0.67
5:C:64:VAL:HB	5:C:99:VAL:CB	2.25	0.66
19:Q:12:SER:HB3	19:Q:20:THR:HB	1.77	0.66
7:E:150:ARG:HH11	7:E:150:ARG:HG3	1.59	0.66
11:I:127:LYS:HD3	15:M:126:LYS:HE2	1.77	0.66
13:K:54:ARG:O	13:K:57:THR:HG22	1.95	0.66
17:O:45:VAL:HG12	17:O:46:HIS:N	2.10	0.66
1:A:478:A:C2'	1:A:479:C:H5'	2.24	0.66
6:D:25:ARG:C	6:D:27:TYR:H	1.96	0.66
9:G:15:ASP:HB3	9:G:19:GLY:N	2.11	0.66
9:G:22:LEU:HG	9:G:62:PHE:HE2	1.59	0.66
10:H:77:GLU:HG2	10:H:78:GLN:H	1.60	0.66
22:T:36:LEU:HD12	22:T:62:LEU:HD12	1.76	0.66
1:A:1229:A:H2'	1:A:1230:C:H6	1.58	0.66
1:A:147:G:O2'	1:A:148:G:H5'	1.96	0.66
1:A:370:C:O2'	1:A:371:G:H5'	1.95	0.66
11:I:6:GLY:H	11:I:84:ALA:HB2	1.60	0.66
1:A:1372:U:OP1	11:I:71:SER:HB3	1.95	0.66
6:D:3:ARG:HH11	6:D:3:ARG:HA	1.60	0.66
8:F:10:LEU:HD12	8:F:10:LEU:H	1.59	0.66
9:G:155:ARG:HA	9:G:155:ARG:HH11	1.61	0.66
15:M:117:VAL:HG12	15:M:118:ALA:N	2.10	0.66
15:M:23:TYR:CB	15:M:67:GLU:HA	2.26	0.66
22:T:49:ALA:HB3	22:T:99:LEU:HG	1.77	0.66
1:A:1118:C:H1'	1:A:1179:A:C4	2.31	0.66
1:A:403:C:O2'	1:A:404:U:H5'	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD23	5:C:118:GLN:OE1	1.95	0.66
7:E:76:ILE:HG22	7:E:78:HIS:H	1.60	0.66
8:F:33:TYR:HA	8:F:71:ARG:NH2	2.09	0.66
9:G:78:ARG:HB2	9:G:156:TRP:HZ3	1.60	0.66
12:J:46:ARG:HG2	12:J:46:ARG:NH1	2.10	0.66
1:A:1047:G:H5''	16:N:4:LYS:HD3	1.78	0.66
1:A:1428:A:H2'	1:A:1429:C:C6	2.31	0.66
1:A:344:A:H4'	1:A:345:C:OP2	1.95	0.66
1:A:946:A:H2'	1:A:947:G:C8	2.31	0.66
4:B:36:ARG:HB2	4:B:41:ILE:HD11	1.77	0.66
6:D:3:ARG:H	6:D:3:ARG:NH1	1.93	0.66
11:I:100:GLY:O	11:I:102:LEU:N	2.27	0.66
14:L:28:LYS:C	14:L:30:ALA:H	1.98	0.66
5:C:15:THR:O	5:C:16:ARG:HB2	1.94	0.66
10:H:51:VAL:HG11	10:H:60:ARG:NH2	2.11	0.66
18:P:81:ARG:CA	18:P:81:ARG:HE	2.09	0.66
1:A:1132:C:H2'	1:A:1133:G:C8	2.30	0.66
1:A:390:C:H2'	1:A:391:G:C8	2.31	0.66
18:P:80:PHE:O	18:P:82:GLN:N	2.29	0.66
1:A:1161:C:H2'	1:A:1162:C:H6	1.61	0.65
1:A:1278:U:H5''	1:A:1279:A:O4'	1.96	0.65
1:A:1352:C:H2'	1:A:1353:G:C8	2.31	0.65
1:A:1412:C:H2'	1:A:1413:A:C8	2.32	0.65
9:G:75:VAL:HG21	9:G:86:GLN:HB3	1.76	0.65
15:M:19:LEU:O	15:M:22:ILE:HD13	1.96	0.65
15:M:78:ILE:HA	15:M:81:LEU:HD12	1.78	0.65
21:S:41:VAL:HG23	21:S:43:GLU:HG2	1.78	0.65
1:A:1154:G:H2'	1:A:1155:G:H8	1.61	0.65
1:A:673:G:H2'	1:A:674:G:C8	2.31	0.65
5:C:139:GLN:NE2	5:C:139:GLN:HA	2.11	0.65
5:C:86:VAL:O	5:C:89:GLU:HB3	1.96	0.65
1:A:1202:G:O2'	1:A:1203:C:H5'	1.96	0.65
9:G:115:ARG:HB2	9:G:118:VAL:HG23	1.79	0.65
1:A:695:A:OP2	13:K:53:SER:HB2	1.97	0.65
20:R:36:ASN:O	20:R:39:VAL:HG12	1.96	0.65
1:A:1230:C:O2'	1:A:1231:G:H5'	1.95	0.65
4:B:132:LYS:C	4:B:134:GLU:H	2.00	0.65
13:K:15:ALA:HA	13:K:77:MET:HA	1.78	0.65
14:L:55:VAL:CG1	14:L:67:THR:HG23	2.27	0.65
17:O:77:ARG:O	17:O:80:ALA:HB3	1.96	0.65
21:S:33:THR:HG22	21:S:34:TRP:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:C:O2'	1:A:1235:U:H5'	1.96	0.65
5:C:139:GLN:HE21	5:C:139:GLN:CA	2.10	0.65
14:L:43:VAL:HG12	14:L:44:THR:N	2.10	0.65
14:L:54:LYS:HE3	14:L:54:LYS:N	2.11	0.65
21:S:44:MET:O	21:S:62:ILE:HG21	1.96	0.65
1:A:406:G:H21	6:D:119:GLN:HE22	1.43	0.65
1:A:430:A:C2'	1:A:431:A:H5''	2.26	0.65
5:C:139:GLN:O	5:C:143:GLU:HG3	1.97	0.65
5:C:40:ARG:HB3	5:C:44:GLU:OE2	1.97	0.65
9:G:18:TYR:HB3	9:G:59:LEU:HD22	1.78	0.65
15:M:26:GLY:O	15:M:28:ALA:N	2.29	0.65
15:M:49:THR:HG22	15:M:51:ALA:N	2.12	0.65
15:M:37:THR:CG2	15:M:55:ARG:HD2	2.26	0.65
1:A:1229:A:H1'	15:M:125:ARG:HD3	1.78	0.65
1:A:1363:A:H1'	1:A:1365:G:N7	2.12	0.65
4:B:178:ARG:CG	4:B:178:ARG:HH11	2.07	0.65
5:C:3:ASN:O	5:C:4:LYS:HB2	1.97	0.65
7:E:126:ARG:HG3	7:E:126:ARG:NH1	2.00	0.65
14:L:54:LYS:HG2	14:L:75:HIS:CE1	2.32	0.65
15:M:37:THR:HG22	15:M:39:ILE:HG13	1.77	0.65
1:A:1223:C:P	21:S:78:ARG:NH1	2.70	0.65
1:A:444:C:H2'	1:A:445:G:H8	1.62	0.65
1:A:691:G:O6	13:K:52:GLY:HA2	1.97	0.65
12:J:45:ARG:O	12:J:64:GLU:HA	1.97	0.65
19:Q:9:VAL:HG21	19:Q:84:LEU:HD13	1.77	0.65
8:F:97:PHE:HB2	20:R:32:ARG:NH2	2.12	0.65
12:J:90:LEU:N	12:J:91:PRO:CD	2.60	0.64
1:A:1151:A:HO2'	1:A:1152:A:H8	1.45	0.64
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.97	0.64
1:A:392:G:H2'	1:A:393:A:C8	2.33	0.64
1:A:76:C:O2'	1:A:77:G:H5'	1.98	0.64
7:E:101:ILE:HD12	7:E:119:LEU:CD2	2.27	0.64
7:E:75:THR:HG23	7:E:76:ILE:N	2.12	0.64
13:K:14:VAL:HG21	13:K:40:ILE:HD11	1.77	0.64
20:R:46:GLU:CD	20:R:46:GLU:H	1.99	0.64
1:A:1256:A:H5'	1:A:1258:G:H1'	1.78	0.64
4:B:72:GLY:HA3	4:B:81:VAL:HG21	1.79	0.64
5:C:107:GLN:H	5:C:107:GLN:CD	1.99	0.64
1:A:1148:U:H2'	1:A:1149:C:O4'	1.96	0.64
1:A:314:C:O2'	1:A:315:A:H5'	1.97	0.64
1:A:350:G:H5'	1:A:350:G:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:A:N6	1:A:463:A:C6	2.65	0.64
1:A:501:C:H2'	1:A:502:G:H8	1.62	0.64
1:A:939:G:H2'	1:A:940:C:C6	2.32	0.64
4:B:102:LEU:HD21	4:B:162:ILE:CD1	2.28	0.64
5:C:134:ILE:HD11	5:C:153:VAL:CG2	2.27	0.64
8:F:80:ARG:NH1	8:F:88:VAL:HB	2.12	0.64
15:M:4:ILE:HG22	15:M:5:ALA:N	2.13	0.64
1:A:1477:C:H2'	1:A:1478:C:C6	2.33	0.64
1:A:590:C:O2'	1:A:591:U:H5'	1.98	0.64
4:B:30:ARG:HG3	4:B:31:TYR:N	2.12	0.64
5:C:14:ILE:HG22	5:C:15:THR:N	2.09	0.64
1:A:1112:C:H1'	5:C:179:ARG:HH21	1.61	0.64
6:D:8:VAL:HB	6:D:21:LEU:HD12	1.79	0.64
10:H:92:ARG:HH11	10:H:92:ARG:CG	2.10	0.64
19:Q:97:SER:HA	19:Q:102:GLY:O	1.97	0.64
21:S:15:LEU:HD12	21:S:16:LEU:N	2.13	0.64
1:A:390:C:H2'	1:A:391:G:H8	1.62	0.64
12:J:29:ARG:N	12:J:29:ARG:HD3	2.12	0.64
15:M:88:ARG:HG3	15:M:98:VAL:HG11	1.79	0.64
5:C:79:ARG:HG2	5:C:82:GLU:CB	2.23	0.64
12:J:32:ALA:CB	12:J:75:ILE:HB	2.27	0.64
1:A:1182:G:O2'	1:A:1183:A:OP2	2.15	0.64
4:B:84:GLU:HB3	4:B:219:VAL:CG2	2.25	0.64
10:H:83:ILE:O	10:H:83:ILE:HG23	1.98	0.64
14:L:27:LEU:C	14:L:29:GLY:N	2.50	0.64
14:L:75:HIS:HD2	14:L:77:LEU:H	1.44	0.64
1:A:1368:G:O2'	1:A:1369:C:H5'	1.97	0.64
1:A:723:U:O2	1:A:723:U:H2'	1.98	0.64
12:J:39:PRO:O	12:J:40:LEU:HB2	1.98	0.64
5:C:191:THR:CG2	5:C:192:THR:N	2.60	0.64
1:A:1145:C:O2'	1:A:1146:A:H8	1.81	0.63
6:D:62:GLN:NE2	6:D:65:ARG:HH12	1.96	0.63
10:H:38:ILE:H	10:H:38:ILE:HD12	1.61	0.63
14:L:89:ARG:HA	14:L:97:ARG:HA	1.80	0.63
1:A:1320:C:N3	21:S:36:ARG:HD3	2.12	0.63
1:A:28:G:O2'	1:A:296:U:OP1	2.16	0.63
1:A:107:G:C2'	1:A:108:G:H5'	2.28	0.63
1:A:1161:C:H2'	1:A:1162:C:C6	2.34	0.63
4:B:77:ALA:HB2	4:B:211:ILE:HD13	1.80	0.63
11:I:70:LYS:O	11:I:74:ILE:HG13	1.98	0.63
1:A:1064:G:H4'	1:A:1065:U:C5'	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:G:H2'	1:A:1134:G:H8	1.63	0.63
1:A:1149:C:H2'	1:A:1150:U:C6	2.34	0.63
15:M:15:VAL:HG23	15:M:43:THR:O	1.99	0.63
1:A:748:C:HO2'	1:A:749:C:H6	1.41	0.63
4:B:178:ARG:NH1	4:B:178:ARG:HG3	2.12	0.63
14:L:101:VAL:O	14:L:101:VAL:HG12	1.96	0.63
1:A:895:G:H2'	1:A:896:C:H6	1.64	0.63
1:A:1330:U:H2'	1:A:1331:G:H5'	1.80	0.63
4:B:84:GLU:OE1	4:B:216:SER:HA	1.99	0.63
5:C:180:ALA:CB	5:C:182:ILE:HG13	2.29	0.63
9:G:78:ARG:HB2	9:G:156:TRP:CZ3	2.33	0.63
1:A:1095:U:H2'	1:A:1096:C:C6	2.34	0.63
1:A:1351:U:O2'	1:A:1352:C:H5'	1.99	0.63
1:A:1370:G:O2'	1:A:1371:G:H5'	1.99	0.63
1:A:627:G:O2'	1:A:628:G:H5'	1.99	0.63
4:B:19:HIS:HE2	4:B:206:ASP:CB	2.10	0.63
10:H:20:TYR:HE2	10:H:75:ARG:HD2	1.63	0.63
12:J:75:ILE:HG22	12:J:76:ASN:H	1.64	0.63
5:C:193:TYR:HE1	5:C:196:LEU:HD21	1.63	0.62
12:J:71:LEU:O	12:J:72:VAL:HB	1.98	0.62
9:G:59:LEU:O	9:G:63:LYS:HG2	2.00	0.62
10:H:38:ILE:N	10:H:38:ILE:HD12	2.14	0.62
12:J:36:GLY:O	12:J:72:VAL:HA	1.98	0.62
14:L:46:LYS:HG2	14:L:92:ASP:O	1.99	0.62
18:P:81:ARG:C	18:P:83:GLU:H	2.01	0.62
11:I:127:LYS:HE3	11:I:127:LYS:N	2.14	0.62
15:M:49:THR:HB	15:M:52:GLU:OE1	1.98	0.62
1:A:1010:G:H2'	1:A:1011:G:H8	1.65	0.62
1:A:666:G:H5'	1:A:726:C:H1'	1.82	0.62
5:C:47:LEU:CD2	5:C:68:VAL:HG11	2.29	0.62
5:C:58:GLU:HB3	12:J:92:THR:CG2	2.28	0.62
1:A:1144:G:N2	1:A:1146:A:H62	1.97	0.62
1:A:328:C:O2	1:A:328:C:C2'	2.48	0.62
1:A:392:G:H2'	1:A:393:A:H8	1.64	0.62
14:L:33:ARG:HG2	14:L:62:SER:HB3	1.81	0.62
13:K:110:ASP:HB2	20:R:88:LYS:NZ	2.15	0.62
1:A:190(L):U:O2'	1:A:191:G:H5'	1.99	0.62
5:C:148:GLY:HA3	5:C:172:ARG:O	1.99	0.62
12:J:31:GLY:CA	12:J:76:ASN:HD21	2.11	0.62
1:A:1495:U:H2'	1:A:1496:C:H6	1.64	0.62
1:A:188:C:H5''	1:A:188:C:H6	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:G:O2'	1:A:640:A:H5'	1.99	0.62
4:B:25:ASN:ND2	4:B:25:ASN:C	2.53	0.62
1:A:1298:C:H2'	9:G:114:ARG:HH12	1.63	0.62
1:A:528:C:H5'	1:A:535:A:C6	2.35	0.62
11:I:93:ARG:HB3	11:I:93:ARG:NH1	2.14	0.62
16:N:58:LYS:HZ2	16:N:58:LYS:HB3	1.65	0.62
21:S:63:THR:HG22	21:S:64:GLU:N	2.15	0.62
1:A:1488:G:O2'	1:A:1489:G:H5'	1.99	0.62
18:P:59:TRP:HB3	18:P:64:ALA:HB2	1.81	0.62
1:A:1152:A:H2'	1:A:1153:C:H6	1.64	0.62
8:F:23:LYS:O	8:F:27:GLN:HG2	2.00	0.62
1:A:107:G:H2'	1:A:108:G:H5'	1.82	0.61
1:A:1196:U:H4'	1:A:1197:G:OP2	1.99	0.61
10:H:116:LYS:NZ	10:H:127:LEU:HB3	2.16	0.61
13:K:121:PRO:HG2	13:K:126:ARG:HG2	1.82	0.61
15:M:3:ARG:HB2	15:M:3:ARG:NH1	2.14	0.61
21:S:71:LEU:H	21:S:71:LEU:HD12	1.65	0.61
1:A:1003:G:N2	1:A:1004:A:H1'	2.16	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.14	0.61
1:A:1521:G:H2'	1:A:1522:U:C6	2.35	0.61
1:A:409:G:OP2	1:A:431:A:H8	1.82	0.61
1:A:412:A:H5'	1:A:417:C:C5	2.35	0.61
1:A:437:U:C2'	1:A:438:G:H5'	2.30	0.61
1:A:919:A:O2'	1:A:920:U:H5'	1.99	0.61
1:A:975:A:H5'	1:A:975:A:H8	1.65	0.61
20:R:47:THR:HG22	20:R:48:GLY:N	2.14	0.61
23:V:23:PRO:C	23:V:25:LYS:H	2.03	0.61
1:A:1104:G:OP1	4:B:111:ARG:HD2	2.00	0.61
4:B:124:SER:O	4:B:127:ILE:HG12	2.00	0.61
16:N:37:PHE:CE2	16:N:53:LEU:HD13	2.35	0.61
1:A:575:G:OP1	1:A:575:G:H4'	1.99	0.61
4:B:8:LYS:HD3	4:B:9:GLU:H	1.65	0.61
5:C:54:ARG:HG3	5:C:55:VAL:H	1.65	0.61
5:C:40:ARG:HG2	5:C:55:VAL:HG11	1.82	0.61
14:L:75:HIS:CD2	14:L:77:LEU:H	2.17	0.61
1:A:791:G:H2'	1:A:792:A:C5'	2.31	0.61
20:R:38:GLU:CD	20:R:38:GLU:H	2.04	0.61
1:A:1005:A:H1'	1:A:1026:G:H22	1.64	0.61
1:A:1068:G:H8	1:A:1068:G:OP2	1.82	0.61
8:F:66:GLU:O	8:F:66:GLU:HG3	2.01	0.61
7:E:57:LYS:HG2	7:E:61:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:10:LEU:HD22	10:H:83:ILE:HD11	1.82	0.61
23:V:6:ARG:HG3	23:V:7:ARG:HD2	1.83	0.61
1:A:26:A:N6	1:A:558:G:H1'	2.16	0.61
4:B:219:VAL:C	4:B:221:LEU:H	2.04	0.61
17:O:33:THR:HG23	17:O:63:ARG:NH1	2.15	0.61
21:S:40:ILE:HG21	21:S:62:ILE:CD1	2.31	0.61
1:A:1391:U:H2'	1:A:1392:G:H8	1.64	0.60
1:A:996:A:H2'	1:A:997:U:C6	2.36	0.60
4:B:178:ARG:NH2	4:B:196:LEU:HA	2.16	0.60
5:C:10:PHE:CE2	5:C:178:LEU:HD13	2.36	0.60
5:C:21:ARG:HD3	5:C:58:GLU:HG2	1.82	0.60
1:A:1124:G:H5'	12:J:35:SER:HB3	1.82	0.60
12:J:45:ARG:NH2	16:N:36:PHE:CD2	2.69	0.60
12:J:47:PHE:CE2	16:N:37:PHE:HE1	2.19	0.60
15:M:40:ASN:ND2	15:M:42:ALA:H	1.99	0.60
22:T:56:MET:HE2	22:T:85:MET:HA	1.83	0.60
5:C:41:GLY:O	5:C:45:LYS:HG2	2.01	0.60
11:I:118:LYS:O	11:I:119:ALA:CB	2.49	0.60
12:J:51:ARG:H	12:J:59:SER:HB2	1.66	0.60
1:A:184:G:H2'	1:A:185:A:H8	1.66	0.60
1:A:409:G:H3'	1:A:431:A:N7	2.17	0.60
4:B:139:LYS:NZ	4:B:142:LEU:HD23	2.15	0.60
1:A:269:C:H2'	1:A:270:A:C8	2.36	0.60
1:A:352:C:H4'	1:A:354:G:OP1	2.01	0.60
1:A:413:G:H1'	1:A:416:G:OP1	2.02	0.60
1:A:794:A:H2'	1:A:795:C:C6	2.35	0.60
1:A:975:A:H5'	1:A:975:A:C8	2.36	0.60
5:C:89:GLU:O	5:C:93:LYS:HB2	2.00	0.60
15:M:97:PRO:HB2	15:M:101:GLN:OE1	2.00	0.60
22:T:21:LYS:HZ2	22:T:21:LYS:HB2	1.65	0.60
1:A:1443:G:H5''	1:A:1446:A:H5'	1.83	0.60
1:A:1527:C:O2'	1:A:1528:U:H5'	2.01	0.60
1:A:664:G:OP1	20:R:64:ARG:HD2	2.00	0.60
4:B:132:LYS:HD3	4:B:135:GLN:HB2	1.83	0.60
4:B:25:ASN:ND2	4:B:27:LYS:H	1.99	0.60
4:B:96:ARG:O	4:B:98:LEU:HD23	2.01	0.60
5:C:22:TRP:CH2	5:C:32:LEU:HB2	2.37	0.60
12:J:21:GLN:HE21	12:J:25:GLU:HG2	1.66	0.60
12:J:75:ILE:HG22	12:J:76:ASN:N	2.17	0.60
19:Q:69:LYS:H	19:Q:70:ARG:HD2	1.67	0.60
1:A:1347:G:O2'	1:A:1348:U:P	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:111:ARG:HB3	4:B:149:LEU:HD11	1.83	0.60
5:C:83:ARG:C	5:C:85:ARG:H	2.04	0.60
6:D:8:VAL:C	6:D:10:ARG:H	2.05	0.60
12:J:49:VAL:CG2	16:N:41:ARG:HB2	2.30	0.60
21:S:6:LYS:CD	21:S:6:LYS:H	2.11	0.60
1:A:1152:A:H5'	12:J:70:ARG:HH22	1.67	0.60
1:A:547:A:H4'	1:A:548:G:O5'	2.01	0.60
5:C:47:LEU:HD12	5:C:47:LEU:H	1.67	0.60
11:I:89:ASN:HD21	11:I:91:ASP:HB2	1.67	0.60
15:M:48:LEU:HD12	15:M:53:VAL:HG22	1.82	0.60
17:O:39:LEU:HD22	17:O:56:LEU:HB2	1.83	0.60
6:D:23:GLY:HA3	6:D:113:SER:HB3	1.84	0.60
9:G:37:ASN:O	9:G:41:ARG:HG3	2.01	0.60
12:J:3:LYS:N	12:J:3:LYS:HD2	2.17	0.60
17:O:76:GLU:HA	17:O:79:ARG:HH21	1.65	0.60
1:A:1128:C:O2'	1:A:1130:A:H8	1.84	0.60
1:A:1497:G:C2'	1:A:1498:U:H5'	2.31	0.60
1:A:149:A:H2'	1:A:150:C:C6	2.37	0.60
1:A:189:G:C2'	1:A:190:C:H5'	2.25	0.60
1:A:190:C:H5'	1:A:190(K):G:N2	2.17	0.60
14:L:26:ALA:O	14:L:27:LEU:O	2.20	0.60
14:L:58:VAL:O	14:L:65:GLU:HA	2.01	0.60
19:Q:76:LEU:HD23	19:Q:77:VAL:N	2.17	0.60
1:A:408:A:C4'	1:A:429:U:O2	2.48	0.60
1:A:620:C:N1	6:D:135:LEU:HD13	2.16	0.60
16:N:9:LYS:C	16:N:11:LYS:H	2.05	0.60
1:A:453:A:H4'	18:P:72:ARG:HG3	1.84	0.60
21:S:42:PRO:O	21:S:45:VAL:HG23	2.00	0.60
13:K:126:ARG:O	13:K:128:ALA:N	2.35	0.59
15:M:48:LEU:HD12	15:M:53:VAL:CG2	2.32	0.59
17:O:39:LEU:O	17:O:39:LEU:HD23	2.02	0.59
1:A:255:G:H1'	19:Q:16:GLN:OE1	2.02	0.59
1:A:1020:U:H2'	1:A:1021:G:C8	2.37	0.59
1:A:748:C:O2'	1:A:749:C:C6	2.54	0.59
4:B:177:ALA:O	4:B:180:LEU:N	2.29	0.59
6:D:126:ILE:HG22	6:D:127:THR:H	1.66	0.59
8:F:25:ILE:HD12	8:F:82:ARG:HH11	1.67	0.59
13:K:14:VAL:HG12	13:K:16:SER:H	1.66	0.59
19:Q:101:ARG:HE	19:Q:101:ARG:HA	1.65	0.59
1:A:1062:U:H2'	1:A:1063:C:C6	2.36	0.59
1:A:502:G:H4'	1:A:550:G:H4'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:G:N3	17:O:23:GLY:HA3	2.17	0.59
4:B:185:ILE:HD12	4:B:185:ILE:N	2.16	0.59
5:C:18:TRP:HE3	5:C:18:TRP:H	1.49	0.59
11:I:86:VAL:HG13	11:I:90:PRO:HA	1.83	0.59
13:K:126:ARG:C	13:K:128:ALA:H	2.04	0.59
1:A:1121:U:O2'	1:A:1122:U:H5'	2.01	0.59
1:A:1367:C:H5'	12:J:60:ARG:NH1	2.17	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.59
4:B:166:ASP:OD2	4:B:169:LYS:HB2	2.02	0.59
1:A:1251:A:H4'	11:I:12:GLU:OE2	2.03	0.59
12:J:4:ILE:HD11	12:J:74:ILE:CD1	2.25	0.59
16:N:26:ARG:HH11	16:N:43:CYS:HB3	1.66	0.59
19:Q:14:LYS:CD	19:Q:14:LYS:H	2.14	0.59
1:A:730:G:H21	1:A:765:G:H5''	1.67	0.59
4:B:178:ARG:NH1	4:B:178:ARG:CG	2.65	0.59
4:B:17:PHE:HA	4:B:42:ILE:HB	1.84	0.59
5:C:91:LEU:HD21	5:C:99:VAL:HG22	1.83	0.59
7:E:9:LYS:HB3	7:E:33:VAL:HG23	1.82	0.59
13:K:51:LYS:HE2	13:K:52:GLY:N	2.18	0.59
1:A:266:G:C8	1:A:266:G:H5'	2.37	0.59
1:A:960:U:O2	1:A:960:U:H2'	2.03	0.59
4:B:103:THR:HG23	4:B:176:GLU:OE1	2.02	0.59
4:B:22:LYS:HG3	4:B:35:GLU:OE1	2.02	0.59
7:E:33:VAL:CG1	7:E:109:ILE:HG12	2.25	0.59
7:E:36:ASP:OD1	7:E:38:GLN:N	2.31	0.59
13:K:22:HIS:HB3	13:K:29:ILE:HG13	1.85	0.59
14:L:39:VAL:H	14:L:57:LYS:HB2	1.67	0.59
4:B:139:LYS:C	4:B:139:LYS:HD3	2.22	0.59
5:C:55:VAL:HG12	5:C:55:VAL:O	2.01	0.59
7:E:53:LEU:H	7:E:53:LEU:CD1	2.15	0.59
9:G:115:ARG:HB2	9:G:118:VAL:CG2	2.33	0.59
18:P:67:THR:HG22	18:P:68:ASP:N	2.17	0.59
1:A:1091:U:O2	1:A:1093:A:C8	2.56	0.59
5:C:91:LEU:HD23	5:C:92:ALA:H	1.67	0.59
7:E:103:GLY:O	7:E:106:PRO:HD2	2.03	0.59
11:I:9:ARG:CG	11:I:14:VAL:HG22	2.32	0.59
1:A:996:A:H2	1:A:1045:C:HO2'	1.50	0.59
1:A:882:C:O2'	1:A:883:C:H5'	2.02	0.59
4:B:223:ILE:C	4:B:225:ALA:H	2.05	0.59
6:D:187:ARG:HD2	6:D:188:LEU:H	1.67	0.59
7:E:9:LYS:HB3	7:E:33:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:57:THR:OG1	13:K:58:PRO:HD2	2.03	0.59
18:P:81:ARG:HH21	18:P:82:GLN:HG2	1.66	0.59
1:A:1020:U:H2'	1:A:1021:G:H8	1.67	0.59
1:A:1117:G:H21	1:A:1180:A:H1'	1.68	0.59
1:A:1216:G:O2'	1:A:1217:C:H5'	2.03	0.59
7:E:37:ARG:HG2	7:E:37:ARG:HH11	1.68	0.59
10:H:69:ARG:NH1	10:H:75:ARG:O	2.35	0.59
12:J:5:ARG:HA	12:J:73:ASP:OD1	2.02	0.59
14:L:27:LEU:HG	14:L:28:LYS:H	1.68	0.59
15:M:9:ILE:N	15:M:9:ILE:HD12	2.17	0.59
20:R:39:VAL:O	20:R:42:ARG:HB2	2.03	0.59
1:A:254:G:OP1	19:Q:67:LYS:O	2.20	0.58
1:A:344:A:H5''	1:A:345:C:H5	1.67	0.58
1:A:662:G:H2'	1:A:663:A:C8	2.38	0.58
1:A:694:A:C3'	1:A:695:A:H5''	2.32	0.58
16:N:3:ARG:NH1	16:N:6:LEU:HD11	2.17	0.58
5:C:134:ILE:O	5:C:138:VAL:HG23	2.02	0.58
5:C:154:SER:O	5:C:165:THR:HA	2.02	0.58
5:C:116:VAL:HG21	5:C:202:ILE:HD11	1.85	0.58
5:C:46:GLU:O	5:C:48:TYR:N	2.36	0.58
10:H:51:VAL:HG12	10:H:52:ASP:N	2.18	0.58
10:H:63:LEU:H	10:H:63:LEU:HD22	1.68	0.58
10:H:77:GLU:HG2	10:H:78:GLN:N	2.19	0.58
22:T:54:LYS:HG3	22:T:100:ILE:HD12	1.85	0.58
1:A:977:A:C2'	1:A:978:A:H5''	2.33	0.58
4:B:184:VAL:HG12	4:B:197:VAL:HG13	1.85	0.58
4:B:206:ASP:O	4:B:207:ALA:HB3	2.03	0.58
4:B:8:LYS:CD	4:B:9:GLU:H	2.16	0.58
5:C:19:GLU:HB3	5:C:40:ARG:HH21	1.67	0.58
1:A:302:G:H5''	14:L:17:LYS:HZ1	1.68	0.58
15:M:125:ARG:HD2	15:M:125:ARG:O	2.02	0.58
1:A:839:U:O2	1:A:839:U:H2'	2.02	0.58
4:B:83:MET:HE3	4:B:235:SER:HA	1.84	0.58
5:C:108:ASN:HD22	5:C:111:LEU:HG	1.68	0.58
5:C:34:LEU:HG	16:N:25:VAL:HG21	1.83	0.58
9:G:135:VAL:O	9:G:139:GLU:HG3	2.02	0.58
20:R:42:ARG:HH11	20:R:42:ARG:HG3	1.69	0.58
21:S:15:LEU:O	21:S:19:VAL:HG12	2.03	0.58
1:A:459:G:H3'	1:A:460:A:H5''	1.84	0.58
1:A:792:A:H1'	1:A:794:A:N7	2.19	0.58
4:B:24:TRP:HB3	4:B:40:HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:33:TYR:O	8:F:35:ALA:N	2.36	0.58
10:H:103:VAL:CG2	10:H:110:ALA:HB2	2.33	0.58
14:L:46:LYS:HE3	14:L:47:LYS:HB2	1.86	0.58
17:O:17:ARG:NH1	17:O:77:ARG:NH1	2.51	0.58
22:T:54:LYS:HE3	22:T:100:ILE:HD11	1.85	0.58
1:A:1117:G:H5'	1:A:1117:G:H8	1.68	0.58
1:A:1216:G:H5''	16:N:5:ALA:CB	2.34	0.58
1:A:883:C:O2'	1:A:884:U:H5'	2.04	0.58
6:D:36:ARG:HH11	6:D:36:ARG:HG2	1.68	0.58
22:T:24:LEU:HA	22:T:27:LYS:HE2	1.84	0.58
1:A:1225:A:N3	1:A:1225:A:H2'	2.18	0.58
1:A:1407:C:O2'	1:A:1408:A:H5'	2.03	0.58
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.58
1:A:413:G:OP2	1:A:417:C:H5''	2.03	0.58
1:A:560:U:H5'	1:A:566:G:N2	2.18	0.58
5:C:34:LEU:HD23	5:C:34:LEU:O	2.02	0.58
14:L:50:SER:O	14:L:51:ALA:HB2	2.03	0.58
14:L:67:THR:HG21	14:L:96:VAL:HG22	1.84	0.58
17:O:39:LEU:C	17:O:39:LEU:HD23	2.24	0.58
5:C:47:LEU:N	5:C:47:LEU:HD12	2.19	0.58
9:G:121:ALA:O	9:G:125:MET:HG3	2.03	0.58
12:J:32:ALA:HB1	12:J:75:ILE:HD13	1.85	0.58
19:Q:45:HIS:CD2	19:Q:47:PRO:HG3	2.38	0.58
22:T:70:SER:HA	22:T:73:HIS:CD2	2.38	0.58
22:T:75:ASN:N	22:T:75:ASN:OD1	2.35	0.58
1:A:1016:A:H2'	1:A:1017:G:O4'	2.04	0.58
1:A:1033:G:H2'	1:A:1034:G:H8	1.68	0.58
1:A:1072:G:H2'	1:A:1073:U:C6	2.39	0.58
1:A:45:U:H2'	1:A:46:G:C8	2.39	0.58
1:A:748:C:OP2	1:A:748:C:H6	1.87	0.58
4:B:25:ASN:ND2	4:B:27:LYS:N	2.51	0.58
4:B:95:GLN:C	4:B:96:ARG:HD2	2.24	0.58
12:J:29:ARG:HH12	12:J:84:GLN:NE2	1.95	0.58
15:M:32:GLU:OE1	15:M:64:TRP:HZ2	1.87	0.58
15:M:94:ARG:NH1	15:M:94:ARG:HG3	2.17	0.58
16:N:11:LYS:HB2	16:N:11:LYS:NZ	2.19	0.58
20:R:43:PHE:HA	20:R:51:LEU:HD12	1.86	0.58
1:A:1277:C:H2'	1:A:1278:U:H5'	1.86	0.58
1:A:1402:C:O2	1:A:1500:A:N1	2.37	0.58
1:A:731:G:OP1	1:A:766:A:H1'	2.04	0.58
4:B:98:LEU:O	4:B:101:MET:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:75:LYS:HE2	4:B:96:ARG:HH12	1.69	0.58
4:B:98:LEU:N	4:B:98:LEU:HD23	2.19	0.58
5:C:47:LEU:CD1	5:C:47:LEU:H	2.17	0.58
7:E:79:GLU:HG3	7:E:93:PRO:CD	2.33	0.58
14:L:46:LYS:CG	14:L:47:LYS:H	2.16	0.58
1:A:1435:G:H2'	1:A:1436:U:H6	1.67	0.57
1:A:371:G:C2'	1:A:372:C:H5'	2.34	0.57
1:A:409:G:H5'	1:A:430:A:C6	2.38	0.57
1:A:865:A:H5'	1:A:1078:U:O4	2.04	0.57
6:D:61:LYS:HD2	6:D:207:TYR:OH	2.03	0.57
7:E:76:ILE:HD12	7:E:118:ILE:HD12	1.85	0.57
10:H:60:ARG:HG3	10:H:60:ARG:HH11	1.69	0.57
13:K:70:LYS:O	13:K:73:MET:N	2.36	0.57
13:K:84:VAL:HG21	20:R:88:LYS:HD2	1.86	0.57
21:S:63:THR:HG22	21:S:65:ASN:H	1.69	0.57
1:A:1066:C:O2'	1:A:1067:A:H5'	2.04	0.57
5:C:60:ALA:O	5:C:61:ALA:HB2	2.04	0.57
1:A:427:U:OP1	6:D:13:ARG:NH2	2.36	0.57
6:D:158:ILE:HG23	6:D:162:LEU:HD12	1.86	0.57
8:F:86:ARG:O	8:F:87:ARG:HG2	2.04	0.57
9:G:15:ASP:HB3	9:G:19:GLY:H	1.67	0.57
22:T:96:GLY:O	22:T:97:ALA:HB3	2.03	0.57
7:E:79:GLU:N	7:E:79:GLU:OE1	2.37	0.57
8:F:93:SER:O	8:F:94:GLN:HG3	2.03	0.57
1:A:409:G:H22	1:A:432:A:C3'	2.17	0.57
1:A:423:G:C8	1:A:424:G:N3	2.72	0.57
1:A:556:C:C2'	1:A:557:G:H5'	2.33	0.57
7:E:144:THR:HB	7:E:147:ASP:OD1	2.05	0.57
21:S:30:LEU:O	21:S:31:ILE:HD13	2.04	0.57
1:A:1195:C:H3'	1:A:1196:U:H5'	1.86	0.57
1:A:1330:U:C2'	1:A:1331:G:H5'	2.33	0.57
1:A:425:G:O2'	1:A:426:G:H5'	2.05	0.57
4:B:80:ILE:HD13	4:B:212:GLN:HB2	1.85	0.57
12:J:12:ASP:OD1	12:J:14:LYS:N	2.36	0.57
15:M:23:TYR:HB3	15:M:67:GLU:CA	2.34	0.57
1:A:376:G:OP2	18:P:67:THR:HG21	2.04	0.57
21:S:28:LYS:CG	21:S:29:ARG:H	2.14	0.57
1:A:1121:U:H2'	1:A:1122:U:H6	1.69	0.57
1:A:1262:C:H2'	1:A:1263:C:H6	1.69	0.57
4:B:18:GLY:N	4:B:42:ILE:H	2.02	0.57
1:A:429:U:H2'	6:D:25:ARG:HH12	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:144:THR:HG22	7:E:146:ALA:N	2.18	0.57
9:G:78:ARG:NH1	9:G:154:TYR:HB3	2.19	0.57
18:P:81:ARG:CA	18:P:81:ARG:NE	2.65	0.57
1:A:1006:C:H2'	1:A:1007:C:C6	2.33	0.57
1:A:617:G:H5'	18:P:45:THR:HG22	1.87	0.57
19:Q:80:GLY:O	19:Q:81:ARG:HB3	2.04	0.57
21:S:51:VAL:HG21	21:S:71:LEU:HB3	1.86	0.57
21:S:51:VAL:O	21:S:58:VAL:N	2.37	0.57
1:A:474:G:H5'	1:A:475:G:C8	2.40	0.57
1:A:476:G:H21	1:A:478:A:H5''	1.68	0.57
4:B:39:ILE:HD12	4:B:39:ILE:N	2.19	0.57
4:B:35:GLU:HA	4:B:39:ILE:O	2.04	0.57
5:C:30:ARG:HH11	5:C:30:ARG:HG2	1.69	0.57
1:A:1016:A:O5'	1:A:1016:A:H8	1.87	0.57
1:A:1279:A:H5''	1:A:1280:A:OP1	2.05	0.57
1:A:112:G:H4'	1:A:389:A:H5''	1.86	0.57
1:A:1103:C:H5''	4:B:98:LEU:CD1	2.35	0.57
9:G:80:VAL:HG22	9:G:83:ALA:O	2.04	0.57
9:G:75:VAL:CG2	9:G:86:GLN:HB3	2.34	0.57
1:A:1112:C:H1'	5:C:179:ARG:NH2	2.20	0.57
1:A:918:A:H2'	1:A:919:A:C8	2.39	0.57
4:B:15:VAL:HG13	4:B:209:ARG:HG3	1.87	0.57
4:B:30:ARG:HG3	4:B:31:TYR:H	1.69	0.57
5:C:79:ARG:CG	5:C:82:GLU:HB2	2.22	0.57
7:E:24:ARG:HH11	7:E:24:ARG:CB	2.18	0.57
8:F:71:ARG:O	8:F:73:ASN:N	2.38	0.57
9:G:23:VAL:HG13	9:G:43:PHE:CE2	2.40	0.57
10:H:46:LYS:N	10:H:64:LYS:HG3	2.20	0.57
1:A:1280:A:O4'	12:J:41:PRO:HG3	2.04	0.57
14:L:24:VAL:HG12	14:L:24:VAL:O	2.03	0.57
15:M:8:GLU:OE1	15:M:22:ILE:HA	2.04	0.57
1:A:1329:A:P	15:M:28:ALA:HB3	2.45	0.56
1:A:113:G:H1'	1:A:354:G:C5'	2.35	0.56
4:B:224:GLN:O	4:B:224:GLN:HG2	2.05	0.56
10:H:120:THR:HG23	10:H:123:GLU:OE2	2.05	0.56
12:J:44:VAL:HG21	12:J:66:ARG:HH21	1.70	0.56
12:J:90:LEU:H	12:J:91:PRO:HD3	1.68	0.56
17:O:74:ASP:OD1	17:O:76:GLU:HB3	2.04	0.56
1:A:1244:C:O2'	1:A:1245:A:H5'	2.06	0.56
1:A:1286:A:C8	1:A:1287:A:H4'	2.41	0.56
1:A:188:C:C6	1:A:188:C:H5''	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:62:GLN:HE22	6:D:65:ARG:NH1	2.01	0.56
10:H:97:VAL:HG21	10:H:128:GLY:HA2	1.86	0.56
11:I:3:GLN:HB2	11:I:20:ARG:HD3	1.87	0.56
12:J:4:ILE:HA	12:J:100:THR:CB	2.35	0.56
1:A:1103:C:H5''	4:B:98:LEU:HD13	1.86	0.56
1:A:1251:A:H2'	1:A:1252:A:H8	1.66	0.56
1:A:112:G:H21	1:A:354:G:C5'	2.15	0.56
5:C:107:GLN:O	5:C:108:ASN:HB3	2.05	0.56
6:D:162:LEU:HD13	6:D:181:MET:CG	2.35	0.56
10:H:24:THR:HG23	10:H:61:VAL:HB	1.86	0.56
10:H:24:THR:HG22	10:H:63:LEU:HD21	1.86	0.56
10:H:63:LEU:HD22	10:H:63:LEU:N	2.21	0.56
11:I:10:ARG:HE	11:I:11:LYS:HB2	1.71	0.56
15:M:25:ILE:HG22	15:M:26:GLY:N	2.20	0.56
1:A:1229:A:H2'	1:A:1230:C:C6	2.40	0.56
1:A:1405:G:O2'	1:A:1406:U:H5'	2.04	0.56
6:D:153:ARG:HE	6:D:181:MET:HE3	1.71	0.56
12:J:6:ILE:HD12	12:J:72:VAL:HG11	1.87	0.56
17:O:17:ARG:HG3	17:O:17:ARG:NH1	2.20	0.56
1:A:1117:G:N2	1:A:1180:A:H1'	2.19	0.56
1:A:168:G:O2'	1:A:169:C:H5'	2.04	0.56
1:A:421:U:H2'	1:A:423:G:OP1	2.04	0.56
1:A:953:G:H1'	15:M:125:ARG:CA	2.35	0.56
4:B:18:GLY:H	4:B:42:ILE:N	2.02	0.56
5:C:10:PHE:CZ	5:C:178:LEU:HD13	2.41	0.56
5:C:90:GLU:O	5:C:94:LEU:HD13	2.05	0.56
6:D:64:LEU:HD12	6:D:75:PHE:CZ	2.41	0.56
10:H:36:LEU:CD1	10:H:59:LEU:HD13	2.36	0.56
15:M:50:GLU:O	15:M:54:VAL:HG23	2.06	0.56
1:A:1256:A:O3'	1:A:1257:U:H4'	2.06	0.56
1:A:1366:C:H2'	1:A:1367:C:C6	2.40	0.56
1:A:376:G:H2'	1:A:377:G:H8	1.71	0.56
1:A:411:A:N6	1:A:426:G:H22	2.04	0.56
1:A:730:G:N2	1:A:765:G:H5''	2.20	0.56
4:B:38:GLY:C	4:B:39:ILE:HD12	2.26	0.56
6:D:105:VAL:HG12	6:D:117:ALA:HB1	1.86	0.56
6:D:205:GLU:HA	6:D:208:SER:OG	2.06	0.56
9:G:149:ARG:O	9:G:149:ARG:HG2	2.06	0.56
1:A:1090:U:O2'	1:A:1091:U:H5'	2.06	0.56
1:A:1106:G:H5''	5:C:172:ARG:HG2	1.87	0.56
5:C:188:LEU:HD13	5:C:189:ALA:N	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:102:ALA:HB1	7:E:120:THR:HG21	1.88	0.56
9:G:51:GLN:C	9:G:53:LYS:H	2.09	0.56
1:A:972:C:H4'	12:J:57:LYS:HE2	1.87	0.56
15:M:34:LEU:HD13	15:M:41:PRO:CA	2.32	0.56
22:T:67:ALA:HA	22:T:73:HIS:H	1.69	0.56
1:A:1014:A:C2	1:A:1219:U:H1'	2.40	0.56
1:A:41:G:H2'	1:A:42:G:C8	2.41	0.56
1:A:437:U:H2'	1:A:438:G:H5'	1.88	0.56
1:A:1206:G:H1'	5:C:193:TYR:O	2.06	0.56
5:C:66:VAL:O	5:C:66:VAL:HG12	2.06	0.56
6:D:15:GLU:HG2	6:D:63:LYS:HG3	1.88	0.56
10:H:48:TYR:HB2	10:H:60:ARG:O	2.06	0.56
12:J:19:SER:OG	12:J:91:PRO:HD3	2.06	0.56
15:M:121:LYS:O	15:M:122:LYS:HB2	2.05	0.56
18:P:81:ARG:O	18:P:83:GLU:N	2.28	0.56
22:T:79:ARG:O	22:T:83:ARG:HG3	2.05	0.56
2:X:39:C:O5'	2:X:39:C:H6	1.89	0.56
1:A:1262:C:H2'	1:A:1263:C:C6	2.40	0.56
1:A:1475:G:H2'	1:A:1476:G:H8	1.69	0.56
1:A:397:A:H5'	1:A:398:C:OP1	2.05	0.56
5:C:54:ARG:HG3	5:C:55:VAL:N	2.21	0.56
6:D:11:LEU:HD22	6:D:66:ARG:CZ	2.36	0.56
10:H:119:LEU:HD23	10:H:119:LEU:N	2.19	0.56
1:A:591:U:OP1	10:H:30:ARG:NE	2.36	0.56
13:K:92:GLU:HA	13:K:92:GLU:OE1	2.06	0.56
16:N:14:PRO:O	16:N:15:LYS:CB	2.54	0.56
1:A:463:A:N3	18:P:82:GLN:HB2	2.20	0.56
22:T:57:ARG:NH1	22:T:57:ARG:HB2	2.19	0.56
1:A:129:U:H5'	1:A:129(A):G:OP1	2.05	0.56
1:A:697:U:H2'	1:A:698:G:H5'	1.88	0.56
4:B:71:VAL:CG2	4:B:164:VAL:HA	2.36	0.56
8:F:27:GLN:O	8:F:31:GLU:HG3	2.06	0.56
10:H:31:PHE:HZ	10:H:134:ILE:HD11	1.69	0.56
12:J:24:VAL:O	12:J:28:ARG:HB2	2.05	0.56
14:L:25:PRO:C	14:L:27:LEU:H	2.07	0.56
18:P:11:SER:HB3	18:P:14:ASN:HD22	1.70	0.56
21:S:28:LYS:HD3	21:S:31:ILE:CD1	2.36	0.56
1:A:1381:U:O2'	1:A:1382:C:H5'	2.05	0.56
1:A:791:G:H2'	1:A:792:A:H5'	1.87	0.56
4:B:95:GLN:HG3	4:B:148:TYR:HD2	1.71	0.56
5:C:50:ALA:HA	5:C:72:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:C:H2'	1:A:835:U:H6	1.71	0.55
1:A:877:C:O2'	1:A:878:G:H5'	2.05	0.55
4:B:112:VAL:C	4:B:114:ARG:H	2.08	0.55
11:I:8:GLY:CA	11:I:79:LEU:HB3	2.37	0.55
16:N:8:GLU:OE1	16:N:8:GLU:C	2.45	0.55
21:S:6:LYS:CD	21:S:6:LYS:N	2.64	0.55
1:A:418:C:H2'	1:A:419:C:C2	2.41	0.55
4:B:231:GLU:H	4:B:231:GLU:CD	2.08	0.55
8:F:43:LEU:N	8:F:43:LEU:HD22	2.20	0.55
8:F:10:LEU:HD12	8:F:59:TYR:O	2.07	0.55
7:E:152:ARG:HA	10:H:64:LYS:NZ	2.21	0.55
19:Q:66:SER:O	19:Q:70:ARG:NH1	2.39	0.55
21:S:45:VAL:HA	21:S:62:ILE:HG13	1.87	0.55
1:A:1443:G:H5''	1:A:1446:A:C5'	2.37	0.55
1:A:1513:A:H2'	1:A:1514:C:C6	2.41	0.55
1:A:1515:C:O2'	1:A:1516:G:H5'	2.06	0.55
1:A:163:C:O2'	1:A:164:U:H5'	2.07	0.55
1:A:35:G:H2'	1:A:36:C:H6	1.69	0.55
1:A:382:A:H2'	1:A:383:A:C8	2.40	0.55
5:C:93:LYS:HB3	5:C:94:LEU:HD12	1.88	0.55
14:L:41:ARG:HH21	14:L:57:LYS:HE2	1.72	0.55
1:A:190(E):U:O2'	19:Q:63:ARG:NH2	2.38	0.55
7:E:109:ILE:HG22	7:E:109:ILE:O	2.06	0.55
11:I:28:VAL:HA	11:I:63:ILE:O	2.06	0.55
18:P:4:ILE:HG13	18:P:64:ALA:HB1	1.88	0.55
13:K:110:ASP:HB2	20:R:88:LYS:CE	2.37	0.55
22:T:24:LEU:O	22:T:24:LEU:HD12	2.06	0.55
1:A:1298:C:H4'	1:A:1299:A:O4'	2.06	0.55
1:A:780:A:O2'	1:A:781:A:H5''	2.07	0.55
4:B:144:ARG:O	4:B:147:LYS:N	2.39	0.55
4:B:207:ALA:O	4:B:210:SER:HB3	2.06	0.55
5:C:180:ALA:HB1	5:C:182:ILE:HG13	1.89	0.55
14:L:117:ARG:NH2	14:L:124:LYS:HA	2.22	0.55
1:A:975:A:O2'	16:N:32:SER:HA	2.06	0.55
20:R:37:VAL:HG12	20:R:41:LYS:HD3	1.89	0.55
21:S:41:VAL:HG22	21:S:44:MET:CE	2.37	0.55
5:C:154:SER:HB3	5:C:197:GLY:H	1.72	0.55
6:D:148:VAL:CG1	6:D:158:ILE:HD13	2.36	0.55
11:I:127:LYS:CD	15:M:126:LYS:HE2	2.36	0.55
12:J:29:ARG:NH1	12:J:84:GLN:HE22	1.98	0.55
1:A:1238:A:H5'	1:A:1336:C:N4	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H4'	1:A:976:G:O5'	2.07	0.55
5:C:58:GLU:O	5:C:59:ARG:HG3	2.06	0.55
8:F:21:LEU:O	8:F:24:GLU:HB3	2.07	0.55
20:R:59:SER:OG	20:R:62:GLU:HG3	2.06	0.55
1:A:1126:U:N3	1:A:1127:G:C2	2.75	0.55
1:A:1131:G:H2'	1:A:1132:C:C6	2.41	0.55
1:A:1167:A:H2'	1:A:1168:A:C8	2.42	0.55
1:A:393:A:O2'	1:A:394:G:H5'	2.07	0.55
4:B:77:ALA:CB	4:B:211:ILE:HD13	2.36	0.55
8:F:19:LEU:HD23	8:F:19:LEU:C	2.27	0.55
10:H:103:VAL:HG21	10:H:110:ALA:HB2	1.88	0.55
10:H:35:ILE:HG23	10:H:111:ILE:HG21	1.88	0.55
15:M:11:ARG:HG3	15:M:12:ASN:N	2.21	0.55
15:M:36:LYS:HD2	15:M:59:TYR:CZ	2.42	0.55
15:M:69:GLU:O	15:M:72:ALA:HB3	2.07	0.55
1:A:958:A:C8	21:S:55:LYS:HD2	2.42	0.55
1:A:959:A:C2	1:A:1222:G:O4'	2.60	0.55
1:A:349:A:C3'	1:A:350:G:H5''	2.36	0.55
1:A:353:A:H8	1:A:353:A:C5'	2.20	0.55
1:A:409:G:H5''	1:A:431:A:N7	2.20	0.55
1:A:463:A:H3'	1:A:475:G:O6	2.07	0.55
5:C:34:LEU:HD22	5:C:38:ARG:NH2	2.21	0.55
10:H:112:LEU:HD12	10:H:112:LEU:C	2.27	0.55
7:E:152:ARG:HB3	10:H:43:GLY:O	2.07	0.55
15:M:19:LEU:HA	15:M:22:ILE:HD13	1.89	0.55
15:M:62:ASN:O	15:M:63:THR:CB	2.55	0.55
1:A:1116:C:H2'	1:A:1117:G:C5'	2.28	0.55
1:A:1125:U:H5''	1:A:1126:U:C5	2.42	0.55
1:A:1316:G:H4'	16:N:18:VAL:CG1	2.36	0.55
4:B:115:LEU:HG	4:B:116:GLU:N	2.22	0.55
5:C:73:PRO:O	5:C:76:VAL:HB	2.07	0.55
5:C:84:ILE:O	5:C:88:ARG:HB2	2.06	0.55
5:C:64:VAL:HB	5:C:99:VAL:CG2	2.37	0.55
15:M:3:ARG:CB	15:M:3:ARG:HH11	2.17	0.55
1:A:1289:A:H2'	1:A:1290:G:H5'	1.89	0.54
1:A:189:G:C2'	1:A:190(K):G:N2	2.62	0.54
1:A:427:U:OP2	6:D:36:ARG:NH2	2.40	0.54
4:B:74:LYS:HZ1	4:B:206:ASP:HB2	1.72	0.54
5:C:83:ARG:C	5:C:85:ARG:N	2.61	0.54
11:I:7:THR:HG22	11:I:8:GLY:N	2.23	0.54
14:L:41:ARG:NH2	14:L:57:LYS:HE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:9:LYS:C	16:N:11:LYS:N	2.60	0.54
16:N:9:LYS:HD3	16:N:9:LYS:C	2.28	0.54
18:P:28:ARG:HG2	18:P:28:ARG:NH1	2.21	0.54
1:A:760:G:H1	19:Q:105:ALA:HA	1.72	0.54
21:S:63:THR:HG21	21:S:65:ASN:ND2	2.22	0.54
1:A:1392:G:N2	1:A:1502:A:H8	2.04	0.54
1:A:457:C:N4	1:A:475:G:H22	2.05	0.54
1:A:959:A:H3'	1:A:960:U:H5''	1.89	0.54
4:B:184:VAL:N	4:B:198:ASP:OD2	2.40	0.54
4:B:21:ARG:N	4:B:21:ARG:HD2	2.22	0.54
1:A:532:A:H5''	5:C:161:GLU:OE1	2.07	0.54
1:A:644:G:O2'	1:A:645:C:H5'	2.06	0.54
4:B:213:LEU:HD23	4:B:213:LEU:C	2.27	0.54
4:B:81:VAL:HG12	4:B:81:VAL:O	2.05	0.54
5:C:64:VAL:HB	5:C:99:VAL:HG21	1.90	0.54
7:E:96:PRO:HA	7:E:117:ASP:OD2	2.08	0.54
7:E:40:ARG:HG2	7:E:68:GLU:OE1	2.07	0.54
21:S:22:LEU:C	21:S:24:ALA:H	2.11	0.54
1:A:477:G:O2'	1:A:478:A:H5'	2.07	0.54
6:D:111:ALA:HB2	6:D:120:LEU:HD12	1.89	0.54
6:D:173:TRP:CD2	6:D:189:PRO:HB3	2.43	0.54
6:D:173:TRP:O	6:D:186:LEU:HB2	2.07	0.54
7:E:101:ILE:HD12	7:E:119:LEU:HD21	1.89	0.54
10:H:116:LYS:HD3	10:H:127:LEU:CD1	2.37	0.54
12:J:32:ALA:HB2	12:J:76:ASN:OD1	2.07	0.54
1:A:974:A:OP2	16:N:41:ARG:NH1	2.40	0.54
1:A:1532:U:O2'	1:A:1533:C:H4'	2.07	0.54
1:A:613:C:O2'	1:A:614:A:H5'	2.08	0.54
5:C:13:GLY:O	5:C:14:ILE:HD13	2.07	0.54
9:G:38:LEU:HD12	9:G:38:LEU:O	2.07	0.54
9:G:54:THR:HG22	9:G:56:GLN:N	2.22	0.54
11:I:10:ARG:HH21	11:I:11:LYS:HD2	1.73	0.54
11:I:28:VAL:HG12	11:I:63:ILE:HB	1.89	0.54
17:O:87:ILE:O	17:O:88:ARG:HB2	2.08	0.54
4:B:71:VAL:HG21	4:B:164:VAL:HG22	1.89	0.54
5:C:22:TRP:CZ3	5:C:32:LEU:HB2	2.42	0.54
6:D:102:ASP:OD2	6:D:103:ASN:N	2.41	0.54
9:G:146:GLU:HA	9:G:149:ARG:HB2	1.89	0.54
9:G:79:ARG:HH11	9:G:79:ARG:HG2	1.71	0.54
11:I:114:TYR:CE1	12:J:59:SER:O	2.61	0.54
15:M:88:ARG:HH11	15:M:88:ARG:CB	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:10:LEU:HB3	19:Q:32:TYR:CE1	2.42	0.54
1:A:1263:C:H2'	1:A:1264:C:H6	1.68	0.54
7:E:87:SER:HB3	7:E:131:ILE:HD13	1.90	0.54
9:G:59:LEU:HD11	9:G:63:LYS:HE2	1.89	0.54
10:H:45:ILE:O	10:H:46:LYS:C	2.46	0.54
12:J:60:ARG:H	12:J:60:ARG:HD2	1.69	0.54
15:M:40:ASN:HD22	15:M:40:ASN:C	2.07	0.54
13:K:110:ASP:HB2	20:R:88:LYS:HE3	1.89	0.54
1:A:1427:U:O2'	1:A:1428:A:H5'	2.08	0.54
4:B:53:ARG:NH1	4:B:199:TYR:HD2	2.05	0.54
4:B:21:ARG:H	4:B:21:ARG:HD2	1.73	0.54
5:C:155:GLY:O	5:C:156:ARG:HB2	2.07	0.54
5:C:195:VAL:O	5:C:196:LEU:HD22	2.08	0.54
5:C:50:ALA:HB1	5:C:70:VAL:HG11	1.88	0.54
6:D:165:MET:SD	6:D:168:ARG:HD2	2.48	0.54
10:H:119:LEU:HB2	10:H:123:GLU:HB2	1.90	0.54
11:I:11:LYS:O	11:I:11:LYS:HG2	2.08	0.54
11:I:9:ARG:HA	11:I:13:ALA:O	2.08	0.54
18:P:20:VAL:HG11	18:P:32:TYR:HB3	1.90	0.54
1:A:1037:C:H2'	1:A:1038:C:C6	2.43	0.54
1:A:189:G:C2'	1:A:190(K):G:H22	2.21	0.54
5:C:187:ALA:O	5:C:198:VAL:HG23	2.08	0.54
5:C:83:ARG:O	5:C:86:VAL:N	2.41	0.54
6:D:17:VAL:HG12	6:D:18:LYS:N	2.23	0.54
6:D:70:ILE:HG22	6:D:71:SER:N	2.21	0.54
10:H:45:ILE:O	10:H:45:ILE:HG13	2.07	0.54
10:H:64:LYS:CB	10:H:79:VAL:HG21	2.38	0.54
12:J:30:SER:OG	12:J:81:THR:HA	2.08	0.54
1:A:707:C:OP1	13:K:85:ARG:NH1	2.41	0.54
14:L:113:ARG:HB2	14:L:122:THR:HG21	1.88	0.54
1:A:141:A:O2'	1:A:142:G:H5'	2.08	0.54
1:A:701:C:O2'	1:A:702:A:OP2	2.24	0.54
1:A:986:A:H1'	21:S:54:GLY:O	2.08	0.54
4:B:184:VAL:CG1	4:B:197:VAL:HG13	2.38	0.54
5:C:47:LEU:HD23	5:C:68:VAL:HG11	1.89	0.54
12:J:27:ALA:HB2	12:J:85:LEU:HD21	1.90	0.54
14:L:55:VAL:CG1	14:L:56:ALA:N	2.71	0.54
16:N:12:ARG:HA	16:N:12:ARG:HE	1.73	0.54
16:N:26:ARG:HD3	16:N:43:CYS:HB3	1.90	0.54
18:P:28:ARG:HG2	18:P:29:ASP:OD2	2.08	0.54
1:A:130:A:C8	19:Q:63:ARG:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:30:LYS:O	22:T:33:ILE:HB	2.08	0.54
1:A:1112:C:C1'	5:C:179:ARG:HH21	2.20	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
1:A:101:A:O2'	1:A:102:G:H5'	2.07	0.53
1:A:1347:G:C6	11:I:107:ARG:NH2	2.76	0.53
1:A:1505:G:H2'	1:A:1541:U:OP2	2.08	0.53
1:A:867:G:O2'	1:A:868:C:H5'	2.08	0.53
1:A:952:U:O2'	1:A:953:G:H5'	2.08	0.53
4:B:20:GLU:HA	4:B:20:GLU:OE2	2.08	0.53
4:B:239:VAL:HB	4:B:240:GLN:HE22	1.73	0.53
6:D:23:GLY:CA	6:D:113:SER:HB3	2.38	0.53
6:D:194:LEU:H	6:D:194:LEU:HD22	1.73	0.53
9:G:110:GLN:OE1	9:G:110:GLN:HA	2.07	0.53
10:H:102:ARG:HG3	10:H:102:ARG:O	2.09	0.53
19:Q:82:MET:HA	19:Q:85:VAL:HG23	1.89	0.53
1:A:1095:U:H5''	1:A:1109:C:O2	2.08	0.53
1:A:1539:C:O2'	1:A:1540:U:H5'	2.07	0.53
1:A:16:A:O2'	1:A:17:U:H5'	2.08	0.53
4:B:139:LYS:O	4:B:143:GLU:HG2	2.08	0.53
6:D:15:GLU:CG	6:D:63:LYS:HG3	2.38	0.53
7:E:53:LEU:N	7:E:53:LEU:HD12	2.18	0.53
8:F:37:VAL:HA	8:F:65:VAL:HG12	1.89	0.53
11:I:8:GLY:HA2	11:I:79:LEU:HB3	1.90	0.53
1:A:1152:A:H5''	12:J:13:HIS:CG	2.42	0.53
12:J:29:ARG:NH1	12:J:29:ARG:HB2	2.24	0.53
12:J:96:ILE:HG22	12:J:97:GLU:N	2.24	0.53
13:K:106:LYS:CE	13:K:106:LYS:HA	2.25	0.53
15:M:22:ILE:HB	15:M:25:ILE:HD12	1.90	0.53
16:N:24:CYS:HB3	16:N:28:GLY:H	1.72	0.53
17:O:45:VAL:HG12	17:O:46:HIS:ND1	2.23	0.53
19:Q:81:ARG:O	19:Q:81:ARG:HG3	2.08	0.53
22:T:39:LYS:CD	22:T:55:ILE:HD13	2.38	0.53
1:A:1243:C:H2'	1:A:1244:C:C6	2.43	0.53
1:A:338:A:H2'	1:A:339:C:C6	2.44	0.53
5:C:156:ARG:NH2	5:C:161:GLU:HA	2.23	0.53
6:D:64:LEU:HD12	6:D:75:PHE:HZ	1.72	0.53
17:O:66:LEU:O	17:O:69:TYR:HB3	2.09	0.53
17:O:87:ILE:HG22	17:O:88:ARG:N	2.23	0.53
1:A:404:U:H2'	1:A:405:U:H6	1.74	0.53
1:A:983:A:H5'	1:A:984:C:OP2	2.08	0.53
4:B:140:HIS:HA	4:B:143:GLU:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:178:LEU:O	5:C:179:ARG:CB	2.56	0.53
5:C:30:ARG:HG2	5:C:30:ARG:NH1	2.24	0.53
11:I:4:TYR:CZ	11:I:88:TYR:HD1	2.27	0.53
13:K:91:ARG:NH1	20:R:88:LYS:HZ3	2.05	0.53
22:T:54:LYS:HG3	22:T:100:ILE:CD1	2.38	0.53
1:A:1064:G:H4'	1:A:1065:U:H5'	1.89	0.53
1:A:1121:U:H2'	1:A:1122:U:C6	2.43	0.53
1:A:1190:G:C3'	5:C:3:ASN:OD1	2.56	0.53
7:E:126:ARG:CG	7:E:126:ARG:NH1	2.63	0.53
9:G:15:ASP:O	9:G:19:GLY:HA2	2.08	0.53
9:G:77:SER:HB2	9:G:86:GLN:HE22	1.74	0.53
10:H:51:VAL:HG21	10:H:60:ARG:HG3	1.91	0.53
17:O:16:ALA:HB1	17:O:21:ASP:HB3	1.89	0.53
1:A:1423:G:O2'	1:A:1424:C:H5'	2.08	0.53
1:A:404:U:O2'	1:A:405:U:H5'	2.09	0.53
1:A:9:G:H5'	7:E:122:GLU:OE2	2.08	0.53
1:A:1101:A:C8	4:B:172:ILE:HD13	2.43	0.53
7:E:80:ILE:HG23	10:H:104:ARG:NH2	2.23	0.53
12:J:85:LEU:O	12:J:87:THR:N	2.41	0.53
15:M:110:ARG:HG2	15:M:110:ARG:HH11	1.73	0.53
21:S:6:LYS:HD2	21:S:6:LYS:H	1.68	0.53
22:T:100:ILE:C	22:T:102:GLY:N	2.59	0.53
23:V:13:ILE:O	23:V:16:GLY:N	2.39	0.53
1:A:1043:C:O2'	1:A:1044:A:H5'	2.08	0.53
1:A:1095:U:H2'	1:A:1096:C:H6	1.72	0.53
1:A:333:G:H4'	22:T:16:HIS:CE1	2.44	0.53
1:A:475:G:OP1	1:A:475:G:O4'	2.27	0.53
1:A:858:G:O2'	1:A:859:A:H5'	2.09	0.53
10:H:28:ALA:HB2	10:H:59:LEU:HG	1.91	0.53
12:J:4:ILE:HG22	12:J:100:THR:CB	2.39	0.53
15:M:11:ARG:CD	15:M:12:ASN:H	2.21	0.53
21:S:17:GLU:O	21:S:20:LEU:HG	2.09	0.53
21:S:19:VAL:HG13	21:S:20:LEU:N	2.24	0.53
1:A:1229:A:O2'	15:M:125:ARG:NE	2.41	0.53
6:D:31:CYS:SG	6:D:31:CYS:O	2.66	0.53
6:D:32:ALA:C	6:D:34:GLU:N	2.61	0.53
11:I:40:LEU:O	11:I:41:VAL:C	2.47	0.53
1:A:1124:G:H5'	12:J:35:SER:CB	2.38	0.53
15:M:37:THR:HG23	15:M:55:ARG:CD	2.32	0.53
15:M:7:VAL:HG12	15:M:7:VAL:O	2.09	0.53
1:A:1392:G:H2'	1:A:1393:U:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:G:H4'	1:A:1442:G:C6	2.43	0.53
1:A:386:C:C2'	1:A:387:U:H5'	2.39	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.53
1:A:650:G:O2'	1:A:651:C:H5'	2.09	0.53
4:B:122:PHE:C	4:B:127:ILE:HG21	2.30	0.53
4:B:55:PHE:HD2	4:B:221:LEU:HG	1.74	0.53
6:D:61:LYS:HA	6:D:203:VAL:HG22	1.90	0.53
9:G:31:MET:SD	9:G:34:GLY:HA2	2.49	0.53
9:G:66:VAL:HG12	9:G:70:LYS:HE3	1.90	0.53
1:A:523:A:H61	14:L:92:ASP:HB2	1.74	0.53
18:P:46:PRO:O	18:P:47:ASP:HB2	2.08	0.53
19:Q:12:SER:HA	19:Q:14:LYS:NZ	2.23	0.53
1:A:518:C:H4'	1:A:519:C:O5'	2.08	0.52
1:A:748:C:O2'	1:A:749:C:H6	1.90	0.52
5:C:81:GLY:HA2	5:C:84:ILE:HG22	1.91	0.52
6:D:3:ARG:NH2	6:D:74:GLN:HE21	2.07	0.52
9:G:144:MET:O	9:G:145:ALA:C	2.47	0.52
9:G:71:PRO:HD3	9:G:103:TRP:CZ3	2.44	0.52
1:A:1314:C:N4	21:S:4:SER:HB2	2.24	0.52
1:A:1262:C:O2'	1:A:1263:C:H5'	2.09	0.52
1:A:1313:U:OP2	21:S:6:LYS:HA	2.09	0.52
1:A:1525:G:O2'	1:A:1526:G:H5'	2.09	0.52
1:A:190(A):C:H42	1:A:190(H):G:H1	1.56	0.52
1:A:340:U:H2'	1:A:341:C:C6	2.44	0.52
1:A:357:G:O2'	1:A:358:U:H5'	2.08	0.52
1:A:413:G:H4'	1:A:416:G:N2	2.22	0.52
1:A:740:U:O2'	1:A:741:G:H5'	2.10	0.52
4:B:137:ARG:HH11	4:B:137:ARG:HG2	1.74	0.52
4:B:77:ALA:HB2	4:B:211:ILE:CD1	2.39	0.52
6:D:76:ARG:HH11	6:D:76:ARG:HG2	1.75	0.52
7:E:15:ARG:C	7:E:16:THR:HG23	2.29	0.52
8:F:4:TYR:O	8:F:5:GLU:HG3	2.09	0.52
15:M:16:ASP:OD1	15:M:16:ASP:N	2.40	0.52
16:N:34:TYR:HD1	16:N:34:TYR:H	1.55	0.52
19:Q:27:PHE:HB2	19:Q:28:PRO:HD2	1.91	0.52
20:R:61:LYS:O	20:R:65:ILE:HG13	2.09	0.52
1:A:189:G:C5	1:A:190:C:H3'	2.44	0.52
1:A:195:A:H4'	22:T:68:LYS:CE	2.40	0.52
1:A:460:A:H2'	1:A:461:C:H5"	1.92	0.52
4:B:19:HIS:CE1	4:B:204:ASN:HB3	2.45	0.52
4:B:44:LEU:HA	4:B:47:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:123:GLN:HE22	5:C:140:ARG:NH2	2.06	0.52
5:C:191:THR:HG21	5:C:193:TYR:CE1	2.42	0.52
6:D:148:VAL:HG11	6:D:158:ILE:HD13	1.91	0.52
11:I:5:TYR:HE2	11:I:16:ARG:HB3	1.74	0.52
12:J:34:VAL:HG22	12:J:74:ILE:HG12	1.90	0.52
15:M:22:ILE:HG21	15:M:66:LEU:HD13	1.90	0.52
1:A:1196:U:OP1	1:A:1197:G:H5'	2.08	0.52
1:A:1317:C:H2'	1:A:1318:A:O4'	2.09	0.52
1:A:1539:C:H5	9:G:82:GLY:HA2	1.75	0.52
4:B:12:GLU:OE2	4:B:213:LEU:HD11	2.10	0.52
5:C:34:LEU:HG	16:N:25:VAL:CG2	2.39	0.52
7:E:41:VAL:HG22	7:E:113:ALA:HA	1.90	0.52
9:G:8:GLU:OE1	9:G:8:GLU:O	2.28	0.52
11:I:81:ILE:O	11:I:85:LEU:HB2	2.10	0.52
12:J:55:LYS:HG3	12:J:56:HIS:CD2	2.44	0.52
19:Q:66:SER:OG	19:Q:69:LYS:HB3	2.09	0.52
20:R:43:PHE:C	20:R:51:LEU:HD12	2.30	0.52
1:A:1347:G:C2'	1:A:1348:U:OP2	2.58	0.52
1:A:1522:U:O2'	1:A:1523:G:H5'	2.10	0.52
1:A:129(A):G:N3	1:A:190(E):U:H5'	2.25	0.52
4:B:102:LEU:HD21	4:B:162:ILE:HD12	1.90	0.52
5:C:108:ASN:OD1	5:C:110:ASN:HB2	2.10	0.52
8:F:98:LEU:HD11	8:F:101:ALA:HA	1.92	0.52
12:J:26:ALA:C	12:J:84:GLN:HE21	2.12	0.52
18:P:26:ARG:NH2	18:P:31:LYS:NZ	2.57	0.52
1:A:1260:C:O5'	1:A:1284:C:H4'	2.09	0.52
1:A:258:G:O2'	1:A:259:G:H5'	2.09	0.52
1:A:308:C:H2'	1:A:309:G:H8	1.74	0.52
4:B:51:LEU:HD22	4:B:55:PHE:HE1	1.73	0.52
5:C:112:SER:HB3	5:C:115:LEU:HD12	1.90	0.52
5:C:134:ILE:HD11	5:C:153:VAL:HG23	1.91	0.52
14:L:46:LYS:HG3	14:L:47:LYS:N	2.25	0.52
16:N:23:ARG:NH1	16:N:30:ALA:HB2	2.24	0.52
18:P:55:ARG:O	18:P:58:TYR:HB3	2.09	0.52
20:R:26:LEU:HD12	20:R:27:GLY:N	2.25	0.52
1:A:1154:G:H2'	1:A:1155:G:C8	2.42	0.52
1:A:848:C:H2'	1:A:849:C:C6	2.45	0.52
5:C:20:SER:HB3	5:C:22:TRP:CD1	2.44	0.52
8:F:2:ARG:NH1	8:F:69:GLU:HG2	2.25	0.52
11:I:46:ALA:O	11:I:49:PRO:HD2	2.10	0.52
15:M:12:ASN:CG	15:M:12:ASN:O	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:81:ARG:C	18:P:83:GLU:N	2.63	0.52
19:Q:45:HIS:NE2	19:Q:47:PRO:HG3	2.24	0.52
21:S:43:GLU:H	21:S:43:GLU:CD	2.12	0.52
1:A:1054:C:C6	2:X:34:I:H1'	2.45	0.52
1:A:1031:G:H4'	1:A:1032:G:C8	2.45	0.52
1:A:1124:G:O2'	1:A:1145:C:N4	2.42	0.52
1:A:1141:C:H2'	1:A:1142:G:H8	1.74	0.52
1:A:1307:U:H2'	1:A:1308:U:C6	2.45	0.52
1:A:1495:U:H2'	1:A:1496:C:C6	2.44	0.52
1:A:346:G:H2'	1:A:347:G:O4'	2.09	0.52
1:A:502:G:H2'	1:A:503:C:C6	2.45	0.52
1:A:755:G:OP2	17:O:65:ARG:HD2	2.10	0.52
4:B:18:GLY:HA2	4:B:40:HIS:O	2.09	0.52
4:B:17:PHE:HB3	4:B:44:LEU:HD11	1.91	0.52
4:B:80:ILE:HD11	4:B:208:ILE:CG2	2.37	0.52
5:C:54:ARG:O	5:C:55:VAL:HG23	2.10	0.52
8:F:32:ASN:O	8:F:71:ARG:NH2	2.42	0.52
8:F:47:ARG:N	8:F:47:ARG:HD3	2.24	0.52
9:G:79:ARG:NH1	9:G:79:ARG:HG2	2.25	0.52
10:H:116:LYS:HD3	10:H:127:LEU:HD13	1.92	0.52
11:I:96:LEU:HD12	11:I:96:LEU:N	2.25	0.52
12:J:38:ILE:HD12	12:J:71:LEU:CD1	2.40	0.52
15:M:53:VAL:CG1	15:M:57:ARG:HH21	2.23	0.52
1:A:1487:G:O2'	1:A:1488:G:H5'	2.10	0.52
1:A:831:U:H2'	1:A:832:C:C6	2.44	0.52
4:B:7:VAL:HG12	4:B:221:LEU:HD23	1.91	0.52
5:C:133:ALA:O	5:C:136:GLN:N	2.43	0.52
6:D:150:GLU:OE1	6:D:150:GLU:HA	2.08	0.52
6:D:157:LEU:CD2	6:D:161:ASN:HD21	2.23	0.52
6:D:194:LEU:HD22	6:D:194:LEU:N	2.25	0.52
8:F:28:ARG:HG2	8:F:28:ARG:HH11	1.74	0.52
10:H:31:PHE:HZ	10:H:134:ILE:CD1	2.23	0.52
1:A:1117:G:H4'	11:I:104:ARG:NH1	2.25	0.52
12:J:71:LEU:O	12:J:72:VAL:CB	2.57	0.52
13:K:84:VAL:CG1	13:K:95:ILE:HD11	2.39	0.52
1:A:1202:G:C2	16:N:42:ILE:HG21	2.45	0.52
18:P:38:TYR:CE2	18:P:50:LYS:HB3	2.44	0.52
1:A:1270:C:O2'	1:A:1271:G:H5'	2.10	0.52
1:A:1354:C:H2'	1:A:1355:G:H8	1.74	0.52
1:A:382:A:C2	1:A:383:A:C4	2.98	0.52
1:A:939:G:H2'	1:A:940:C:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:9:GLU:OE2	4:B:12:GLU:HA	2.10	0.52
4:B:236:TYR:HD2	4:B:236:TYR:O	1.92	0.52
4:B:47:THR:O	4:B:51:LEU:HG	2.10	0.52
4:B:87:ARG:O	4:B:88:ALA:CB	2.57	0.52
6:D:25:ARG:C	6:D:27:TYR:N	2.62	0.52
6:D:8:VAL:O	6:D:10:ARG:N	2.37	0.52
15:M:63:THR:HG22	15:M:64:TRP:CD1	2.44	0.52
22:T:63:ILE:HD13	22:T:80:ARG:HB2	1.92	0.52
1:A:1317:C:OP1	16:N:17:LYS:HG2	2.09	0.51
1:A:252:U:H2'	1:A:253:U:C6	2.44	0.51
1:A:478:A:C3'	1:A:479:C:H5'	2.41	0.51
1:A:628:G:H2'	1:A:629:G:C8	2.45	0.51
6:D:3:ARG:HG2	6:D:118:ARG:NE	2.25	0.51
8:F:81:ILE:HG23	8:F:82:ARG:N	2.25	0.51
5:C:29:TYR:CZ	16:N:54:PRO:HG2	2.45	0.51
19:Q:93:GLN:O	19:Q:96:GLN:HG3	2.10	0.51
1:A:15:G:H1'	7:E:24:ARG:HH12	1.75	0.51
1:A:839:U:C2'	1:A:839:U:O2	2.58	0.51
4:B:228:GLY:O	4:B:229:VAL:C	2.47	0.51
4:B:220:ASP:HB3	4:B:230:VAL:HG11	1.92	0.51
4:B:83:MET:HG3	4:B:238:LEU:HD12	1.92	0.51
5:C:107:GLN:O	5:C:108:ASN:CB	2.58	0.51
5:C:195:VAL:C	5:C:196:LEU:HD23	2.30	0.51
6:D:170:VAL:HG13	6:D:174:LEU:HB2	1.92	0.51
6:D:159:ARG:HE	6:D:181:MET:HE1	1.74	0.51
9:G:69:VAL:O	9:G:69:VAL:HG12	2.09	0.51
10:H:31:PHE:CZ	10:H:134:ILE:HD11	2.45	0.51
16:N:58:LYS:HB3	16:N:58:LYS:NZ	2.25	0.51
17:O:39:LEU:CD2	17:O:56:LEU:HB2	2.40	0.51
22:T:21:LYS:HB2	22:T:21:LYS:HZ3	1.76	0.51
1:A:1151:A:O2'	1:A:1152:A:H8	1.92	0.51
1:A:1402:C:H2'	1:A:1403:C:O4'	2.10	0.51
1:A:408:A:O5'	1:A:431:A:OP2	2.27	0.51
1:A:818:G:O2'	1:A:819:A:H5'	2.11	0.51
1:A:841:U:H3'	1:A:848:C:O4'	2.10	0.51
4:B:87:ARG:O	4:B:88:ALA:HB2	2.09	0.51
11:I:10:ARG:HG2	11:I:75:ASP:CB	2.40	0.51
14:L:86:ARG:NH1	14:L:87:GLY:O	2.43	0.51
19:Q:17:LYS:HA	19:Q:46:ASP:O	2.10	0.51
1:A:1366:C:C2	1:A:1367:C:C5	2.98	0.51
4:B:124:SER:HB2	4:B:125:PRO:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:163:GLU:C	6:D:165:MET:H	2.14	0.51
9:G:129:GLU:OE1	9:G:131:LYS:HE2	2.09	0.51
14:L:83:VAL:HG22	14:L:100:ILE:HG23	1.93	0.51
15:M:53:VAL:HG12	15:M:57:ARG:HH21	1.74	0.51
19:Q:97:SER:HB2	19:Q:98:LEU:CD1	2.39	0.51
20:R:53:ARG:HD2	20:R:58:LEU:O	2.10	0.51
1:A:1364:U:O2'	1:A:1365:G:H5'	2.09	0.51
1:A:418:C:H2'	1:A:419:C:O2	2.10	0.51
1:A:591:U:P	10:H:30:ARG:HE	2.32	0.51
5:C:112:SER:OG	5:C:115:LEU:HG	2.10	0.51
6:D:105:VAL:HG12	6:D:117:ALA:CB	2.41	0.51
8:F:96:PRO:O	8:F:98:LEU:N	2.43	0.51
1:A:755:G:H1'	10:H:1:MET:HE3	1.91	0.51
15:M:36:LYS:HD2	15:M:59:TYR:OH	2.11	0.51
17:O:33:THR:HG23	17:O:63:ARG:HH12	1.74	0.51
20:R:42:ARG:HG3	20:R:42:ARG:NH1	2.26	0.51
20:R:86:VAL:CG1	20:R:87:ARG:H	2.23	0.51
21:S:47:HIS:O	21:S:62:ILE:HG22	2.10	0.51
22:T:101:GLY:O	22:T:102:GLY:C	2.48	0.51
1:A:409:G:H5''	1:A:431:A:C8	2.46	0.51
1:A:686:U:HO2'	1:A:687:A:H8	1.57	0.51
1:A:849:C:O2'	1:A:850:U:H5'	2.10	0.51
1:A:959:A:H2'	1:A:960:U:O4'	2.10	0.51
4:B:12:GLU:C	4:B:14:GLY:N	2.63	0.51
6:D:29:PRO:C	6:D:30:LYS:HG2	2.29	0.51
6:D:70:ILE:HD11	6:D:100:ARG:CD	2.40	0.51
8:F:10:LEU:HD12	8:F:59:TYR:HB3	1.92	0.51
8:F:25:ILE:CD1	8:F:82:ARG:HH11	2.23	0.51
10:H:35:ILE:HG22	10:H:39:LEU:CD2	2.41	0.51
10:H:92:ARG:NH1	10:H:92:ARG:CG	2.74	0.51
1:A:127:G:HO2'	19:Q:2:PRO:N	2.09	0.51
19:Q:75:ARG:HG3	19:Q:75:ARG:HH11	1.75	0.51
1:A:179:A:H2'	1:A:180:U:H6	1.75	0.51
1:A:27:G:O2'	1:A:28:G:H5'	2.11	0.51
1:A:865:A:O2'	1:A:866:C:H5'	2.11	0.51
7:E:110:LEU:O	7:E:113:ALA:HB3	2.11	0.51
8:F:35:ALA:HB1	8:F:65:VAL:HG21	1.92	0.51
1:A:972:C:C4'	12:J:57:LYS:HE2	2.41	0.51
14:L:52:LEU:O	14:L:54:LYS:NZ	2.39	0.51
14:L:86:ARG:HG3	14:L:87:GLY:O	2.10	0.51
21:S:24:ALA:O	21:S:25:LYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:12:LYS:HB3	23:V:22:ARG:HD2	1.93	0.51
1:A:1005:A:H1'	1:A:1026:G:N2	2.24	0.51
1:A:475:G:O4'	1:A:475:G:P	2.69	0.51
1:A:659:U:O2'	1:A:660:G:H5'	2.11	0.51
1:A:695:A:H2'	1:A:696:A:C8	2.46	0.51
4:B:76:GLN:NE2	4:B:207:ALA:H	2.09	0.51
4:B:75:LYS:C	4:B:77:ALA:H	2.14	0.51
1:A:711:G:P	8:F:54:LYS:HZ1	2.33	0.51
12:J:39:PRO:O	12:J:69:ASN:O	2.28	0.51
13:K:33:THR:HB	13:K:38:ASN:O	2.10	0.51
15:M:11:ARG:CG	15:M:12:ASN:N	2.74	0.51
1:A:1354:C:O2'	1:A:1355:G:H5'	2.10	0.51
1:A:327:A:O2'	1:A:328:C:O4'	2.25	0.51
4:B:17:PHE:CD1	4:B:17:PHE:C	2.84	0.51
5:C:179:ARG:O	5:C:179:ARG:CG	2.58	0.51
6:D:64:LEU:HB2	6:D:198:VAL:HG11	1.93	0.51
10:H:108:GLY:HA3	10:H:138:TRP:HB3	1.92	0.51
10:H:82:HIS:O	10:H:83:ILE:HB	2.11	0.51
1:A:1250:A:H4'	11:I:68:GLY:CA	2.41	0.51
12:J:4:ILE:HG13	12:J:4:ILE:O	2.10	0.51
18:P:1:MET:CE	18:P:3:LYS:HD2	2.40	0.51
1:A:1157:A:H4'	1:A:1158:C:O5'	2.12	0.51
1:A:1397:C:H4'	1:A:1398:A:OP2	2.11	0.51
1:A:792:A:H4'	1:A:793:U:H5"	1.91	0.51
1:A:834:C:H2'	1:A:835:U:C6	2.46	0.51
5:C:102:ASN:N	5:C:102:ASN:ND2	2.57	0.51
5:C:191:THR:CG2	5:C:192:THR:H	2.22	0.51
7:E:91:LEU:HB3	7:E:118:ILE:HD11	1.93	0.51
13:K:69:ALA:O	13:K:73:MET:HG2	2.09	0.51
20:R:36:ASN:HA	20:R:38:GLU:OE2	2.11	0.51
1:A:1347:G:O2'	1:A:1348:U:OP2	2.29	0.50
1:A:459:G:H3'	1:A:460:A:C5'	2.41	0.50
5:C:167:TRP:O	5:C:168:ALA:HB3	2.11	0.50
10:H:117:GLY:O	10:H:119:LEU:HD23	2.11	0.50
1:A:1142:G:C2	1:A:1143:G:H1'	2.46	0.50
1:A:1149:C:O2'	1:A:1280:A:N1	2.39	0.50
1:A:16:A:C2'	1:A:17:U:H5'	2.41	0.50
1:A:184:G:C4'	1:A:224:C:H4'	2.41	0.50
1:A:189:G:H2'	1:A:190(K):G:H21	1.72	0.50
1:A:954:G:H2'	1:A:955:U:H6	1.76	0.50
5:C:7:PRO:HG2	5:C:184:TYR:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:35:ARG:O	6:D:36:ARG:CB	2.58	0.50
8:F:67:MET:HE2	8:F:71:ARG:HB2	1.93	0.50
12:J:34:VAL:CG2	12:J:74:ILE:HG12	2.41	0.50
12:J:48:THR:HG23	12:J:62:HIS:NE2	2.26	0.50
14:L:93:LEU:HB2	14:L:96:VAL:HG21	1.92	0.50
19:Q:27:PHE:CE1	19:Q:36:ILE:HD11	2.46	0.50
19:Q:64:PRO:HB3	19:Q:70:ARG:NH1	2.26	0.50
21:S:33:THR:HG22	21:S:35:SER:N	2.09	0.50
23:V:6:ARG:HG3	23:V:7:ARG:N	2.27	0.50
1:A:1132:C:H2'	1:A:1133:G:H8	1.74	0.50
1:A:1367:C:C2	1:A:1368:G:C8	2.99	0.50
1:A:1474:G:O2'	1:A:1475:G:H5'	2.10	0.50
1:A:828:A:H2'	1:A:829:G:O4'	2.11	0.50
5:C:134:ILE:HG22	5:C:168:ALA:HB3	1.92	0.50
5:C:173:VAL:HG12	5:C:175:LEU:HD21	1.93	0.50
5:C:56:ASP:O	5:C:57:ILE:HG13	2.10	0.50
7:E:80:ILE:HD12	7:E:80:ILE:O	2.11	0.50
9:G:48:LYS:O	9:G:51:GLN:HB2	2.11	0.50
10:H:103:VAL:HG21	10:H:109:ILE:O	2.12	0.50
11:I:113:LYS:H	11:I:119:ALA:HA	1.76	0.50
11:I:23:ASN:O	11:I:23:ASN:ND2	2.44	0.50
15:M:2:ALA:O	15:M:4:ILE:HG13	2.11	0.50
15:M:6:GLY:O	15:M:7:VAL:HB	2.12	0.50
16:N:22:THR:OG1	16:N:33:VAL:HG21	2.11	0.50
19:Q:68:ARG:O	19:Q:68:ARG:CG	2.51	0.50
21:S:52:TYR:HA	21:S:56:GLN:O	2.12	0.50
1:A:1228:C:H4'	15:M:116:THR:HA	1.93	0.50
4:B:88:ALA:C	4:B:90:MET:N	2.65	0.50
5:C:129:ALA:O	5:C:132:ARG:HB3	2.12	0.50
6:D:126:ILE:CG2	6:D:127:THR:N	2.72	0.50
14:L:40:VAL:O	14:L:40:VAL:HG12	2.11	0.50
14:L:53:ARG:HG3	14:L:93:LEU:HD21	1.92	0.50
1:A:192:U:H4'	22:T:57:ARG:HD2	1.94	0.50
1:A:263:A:OP2	22:T:79:ARG:NH1	2.44	0.50
1:A:781:A:H2'	1:A:782:A:H5'	1.94	0.50
6:D:157:LEU:HD21	6:D:161:ASN:HD21	1.76	0.50
9:G:21:VAL:HG23	9:G:22:LEU:N	2.27	0.50
15:M:25:ILE:HG22	15:M:26:GLY:H	1.76	0.50
15:M:88:ARG:HG3	15:M:98:VAL:CG1	2.42	0.50
17:O:78:TYR:OH	17:O:82:ILE:HD11	2.11	0.50
18:P:52:ASP:CG	18:P:55:ARG:HG3	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:59:ILE:CG2	19:Q:71:PHE:CD1	2.95	0.50
21:S:39:THR:HG22	21:S:40:ILE:N	2.27	0.50
1:A:1152:A:H5''	12:J:13:HIS:HD2	1.72	0.50
1:A:1195:C:H3'	1:A:1196:U:C5'	2.41	0.50
1:A:167:G:O2'	1:A:168:G:H5'	2.10	0.50
1:A:258:G:H2'	1:A:259:G:H8	1.76	0.50
1:A:628:G:H2'	1:A:629:G:H8	1.77	0.50
1:A:807:A:H2'	1:A:808:C:C6	2.47	0.50
4:B:45:GLN:O	4:B:48:MET:HB2	2.11	0.50
4:B:69:LEU:HD12	4:B:155:LEU:CD1	2.40	0.50
6:D:62:GLN:NE2	6:D:65:ARG:NH1	2.58	0.50
7:E:76:ILE:HD12	7:E:118:ILE:CD1	2.42	0.50
7:E:13:ILE:HD12	7:E:13:ILE:C	2.32	0.50
9:G:69:VAL:HG21	9:G:104:LEU:HD21	1.93	0.50
13:K:126:ARG:C	13:K:128:ALA:N	2.65	0.50
14:L:27:LEU:HB3	14:L:62:SER:HB2	1.93	0.50
15:M:16:ASP:HB3	15:M:34:LEU:HD12	1.93	0.50
1:A:1064:G:H4'	1:A:1065:U:H5''	1.92	0.50
1:A:1300:G:O2'	1:A:1301:U:P	2.70	0.50
5:C:76:VAL:HG11	5:C:103:VAL:HG21	1.93	0.50
7:E:51:VAL:O	7:E:54:ALA:HB3	2.12	0.50
7:E:76:ILE:HG23	7:E:77:PRO:CD	2.41	0.50
10:H:31:PHE:O	10:H:34:GLU:HB2	2.12	0.50
19:Q:58:GLU:HB2	19:Q:74:LEU:HB3	1.94	0.50
1:A:463:A:H1'	1:A:474:G:OP1	2.12	0.50
4:B:19:HIS:CE1	4:B:206:ASP:HB3	2.47	0.50
11:I:45:ALA:O	11:I:48:GLU:N	2.44	0.50
12:J:42:THR:HG23	12:J:67:THR:O	2.11	0.50
13:K:67:ASP:OD2	13:K:71:LYS:HE3	2.12	0.50
1:A:521:G:OP1	14:L:73:GLU:O	2.30	0.50
1:A:953:G:H1'	15:M:125:ARG:HA	1.92	0.50
19:Q:59:ILE:HG23	19:Q:71:PHE:HB3	1.93	0.50
19:Q:60:ILE:HD13	19:Q:61:GLU:N	2.27	0.50
21:S:15:LEU:HD12	21:S:15:LEU:C	2.32	0.50
22:T:50:GLU:O	22:T:100:ILE:HD12	2.12	0.50
1:A:530:G:O6	3:W:3:A:H1'	2.12	0.50
4:B:69:LEU:HD23	4:B:69:LEU:C	2.32	0.50
8:F:82:ARG:HB2	8:F:85:VAL:CG2	2.41	0.50
12:J:75:ILE:CD1	12:J:75:ILE:H	2.19	0.50
14:L:101:VAL:O	14:L:103:GLY:N	2.45	0.50
14:L:46:LYS:CG	14:L:47:LYS:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:40:ASN:ND2	15:M:40:ASN:C	2.65	0.50
17:O:60:VAL:O	17:O:64:ARG:HG2	2.12	0.50
21:S:12:ASP:H	21:S:38:SER:HB3	1.77	0.50
1:A:1223:C:OP1	1:A:1224:G:H3'	2.12	0.49
1:A:1411:C:O2'	1:A:1412:C:H5'	2.12	0.49
1:A:1475:G:H2'	1:A:1476:G:C8	2.46	0.49
1:A:163:C:C2'	1:A:164:U:H5'	2.41	0.49
1:A:457:C:H42	1:A:475:G:H22	1.60	0.49
4:B:179:LYS:HB2	4:B:179:LYS:NZ	2.27	0.49
5:C:100:ALA:O	5:C:101:LEU:HB2	2.12	0.49
5:C:83:ARG:O	5:C:85:ARG:N	2.45	0.49
9:G:148:ASN:C	9:G:150:ALA:H	2.16	0.49
9:G:51:GLN:OE1	9:G:51:GLN:HA	2.12	0.49
9:G:78:ARG:NH1	9:G:154:TYR:O	2.45	0.49
11:I:48:GLU:N	11:I:49:PRO:CD	2.73	0.49
1:A:1316:G:H4'	16:N:18:VAL:HG11	1.93	0.49
16:N:3:ARG:O	16:N:7:ILE:HG13	2.12	0.49
1:A:279:A:C4	19:Q:98:LEU:HD23	2.46	0.49
1:A:1305:G:H5''	23:V:4:GLY:C	2.32	0.49
1:A:1316:G:N2	1:A:1318:A:H3'	2.28	0.49
1:A:1333:A:H2'	1:A:1334:G:O4'	2.12	0.49
1:A:188:C:H6	1:A:188:C:C5'	2.25	0.49
4:B:219:VAL:C	4:B:221:LEU:N	2.66	0.49
6:D:8:VAL:HG11	6:D:115:ARG:CZ	2.42	0.49
9:G:18:TYR:CE2	9:G:58:PRO:HG2	2.47	0.49
10:H:87:SER:OG	10:H:92:ARG:HD2	2.12	0.49
12:J:4:ILE:HG12	12:J:74:ILE:HB	1.94	0.49
14:L:8:ASN:O	14:L:12:ARG:HG3	2.11	0.49
14:L:34:ARG:O	14:L:61:THR:HG23	2.12	0.49
15:M:40:ASN:HD22	15:M:41:PRO:HD2	1.74	0.49
17:O:32:LEU:HD13	17:O:63:ARG:HB2	1.93	0.49
1:A:1091:U:O2	1:A:1093:A:H8	1.94	0.49
1:A:1305:G:H2'	1:A:1331:G:N2	2.28	0.49
1:A:359:U:O2'	1:A:360:A:H5'	2.12	0.49
5:C:195:VAL:HG12	5:C:196:LEU:N	2.28	0.49
7:E:128:PRO:O	7:E:129:ILE:C	2.48	0.49
7:E:28:PHE:O	7:E:47:LYS:HA	2.12	0.49
11:I:112:LYS:HD3	11:I:112:LYS:C	2.32	0.49
12:J:89:ASP:HB2	12:J:91:PRO:HD2	1.94	0.49
13:K:74:ALA:C	13:K:76:GLY:H	2.16	0.49
14:L:53:ARG:HG3	14:L:53:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:84:ILE:O	15:M:85:GLY:C	2.50	0.49
22:T:39:LYS:HE2	22:T:55:ILE:CD1	2.41	0.49
1:A:384:G:H2'	1:A:385:C:C6	2.47	0.49
5:C:150:LYS:CG	5:C:169:ALA:HB2	2.40	0.49
6:D:5:ILE:HG22	6:D:5:ILE:O	2.12	0.49
7:E:102:ALA:CB	7:E:120:THR:HG21	2.43	0.49
7:E:51:VAL:O	7:E:55:VAL:HG23	2.13	0.49
8:F:48:LEU:HD13	8:F:52:ILE:HD12	1.94	0.49
10:H:20:TYR:CE1	10:H:76:PRO:HD2	2.48	0.49
11:I:45:ALA:O	11:I:48:GLU:HB2	2.12	0.49
12:J:90:LEU:N	12:J:91:PRO:HD2	2.27	0.49
15:M:11:ARG:HD2	15:M:12:ASN:H	1.76	0.49
19:Q:12:SER:HB3	19:Q:20:THR:CB	2.42	0.49
20:R:37:VAL:O	20:R:41:LYS:HG3	2.12	0.49
8:F:50:TYR:CE1	20:R:77:GLY:HA2	2.47	0.49
1:A:1368:G:OP2	11:I:112:LYS:HD3	2.13	0.49
1:A:476:G:N3	1:A:478:A:OP1	2.46	0.49
1:A:586:C:O3'	10:H:89:PRO:HB2	2.13	0.49
1:A:628:G:O2'	1:A:629:G:H5'	2.12	0.49
1:A:701:C:H5''	1:A:703:G:O4'	2.12	0.49
5:C:110:ASN:HB3	5:C:144:SER:OG	2.12	0.49
7:E:109:ILE:O	7:E:113:ALA:HB2	2.12	0.49
7:E:13:ILE:HD12	7:E:13:ILE:O	2.12	0.49
13:K:38:ASN:HD22	13:K:38:ASN:N	2.09	0.49
14:L:60:LEU:N	14:L:64:TYR:O	2.45	0.49
1:A:269:C:H2'	1:A:270:A:H8	1.77	0.49
1:A:626:U:O2'	1:A:627:G:H5'	2.11	0.49
4:B:127:ILE:HG13	4:B:128:GLU:CD	2.31	0.49
5:C:19:GLU:O	5:C:40:ARG:NH2	2.46	0.49
7:E:107:ARG:O	7:E:108:ALA:C	2.50	0.49
7:E:148:VAL:O	7:E:152:ARG:HG3	2.11	0.49
8:F:2:ARG:O	8:F:66:GLU:HA	2.12	0.49
9:G:85:TYR:HD1	9:G:154:TYR:HE1	1.59	0.49
11:I:8:GLY:HA2	11:I:79:LEU:CD1	2.41	0.49
12:J:21:GLN:O	12:J:25:GLU:HG2	2.13	0.49
12:J:69:ASN:O	12:J:70:ARG:HD3	2.11	0.49
19:Q:76:LEU:HD23	19:Q:76:LEU:C	2.33	0.49
1:A:1104:G:P	4:B:111:ARG:HD2	2.52	0.49
1:A:1250:A:O2'	1:A:1251:A:H5'	2.13	0.49
1:A:1271:G:H5'	1:A:1314:C:OP1	2.12	0.49
5:C:20:SER:HB3	5:C:22:TRP:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:32:LEU:HD22	5:C:59:ARG:NH1	2.27	0.49
9:G:18:TYR:OH	9:G:58:PRO:HG3	2.13	0.49
9:G:71:PRO:HG3	9:G:103:TRP:CH2	2.47	0.49
12:J:34:VAL:C	12:J:36:GLY:H	2.16	0.49
18:P:75:ARG:HG3	18:P:75:ARG:HH11	1.78	0.49
1:A:235:C:H5'	19:Q:70:ARG:HG2	1.95	0.49
20:R:35:ARG:O	20:R:37:VAL:HG23	2.12	0.49
22:T:51:GLU:HA	22:T:54:LYS:HD2	1.95	0.49
1:A:103:C:P	22:T:17:ARG:NH1	2.85	0.49
1:A:1152:A:H5''	12:J:13:HIS:HB2	1.95	0.49
1:A:1178:G:N2	1:A:1180:A:H3'	2.27	0.49
1:A:1521:G:H2'	1:A:1522:U:H6	1.76	0.49
1:A:412:A:H2'	1:A:413:G:H5'	1.94	0.49
1:A:830:G:O2'	1:A:831:U:H5'	2.12	0.49
4:B:12:GLU:C	4:B:14:GLY:H	2.14	0.49
6:D:146:ILE:N	6:D:146:ILE:CD1	2.74	0.49
11:I:10:ARG:HD3	11:I:105:ASP:HB3	1.95	0.49
11:I:44:VAL:HG12	11:I:51:ARG:HH12	1.78	0.49
13:K:74:ALA:O	13:K:76:GLY:N	2.46	0.49
1:A:353:A:C5'	1:A:353:A:C8	2.96	0.49
1:A:995:C:H2'	1:A:995:C:O2	2.13	0.49
4:B:212:GLN:O	4:B:216:SER:HB3	2.13	0.49
5:C:84:ILE:O	5:C:84:ILE:HG12	2.11	0.49
17:O:26:GLU:HA	17:O:81:LEU:HD11	1.95	0.49
21:S:15:LEU:HD21	21:S:38:SER:OG	2.12	0.49
22:T:56:MET:O	22:T:59:ALA:HB3	2.12	0.49
1:A:1269:A:N1	1:A:1312:G:O2'	2.43	0.49
1:A:409:G:N2	1:A:432:A:O2'	2.46	0.49
1:A:502:G:H2'	1:A:503:C:H6	1.78	0.49
1:A:736:C:H2'	1:A:737:A:C8	2.48	0.49
5:C:180:ALA:O	5:C:181:ASN:C	2.52	0.49
7:E:144:THR:O	7:E:148:VAL:HG23	2.13	0.49
10:H:51:VAL:HG21	10:H:60:ARG:CG	2.43	0.49
12:J:6:ILE:HD12	12:J:72:VAL:CG1	2.42	0.49
15:M:90:LEU:O	15:M:93:ARG:HB2	2.12	0.49
21:S:16:LEU:C	21:S:19:VAL:HG12	2.33	0.49
1:A:998:G:N2	1:A:1043:C:O2	2.46	0.48
1:A:1463:C:O2'	1:A:1464:G:H5'	2.13	0.48
4:B:75:LYS:HE2	4:B:96:ARG:NH1	2.27	0.48
1:A:542:G:OP1	6:D:10:ARG:NH2	2.45	0.48
17:O:41:GLU:OE2	17:O:41:GLU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:86:VAL:CG1	20:R:87:ARG:N	2.75	0.48
21:S:50:ALA:HA	21:S:58:VAL:O	2.13	0.48
1:A:1283:G:O2'	1:A:1284:C:H5'	2.12	0.48
1:A:1323:G:H2'	1:A:1324:A:C8	2.48	0.48
1:A:1237:C:H4'	1:A:1334:G:N2	2.28	0.48
1:A:1347:G:H2'	1:A:1373:G:H1	1.78	0.48
1:A:338:A:H2'	1:A:339:C:H6	1.77	0.48
4:B:190:THR:CG2	4:B:190:THR:O	2.60	0.48
6:D:119:GLN:HG2	6:D:123:HIS:CD2	2.48	0.48
8:F:60:PHE:C	8:F:61:LEU:HD23	2.34	0.48
9:G:95:ARG:HH11	9:G:95:ARG:HG3	1.78	0.48
15:M:82:MET:HE3	15:M:93:ARG:HG2	1.94	0.48
17:O:4:THR:OG1	17:O:7:GLU:HB2	2.13	0.48
18:P:67:THR:CG2	18:P:68:ASP:N	2.76	0.48
19:Q:78:GLU:HG3	19:Q:78:GLU:O	2.13	0.48
20:R:39:VAL:HG13	20:R:40:LEU:N	2.26	0.48
1:A:1172:C:O2'	1:A:1173:G:H5'	2.13	0.48
1:A:1226:C:H5''	15:M:103:THR:OG1	2.13	0.48
1:A:359:U:H2'	1:A:360:A:H8	1.78	0.48
1:A:434:U:H2'	1:A:435:C:C6	2.47	0.48
1:A:457:C:H2'	1:A:458:C:H6	1.77	0.48
6:D:199:ASN:HD21	6:D:201:GLN:HB2	1.79	0.48
1:A:8:A:N6	6:D:205:GLU:O	2.46	0.48
7:E:71:LEU:O	7:E:72:GLN:HG3	2.13	0.48
9:G:22:LEU:HG	9:G:62:PHE:CE2	2.43	0.48
11:I:117:HIS:C	11:I:118:LYS:HG3	2.33	0.48
11:I:17:VAL:CG2	11:I:80:GLY:HA3	2.42	0.48
14:L:126:LYS:CD	14:L:126:LYS:H	2.00	0.48
22:T:54:LYS:HA	22:T:57:ARG:HH12	1.78	0.48
1:A:129(A):G:O2'	1:A:130:A:OP2	2.32	0.48
1:A:1396:A:H2	7:E:19:MET:HG3	1.78	0.48
1:A:410:G:N1	1:A:411:A:N7	2.61	0.48
1:A:596:C:O2'	1:A:597:G:H5'	2.13	0.48
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.48
1:A:954:G:H2'	1:A:955:U:C6	2.49	0.48
4:B:128:GLU:C	4:B:129:GLU:OE1	2.52	0.48
5:C:88:ARG:HG3	5:C:101:LEU:HD12	1.95	0.48
6:D:126:ILE:CG2	6:D:127:THR:H	2.27	0.48
7:E:37:ARG:HG2	7:E:37:ARG:NH1	2.27	0.48
8:F:69:GLU:CD	8:F:69:GLU:H	2.15	0.48
11:I:127:LYS:CA	11:I:127:LYS:HE3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:16:ARG:HG2	11:I:16:ARG:NH1	2.28	0.48
14:L:28:LYS:C	14:L:30:ALA:N	2.67	0.48
1:A:1165:C:O2'	1:A:1166:G:H5'	2.13	0.48
1:A:1243:C:H2'	1:A:1244:C:H6	1.78	0.48
1:A:1300:G:HO2'	1:A:1301:U:H6	1.58	0.48
1:A:934:C:H5	1:A:1344:C:H2'	1.78	0.48
1:A:992:U:O2'	1:A:993:G:OP2	2.29	0.48
4:B:55:PHE:HA	4:B:58:ILE:HD12	1.96	0.48
4:B:71:VAL:CG2	4:B:164:VAL:HG22	2.44	0.48
5:C:116:VAL:O	5:C:120:VAL:HG23	2.13	0.48
5:C:139:GLN:O	5:C:143:GLU:N	2.44	0.48
5:C:142:MET:HG3	5:C:170:GLN:HB2	1.95	0.48
5:C:43:LEU:HD22	5:C:68:VAL:HG21	1.96	0.48
5:C:77:ILE:HA	5:C:84:ILE:HB	1.93	0.48
5:C:77:ILE:CD1	5:C:84:ILE:HD12	2.43	0.48
6:D:8:VAL:C	6:D:10:ARG:N	2.67	0.48
9:G:59:LEU:CD1	9:G:63:LYS:HE2	2.43	0.48
13:K:57:THR:CG2	13:K:60:ALA:H	2.24	0.48
14:L:69:TYR:HB2	14:L:90:VAL:HG21	1.95	0.48
20:R:37:VAL:O	20:R:41:LYS:HE2	2.14	0.48
21:S:41:VAL:HG22	21:S:44:MET:HE3	1.94	0.48
1:A:1191:A:OP1	5:C:3:ASN:ND2	2.47	0.48
1:A:1462:G:O2'	1:A:1463:C:H5'	2.13	0.48
1:A:337:C:H2'	1:A:338:A:H8	1.77	0.48
1:A:951:G:O2'	1:A:952:U:H5'	2.14	0.48
6:D:117:ALA:O	6:D:121:VAL:HG23	2.13	0.48
6:D:24:GLU:O	6:D:25:ARG:CB	2.62	0.48
9:G:26:PHE:HB2	9:G:62:PHE:HZ	1.79	0.48
9:G:58:PRO:HG2	9:G:59:LEU:H	1.77	0.48
16:N:14:PRO:HG2	16:N:15:LYS:H	1.79	0.48
1:A:1060:C:O2'	1:A:1061:G:H5'	2.13	0.48
4:B:100:GLY:O	4:B:104:ASN:N	2.47	0.48
4:B:201:ILE:O	4:B:203:GLY:N	2.47	0.48
4:B:71:VAL:O	4:B:71:VAL:HG23	2.14	0.48
5:C:14:ILE:CG2	5:C:15:THR:H	2.07	0.48
8:F:100:ASN:HB2	20:R:23:LYS:HZ2	1.78	0.48
8:F:10:LEU:HD13	8:F:59:TYR:HB3	1.95	0.48
10:H:31:PHE:O	10:H:35:ILE:HG13	2.14	0.48
1:A:1064:G:C4'	1:A:1065:U:H5'	2.43	0.48
1:A:1182:G:H4'	1:A:1183:A:H5''	1.95	0.48
1:A:1281:U:H6	1:A:1281:U:H3'	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:A:O2'	1:A:1500:A:H5'	2.14	0.48
1:A:19:C:H2'	1:A:20:U:H6	1.79	0.48
4:B:61:LEU:CD2	4:B:64:ARG:HD2	2.35	0.48
5:C:118:GLN:O	5:C:122:GLU:HG3	2.14	0.48
5:C:180:ALA:HB3	5:C:182:ILE:HG13	1.94	0.48
1:A:1240:U:OP2	9:G:116:ALA:HB2	2.13	0.48
10:H:114:THR:HG21	10:H:129:VAL:HG23	1.96	0.48
11:I:95:LYS:O	11:I:98:PRO:HD2	2.13	0.48
18:P:7:ALA:O	18:P:17:TYR:HA	2.14	0.48
2:X:33:U:H2'	2:X:35:C:OP2	2.14	0.48
1:A:1256:A:H5'	1:A:1258:G:C1'	2.43	0.48
1:A:1319:A:H5'	1:A:1320:C:OP1	2.14	0.48
1:A:1343:G:H2'	1:A:1344:C:H6	1.74	0.48
1:A:189:G:N3	1:A:190(K):G:N2	2.59	0.48
1:A:26:A:H61	1:A:558:G:H1'	1.79	0.48
7:E:102:ALA:HB2	7:E:120:THR:HB	1.96	0.48
7:E:92:LYS:HB3	7:E:119:LEU:HB2	1.95	0.48
8:F:69:GLU:N	8:F:69:GLU:OE1	2.47	0.48
10:H:116:LYS:HZ2	10:H:127:LEU:HB3	1.78	0.48
11:I:44:VAL:HG12	11:I:51:ARG:NH1	2.28	0.48
5:C:58:GLU:CB	12:J:92:THR:HG21	2.42	0.48
14:L:71:PRO:HG2	14:L:102:ARG:HG2	1.95	0.48
14:L:104:VAL:O	14:L:105:TYR:HB2	2.14	0.48
14:L:86:ARG:HG3	14:L:86:ARG:HH11	1.79	0.48
15:M:33:ALA:HA	15:M:59:TYR:CE2	2.49	0.48
15:M:81:LEU:O	15:M:86:CYS:HB3	2.14	0.48
1:A:1014:A:H2'	1:A:1015:A:C8	2.48	0.48
1:A:1128:C:H5'	11:I:16:ARG:NH2	2.29	0.48
1:A:1305:G:O2'	1:A:1306:A:C8	2.50	0.48
1:A:922:G:N3	1:A:1398:A:H2	2.11	0.48
4:B:76:GLN:O	4:B:208:ILE:HG13	2.14	0.48
1:A:1106:G:H5''	5:C:172:ARG:CG	2.43	0.48
5:C:22:TRP:NE1	5:C:36:ASP:OD1	2.45	0.48
6:D:70:ILE:CG2	6:D:71:SER:N	2.77	0.48
10:H:64:LYS:HB3	10:H:79:VAL:HG21	1.94	0.48
11:I:37:PHE:O	11:I:39:GLY:N	2.47	0.48
14:L:77:LEU:HD21	14:L:107:ALA:HA	1.95	0.48
14:L:92:ASP:O	14:L:94:PRO:HD3	2.14	0.48
18:P:10:GLY:HA3	18:P:15:PRO:HA	1.96	0.48
21:S:71:LEU:HD12	21:S:71:LEU:N	2.29	0.48
1:A:1160:G:O2'	1:A:1161:C:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:U:OP2	6:D:3:ARG:HD3	2.13	0.47
1:A:462:G:N2	18:P:82:GLN:CB	2.61	0.47
1:A:866:C:H2'	1:A:867:G:O4'	2.14	0.47
1:A:942:G:H2'	1:A:943:U:H6	1.78	0.47
4:B:107:THR:C	4:B:109:SER:N	2.66	0.47
4:B:69:LEU:HD23	4:B:70:PHE:N	2.28	0.47
5:C:179:ARG:O	5:C:179:ARG:HG2	2.14	0.47
8:F:6:VAL:HG12	8:F:6:VAL:O	2.14	0.47
9:G:72:ARG:HA	9:G:96:GLN:NE2	2.28	0.47
10:H:134:ILE:HG22	10:H:135:CYS:N	2.28	0.47
11:I:82:ALA:HB1	11:I:96:LEU:HD23	1.96	0.47
14:L:117:ARG:NH2	14:L:124:LYS:CA	2.76	0.47
1:A:1311:G:O6	21:S:2:PRO:HB3	2.14	0.47
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.47
1:A:462:G:H2'	1:A:463:A:H5''	1.96	0.47
1:A:832:C:O2'	1:A:833:U:H5'	2.13	0.47
5:C:145:GLY:O	5:C:146:ALA:HB3	2.14	0.47
5:C:187:ALA:HB3	5:C:198:VAL:HB	1.96	0.47
7:E:12:LEU:HD13	7:E:31:LEU:HB2	1.96	0.47
8:F:33:TYR:CA	8:F:71:ARG:HH21	2.15	0.47
11:I:120:ARG:O	11:I:122:ALA:N	2.47	0.47
12:J:9:ARG:O	12:J:9:ARG:HG3	2.14	0.47
13:K:79:SER:OG	13:K:106:LYS:HG2	2.14	0.47
19:Q:48:GLU:O	19:Q:49:GLU:C	2.52	0.47
1:A:1060:C:O2	1:A:1198:G:C2	2.67	0.47
1:A:1222:G:O2'	1:A:1223:C:H5'	2.15	0.47
1:A:1461:G:O2'	1:A:1462:G:H5'	2.14	0.47
4:B:114:ARG:O	4:B:117:GLU:HB3	2.15	0.47
5:C:3:ASN:N	5:C:3:ASN:ND2	2.39	0.47
6:D:17:VAL:CG1	6:D:18:LYS:N	2.77	0.47
7:E:51:VAL:HB	7:E:52:PRO:CD	2.40	0.47
21:S:11:VAL:HA	21:S:38:SER:HB2	1.96	0.47
22:T:79:ARG:HG2	22:T:83:ARG:HE	1.79	0.47
1:A:434:U:H2'	1:A:435:C:H6	1.79	0.47
1:A:479:C:H5	1:A:480:U:C4	2.32	0.47
1:A:490:G:H2'	1:A:491:G:H8	1.78	0.47
4:B:101:MET:CA	4:B:108:ILE:HG13	2.36	0.47
4:B:59:GLU:O	4:B:62:ALA:HB3	2.14	0.47
4:B:98:LEU:N	4:B:98:LEU:CD2	2.78	0.47
6:D:176:LEU:HD23	6:D:176:LEU:H	1.79	0.47
7:E:144:THR:O	7:E:145:LYS:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:6:ARG:O	9:G:7:ALA:C	2.52	0.47
14:L:29:GLY:O	14:L:30:ALA:O	2.33	0.47
15:M:117:VAL:CG1	15:M:118:ALA:H	2.19	0.47
16:N:26:ARG:HH12	16:N:46:GLU:HB2	1.80	0.47
19:Q:80:GLY:O	19:Q:81:ARG:CB	2.62	0.47
21:S:28:LYS:HD3	21:S:31:ILE:HD11	1.97	0.47
21:S:63:THR:CG2	21:S:64:GLU:N	2.77	0.47
1:A:1313:U:P	21:S:6:LYS:HB3	2.54	0.47
1:A:1101:A:H4'	1:A:1102:A:O5'	2.15	0.47
1:A:114:U:O2'	1:A:115:G:H5'	2.15	0.47
1:A:1326:C:H2'	1:A:1327:C:H6	1.79	0.47
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.14	0.47
1:A:255:G:O6	1:A:266:G:O6	2.31	0.47
1:A:376:G:P	18:P:67:THR:HG21	2.54	0.47
1:A:406:G:H5'	6:D:5:ILE:HD13	1.96	0.47
4:B:88:ALA:CB	4:B:226:ARG:HH22	2.28	0.47
6:D:175:SER:HB3	6:D:186:LEU:HD11	1.96	0.47
7:E:80:ILE:HD11	7:E:91:LEU:HD12	1.94	0.47
1:A:1187:G:OP1	11:I:113:LYS:HE2	2.14	0.47
12:J:33:GLN:OE1	12:J:33:GLN:O	2.33	0.47
13:K:92:GLU:HB3	13:K:96:ARG:HH22	1.79	0.47
14:L:40:VAL:HG21	14:L:77:LEU:O	2.13	0.47
15:M:67:GLU:HB3	15:M:68:GLY:H	1.49	0.47
15:M:88:ARG:HB3	15:M:88:ARG:HH11	1.80	0.47
5:C:29:TYR:OH	16:N:54:PRO:HG2	2.15	0.47
19:Q:9:VAL:HG22	19:Q:56:VAL:HG22	1.97	0.47
22:T:100:ILE:C	22:T:102:GLY:H	2.17	0.47
22:T:56:MET:CE	22:T:85:MET:HA	2.44	0.47
1:A:1347:G:C2'	1:A:1373:G:H1	2.27	0.47
1:A:180:U:H2'	1:A:181:G:H5'	1.96	0.47
1:A:245:C:O2	1:A:283:C:N3	2.47	0.47
1:A:411:A:H62	1:A:426:G:H22	1.62	0.47
1:A:543:C:O2'	1:A:544:G:H5'	2.14	0.47
4:B:239:VAL:HB	4:B:240:GLN:NE2	2.29	0.47
5:C:113:ALA:N	5:C:114:PRO:CD	2.77	0.47
5:C:119:ARG:O	5:C:122:GLU:HB2	2.15	0.47
1:A:620:C:C1'	6:D:135:LEU:HD13	2.45	0.47
7:E:152:ARG:NH2	10:H:107:LEU:O	2.47	0.47
7:E:18:ARG:NH1	7:E:25:ARG:HB2	2.30	0.47
13:K:15:ALA:HA	13:K:77:MET:CA	2.43	0.47
1:A:537:G:OP1	14:L:113:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:119:LYS:O	14:L:120:TYR:HB2	2.15	0.47
1:A:1038:C:H2'	1:A:1039:C:C6	2.49	0.47
1:A:1047:G:O2'	1:A:1048:G:H5'	2.14	0.47
1:A:112:G:H5'	1:A:389:A:H4'	1.96	0.47
1:A:1288:A:H2'	1:A:1289:A:O4'	2.15	0.47
1:A:1290:G:H2'	1:A:1291:G:H8	1.80	0.47
1:A:1343:G:OP1	11:I:125:TYR:HE2	1.96	0.47
4:B:69:LEU:HD22	4:B:71:VAL:HG13	1.97	0.47
8:F:76:ALA:O	8:F:80:ARG:HG3	2.14	0.47
10:H:24:THR:CG2	10:H:63:LEU:HD21	2.45	0.47
10:H:86:ILE:O	10:H:88:LYS:HG3	2.15	0.47
16:N:8:GLU:OE1	16:N:9:LYS:N	2.48	0.47
1:A:1451:A:O2'	1:A:1452:C:OP1	2.25	0.47
1:A:302:G:H5''	14:L:17:LYS:HZ2	1.78	0.47
4:B:51:LEU:O	4:B:55:PHE:HD1	1.98	0.47
5:C:36:ASP:HB3	5:C:40:ARG:HH12	1.80	0.47
7:E:43:LEU:HD11	7:E:132:ALA:HB1	1.97	0.47
12:J:94:VAL:HG12	12:J:95:GLU:N	2.29	0.47
13:K:72:ALA:HB1	13:K:77:MET:HG3	1.96	0.47
13:K:92:GLU:OE1	13:K:95:ILE:HD12	2.15	0.47
14:L:82:VAL:N	14:L:106:ASP:OD1	2.46	0.47
14:L:28:LYS:O	14:L:28:LYS:HG2	2.15	0.47
17:O:39:LEU:HD22	17:O:56:LEU:HD22	1.96	0.47
21:S:45:VAL:HG12	21:S:46:GLY:N	2.30	0.47
1:A:1177:G:O5'	11:I:97:LYS:HE3	2.15	0.47
1:A:390:C:O3'	18:P:28:ARG:NH2	2.48	0.47
1:A:425:G:OP2	1:A:425:G:C8	2.67	0.47
1:A:848:C:H2'	1:A:849:C:H6	1.80	0.47
4:B:10:LEU:O	4:B:12:GLU:N	2.46	0.47
1:A:1298:C:C4	9:G:114:ARG:HD3	2.50	0.47
20:R:39:VAL:CG1	20:R:40:LEU:N	2.76	0.47
21:S:36:ARG:NH2	21:S:75:ALA:HB3	2.29	0.47
23:V:15:ARG:O	23:V:17:THR:HG23	2.15	0.47
1:A:1223:C:H3'	1:A:1224:G:H5''	1.97	0.47
1:A:1329:A:C2'	1:A:1330:U:H5'	2.44	0.47
1:A:1392:G:H2'	1:A:1393:U:C6	2.50	0.47
1:A:1412:C:H2'	1:A:1413:A:H8	1.78	0.47
1:A:1424:C:O2'	1:A:1425:U:H5'	2.15	0.47
1:A:1508:G:O2'	1:A:1509:C:H5'	2.15	0.47
1:A:142:G:O2'	1:A:196:A:N1	2.41	0.47
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:102:LEU:HD21	4:B:162:ILE:HD11	1.96	0.47
4:B:168:THR:O	4:B:171:ALA:HB2	2.14	0.47
4:B:30:ARG:HG3	4:B:31:TYR:CD2	2.50	0.47
6:D:132:ARG:HH11	6:D:132:ARG:HG3	1.80	0.47
14:L:102:ARG:HH22	14:L:110:VAL:HA	1.80	0.47
15:M:22:ILE:CB	15:M:25:ILE:HD12	2.45	0.47
1:A:1129:C:O2'	1:A:1131:G:H3'	2.14	0.47
1:A:1054:C:N4	1:A:1196:U:H5	2.13	0.47
1:A:1014:A:H2	1:A:1219:U:H1'	1.80	0.47
1:A:647:C:H2'	1:A:648:A:H8	1.80	0.47
4:B:71:VAL:HG22	4:B:164:VAL:HA	1.97	0.47
5:C:76:VAL:O	5:C:83:ARG:HG3	2.15	0.47
5:C:92:ALA:O	5:C:96:GLY:HA2	2.15	0.47
6:D:78:LEU:CD2	6:D:96:LEU:HB3	2.42	0.47
9:G:136:LYS:O	9:G:139:GLU:N	2.48	0.47
10:H:118:VAL:C	10:H:119:LEU:HD23	2.36	0.47
12:J:33:GLN:O	12:J:34:VAL:HB	2.14	0.47
13:K:120:ARG:NH2	13:K:126:ARG:NH1	2.63	0.47
14:L:55:VAL:HG12	14:L:56:ALA:H	1.76	0.47
16:N:24:CYS:HB3	16:N:28:GLY:N	2.30	0.47
17:O:87:ILE:HG22	17:O:88:ARG:NE	2.24	0.47
18:P:28:ARG:NH1	18:P:29:ASP:OD2	2.48	0.47
18:P:19:ILE:HG22	18:P:36:ILE:HG13	1.96	0.47
18:P:43:LYS:HG3	18:P:48:TRP:CD2	2.50	0.47
1:A:1262:C:H42	1:A:1273:G:H1	1.63	0.46
1:A:1372:U:O2'	1:A:1373:G:H5'	2.15	0.46
1:A:1511:G:O2'	1:A:1512:U:H5'	2.15	0.46
1:A:437:U:O2'	1:A:438:G:H5'	2.15	0.46
1:A:782:A:H2'	1:A:783:C:O4'	2.15	0.46
1:A:791:G:H2'	1:A:792:A:H5''	1.95	0.46
1:A:861:G:O2'	1:A:862:C:H5'	2.15	0.46
4:B:77:ALA:O	4:B:81:VAL:HG23	2.15	0.46
5:C:129:ALA:HB3	5:C:132:ARG:NE	2.30	0.46
1:A:1060:C:C5	5:C:2:GLY:N	2.83	0.46
11:I:17:VAL:HG11	11:I:81:ILE:HA	1.96	0.46
13:K:87:THR:HG22	13:K:91:ARG:NH2	2.30	0.46
14:L:39:VAL:HG12	14:L:40:VAL:N	2.30	0.46
19:Q:3:LYS:HB3	19:Q:60:ILE:CD1	2.45	0.46
1:A:1373:G:H5''	9:G:36:LYS:HB2	1.98	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.15	0.46
1:A:279:A:H5''	1:A:280:C:H3'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:A:O2'	1:A:641:U:H5'	2.15	0.46
1:A:908:A:H2'	1:A:909:A:C8	2.49	0.46
1:A:973:G:H3'	1:A:974:A:H5''	1.98	0.46
4:B:15:VAL:HG12	4:B:16:HIS:N	2.20	0.46
4:B:82:ARG:HB3	4:B:94:ASN:HD21	1.80	0.46
5:C:52:LEU:H	5:C:52:LEU:CD2	2.28	0.46
7:E:135:THR:O	7:E:138:ALA:HB3	2.15	0.46
9:G:16:LEU:N	9:G:16:LEU:HD22	2.30	0.46
11:I:99:LEU:N	11:I:99:LEU:HD22	2.30	0.46
13:K:33:THR:HB	13:K:38:ASN:C	2.34	0.46
18:P:34:GLU:OE1	18:P:55:ARG:NH1	2.48	0.46
21:S:17:GLU:HA	21:S:20:LEU:CG	2.43	0.46
22:T:39:LYS:HG2	22:T:55:ILE:HD13	1.98	0.46
1:A:1425:U:H3	1:A:1475:G:H1	1.63	0.46
1:A:1476:G:O2'	1:A:1477:C:H5'	2.14	0.46
1:A:1392:G:N2	1:A:1502:A:C8	2.83	0.46
4:B:22:LYS:HG2	4:B:22:LYS:O	2.15	0.46
11:I:85:LEU:O	11:I:92:TYR:HD1	1.98	0.46
12:J:32:ALA:CB	12:J:75:ILE:HD13	2.45	0.46
12:J:4:ILE:CG1	12:J:74:ILE:HB	2.44	0.46
17:O:70:LEU:HD12	17:O:78:TYR:CB	2.45	0.46
19:Q:68:ARG:O	19:Q:69:LYS:HB2	2.15	0.46
19:Q:6:LEU:O	19:Q:59:ILE:N	2.44	0.46
1:A:1250:A:C5'	11:I:68:GLY:N	2.78	0.46
1:A:1294:G:O2'	1:A:1295:G:H5'	2.15	0.46
1:A:1405:G:P	24:A:1545:PAR:O34	2.74	0.46
1:A:166:G:O2'	1:A:167:G:H5'	2.15	0.46
1:A:456:C:O2'	1:A:457:C:H5'	2.15	0.46
4:B:60:ASP:OD1	4:B:64:ARG:NH2	2.49	0.46
5:C:191:THR:HG22	5:C:192:THR:H	1.79	0.46
7:E:106:PRO:O	7:E:110:LEU:HG	2.15	0.46
7:E:144:THR:CG2	7:E:146:ALA:H	2.28	0.46
11:I:5:TYR:HA	11:I:17:VAL:O	2.16	0.46
12:J:48:THR:HA	12:J:62:HIS:CD2	2.45	0.46
20:R:59:SER:O	20:R:60:GLY:C	2.53	0.46
1:A:1202:G:C2'	1:A:1203:C:H5'	2.45	0.46
1:A:1301:U:O2'	1:A:1302:U:P	2.74	0.46
1:A:1406:U:O2'	1:A:1407:C:H5'	2.16	0.46
1:A:192:U:O4'	22:T:103:GLY:HA2	2.14	0.46
1:A:22:G:O2'	1:A:23:C:H5'	2.15	0.46
1:A:386:C:O2'	1:A:387:U:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:A:C2'	1:A:641:U:H5'	2.46	0.46
1:A:706:A:H1'	13:K:29:ILE:CD1	2.45	0.46
1:A:797:C:O2'	1:A:798:G:H5'	2.16	0.46
4:B:159:PRO:HB2	4:B:161:ALA:O	2.16	0.46
9:G:122:HIS:HD2	9:G:125:MET:CE	2.28	0.46
10:H:82:HIS:CB	10:H:138:TRP:CE2	2.98	0.46
14:L:111:LYS:O	14:L:112:ASP:HB2	2.16	0.46
22:T:39:LYS:HE2	22:T:55:ILE:HD11	1.96	0.46
23:V:2:GLY:C	23:V:4:GLY:H	2.19	0.46
1:A:298:A:H2'	1:A:299:G:O4'	2.15	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.46
1:A:803:G:H2'	1:A:804:U:O4'	2.15	0.46
4:B:80:ILE:CD1	4:B:208:ILE:HG23	2.41	0.46
4:B:25:ASN:HD22	4:B:27:LYS:N	2.13	0.46
6:D:31:CYS:O	6:D:32:ALA:HB3	2.15	0.46
7:E:107:ARG:O	7:E:110:LEU:N	2.32	0.46
11:I:93:ARG:CB	11:I:93:ARG:HH11	2.29	0.46
13:K:48:ILE:HD11	13:K:64:ALA:HA	1.98	0.46
1:A:1056:U:H5'	5:C:163:ALA:CB	2.46	0.46
1:A:1237:C:C4'	1:A:1334:G:N2	2.79	0.46
1:A:1296:C:H4'	1:A:1302:U:C5	2.51	0.46
1:A:22:G:H2'	1:A:23:C:C6	2.51	0.46
4:B:88:ALA:O	4:B:90:MET:N	2.47	0.46
6:D:159:ARG:HD3	6:D:159:ARG:HA	1.83	0.46
8:F:43:LEU:N	8:F:43:LEU:CD2	2.79	0.46
10:H:51:VAL:CG1	10:H:52:ASP:N	2.79	0.46
15:M:78:ILE:O	15:M:81:LEU:HB2	2.16	0.46
16:N:43:CYS:O	16:N:44:LEU:C	2.54	0.46
1:A:430:A:C3'	1:A:431:A:H5''	2.45	0.46
1:A:645:C:O2'	1:A:646:U:H5'	2.15	0.46
1:A:646:U:O2'	1:A:647:C:H5'	2.15	0.46
1:A:7:G:H21	7:E:121:LYS:HG2	1.80	0.46
1:A:831:U:H2'	1:A:832:C:H6	1.80	0.46
4:B:95:GLN:OE1	4:B:95:GLN:HA	2.15	0.46
11:I:42:ARG:HH11	11:I:42:ARG:HG2	1.81	0.46
11:I:5:TYR:C	11:I:5:TYR:CD1	2.88	0.46
14:L:59:ARG:NH1	14:L:65:GLU:HG2	2.30	0.46
19:Q:48:GLU:O	19:Q:50:LYS:N	2.49	0.46
1:A:1277:C:C2'	1:A:1278:U:H5'	2.46	0.46
1:A:131:C:H2'	1:A:132:C:C6	2.51	0.46
1:A:624:C:O2'	1:A:625:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:U:O2'	1:A:962:C:H5'	2.16	0.46
1:A:992:U:O2'	1:A:993:G:P	2.73	0.46
4:B:134:GLU:HA	4:B:137:ARG:HB3	1.98	0.46
9:G:140:ASP:O	9:G:143:ARG:HB3	2.15	0.46
9:G:155:ARG:O	9:G:156:TRP:HB3	2.15	0.46
12:J:96:ILE:CG2	12:J:97:GLU:N	2.78	0.46
18:P:31:LYS:HB3	18:P:31:LYS:NZ	2.31	0.46
18:P:21:VAL:HG21	18:P:59:TRP:CD1	2.51	0.46
20:R:87:ARG:O	20:R:88:LYS:HB3	2.16	0.46
1:A:1010:G:N2	1:A:1020:U:H1'	2.31	0.46
1:A:1131:G:H2'	1:A:1132:C:H6	1.79	0.46
1:A:193:C:H2'	1:A:194:C:C6	2.51	0.46
1:A:123:C:OP1	1:A:312:C:H5'	2.16	0.46
1:A:744:C:H2'	1:A:745:C:C6	2.50	0.46
4:B:44:LEU:O	4:B:47:THR:N	2.49	0.46
5:C:32:LEU:HB3	5:C:59:ARG:NH1	2.31	0.46
6:D:4:TYR:O	6:D:5:ILE:HB	2.16	0.46
8:F:100:ASN:CB	20:R:23:LYS:HZ2	2.29	0.46
9:G:107:ALA:O	9:G:110:GLN:HB2	2.16	0.46
10:H:36:LEU:HD12	10:H:59:LEU:HD13	1.97	0.46
18:P:1:MET:HE2	18:P:3:LYS:HD2	1.97	0.46
1:A:119:A:H4'	1:A:120:A:O5'	2.16	0.45
1:A:1320:C:O2'	1:A:1321:C:H5'	2.15	0.45
1:A:1339:A:H2'	1:A:1340:A:O4'	2.16	0.45
1:A:1371:G:O3'	11:I:69:GLY:HA3	2.16	0.45
1:A:925:G:C2	1:A:927:G:C8	3.04	0.45
4:B:210:SER:O	4:B:211:ILE:C	2.54	0.45
4:B:21:ARG:HB2	4:B:22:LYS:H	1.61	0.45
8:F:92:LYS:NZ	8:F:92:LYS:HB2	2.31	0.45
10:H:38:ILE:CG2	10:H:120:THR:HG22	2.46	0.45
1:A:716:A:N3	13:K:117:ASN:O	2.49	0.45
14:L:61:THR:C	14:L:63:GLY:H	2.18	0.45
1:A:178:C:O2'	1:A:179:A:H5'	2.17	0.45
1:A:757:U:H2'	1:A:758:G:O4'	2.16	0.45
1:A:819:A:H4'	1:A:820:U:OP2	2.14	0.45
1:A:826:C:H2'	1:A:827:U:H6	1.80	0.45
1:A:934:C:C4	1:A:1345:U:C5	3.04	0.45
5:C:7:PRO:CB	5:C:11:ARG:HH21	2.28	0.45
6:D:8:VAL:HB	6:D:21:LEU:CD1	2.44	0.45
7:E:80:ILE:CD1	7:E:91:LEU:HD12	2.46	0.45
11:I:27:THR:HG23	11:I:30:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:89:ASN:ND2	11:I:91:ASP:HB2	2.30	0.45
16:N:45:ARG:HG2	16:N:49:HIS:CD2	2.52	0.45
1:A:1033:G:H2'	1:A:1034:G:C8	2.48	0.45
1:A:1110:A:H8	1:A:1110:A:O5'	1.98	0.45
1:A:1281:U:H4'	1:A:1282:C:OP2	2.17	0.45
1:A:359:U:H2'	1:A:360:A:C8	2.51	0.45
4:B:25:ASN:HD21	4:B:27:LYS:HB2	1.81	0.45
4:B:66:GLY:HA2	4:B:160:ASP:OD2	2.16	0.45
4:B:79:ASP:O	4:B:82:ARG:HG2	2.16	0.45
5:C:29:TYR:CD2	5:C:29:TYR:C	2.90	0.45
7:E:11:ILE:CG2	7:E:12:LEU:HD12	2.45	0.45
8:F:55:ASP:CB	8:F:86:ARG:HH12	2.29	0.45
11:I:44:VAL:CG1	11:I:51:ARG:HH12	2.30	0.45
15:M:110:ARG:HH11	15:M:110:ARG:CG	2.29	0.45
21:S:12:ASP:HB3	21:S:14:HIS:CE1	2.52	0.45
23:V:6:ARG:HE	23:V:7:ARG:HE	1.63	0.45
1:A:1279:A:O2'	1:A:1282:C:N4	2.49	0.45
1:A:149:A:O2'	1:A:150:C:H5'	2.17	0.45
1:A:67:C:O2'	1:A:171:A:H1'	2.16	0.45
1:A:190(A):C:N4	1:A:190(H):G:H1	2.15	0.45
1:A:442:C:H2'	1:A:443:C:C6	2.52	0.45
1:A:602:A:O2'	1:A:603:U:H5'	2.16	0.45
5:C:115:LEU:O	5:C:116:VAL:C	2.55	0.45
9:G:120:ILE:HD12	9:G:120:ILE:N	2.31	0.45
12:J:23:ILE:HD12	12:J:23:ILE:N	2.31	0.45
13:K:127:LYS:HA	13:K:127:LYS:HE3	1.98	0.45
12:J:47:PHE:HD2	16:N:34:TYR:CD2	2.34	0.45
16:N:59:ALA:O	16:N:60:SER:HB2	2.16	0.45
1:A:1222:G:O3'	21:S:78:ARG:NH1	2.49	0.45
1:A:1227:A:H2'	1:A:1228:C:O5'	2.17	0.45
1:A:1370:G:C2	1:A:1371:G:N7	2.84	0.45
1:A:622:A:C8	1:A:623:C:C6	3.05	0.45
1:A:718:G:H5'	13:K:117:ASN:OD1	2.16	0.45
1:A:778:G:O2'	1:A:779:C:H5'	2.16	0.45
4:B:74:LYS:NZ	4:B:206:ASP:HB2	2.31	0.45
6:D:107:ARG:HB3	6:D:174:LEU:CD1	2.47	0.45
6:D:118:ARG:HG3	6:D:136:PRO:HB3	1.98	0.45
6:D:54:TYR:O	6:D:55:ALA:C	2.54	0.45
6:D:58:LEU:CD2	6:D:62:GLN:HG2	2.46	0.45
7:E:80:ILE:HD12	7:E:80:ILE:H	1.81	0.45
8:F:27:GLN:NE2	8:F:27:GLN:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:38:THR:O	14:L:79:GLU:HB3	2.16	0.45
15:M:15:VAL:HG11	15:M:34:LEU:HD21	1.98	0.45
21:S:28:LYS:HG2	21:S:29:ARG:N	2.17	0.45
21:S:40:ILE:HG13	21:S:69:HIS:O	2.16	0.45
1:A:1206:G:C6	1:A:1207:G:C5	3.05	0.45
1:A:1494:G:O2'	1:A:1495:U:H5'	2.17	0.45
1:A:942:G:O2'	1:A:943:U:H5'	2.16	0.45
1:A:993:G:H4'	1:A:994:A:OP2	2.16	0.45
4:B:83:MET:HE3	4:B:235:SER:CA	2.45	0.45
1:A:1256:A:H8	5:C:27:LYS:HZ1	1.63	0.45
6:D:173:TRP:CD1	6:D:174:LEU:HG	2.51	0.45
8:F:27:GLN:HE21	8:F:27:GLN:HA	1.82	0.45
12:J:6:ILE:HG23	12:J:98:ILE:CG2	2.46	0.45
13:K:17:GLY:O	13:K:80:VAL:HA	2.16	0.45
14:L:33:ARG:HD2	14:L:33:ARG:HA	1.66	0.45
14:L:83:VAL:CG2	14:L:100:ILE:HG23	2.47	0.45
15:M:44:ARG:HB3	15:M:46:LYS:HG2	1.98	0.45
16:N:14:PRO:O	16:N:15:LYS:HB2	2.16	0.45
23:V:9:ARG:NH1	23:V:22:ARG:HA	2.32	0.45
1:A:105:G:H2'	1:A:106:C:C6	2.51	0.45
1:A:109:A:H2'	1:A:326:G:H21	1.80	0.45
1:A:1136:U:H5''	1:A:1137:C:H5	1.81	0.45
1:A:1184:G:H2'	1:A:1185:G:H8	1.81	0.45
1:A:425:G:H8	1:A:425:G:H5''	1.81	0.45
1:A:429:U:H4'	1:A:430:A:OP1	2.17	0.45
1:A:685:G:O2'	1:A:686:U:H5'	2.16	0.45
4:B:140:HIS:O	4:B:143:GLU:HB2	2.17	0.45
6:D:64:LEU:HD13	6:D:64:LEU:C	2.36	0.45
7:E:129:ILE:HD12	7:E:129:ILE:H	1.82	0.45
12:J:60:ARG:CD	12:J:60:ARG:N	2.74	0.45
14:L:117:ARG:CZ	14:L:124:LYS:HA	2.47	0.45
18:P:20:VAL:CG1	18:P:21:VAL:N	2.78	0.45
1:A:1129:C:HO2'	1:A:1131:G:H8	1.56	0.45
1:A:1438:G:H2'	1:A:1439:C:C6	2.52	0.45
1:A:1417:G:H2'	1:A:1482:G:H22	1.81	0.45
1:A:407:G:O2'	1:A:408:A:OP1	2.31	0.45
1:A:949:A:N7	15:M:106:ASN:ND2	2.65	0.45
6:D:153:ARG:HE	6:D:181:MET:CE	2.29	0.45
6:D:162:LEU:HD13	6:D:181:MET:HG2	1.97	0.45
7:E:51:VAL:CB	7:E:52:PRO:HD3	2.41	0.45
13:K:14:VAL:HG21	13:K:40:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:26:ARG:HG3	18:P:27:LYS:N	2.32	0.45
19:Q:14:LYS:HZ1	19:Q:53:LEU:HD22	1.82	0.45
1:A:1057:G:C5	1:A:1204:A:C2	3.04	0.45
1:A:1370:G:C2	1:A:1371:G:C8	3.05	0.45
1:A:151:A:H2'	1:A:152:A:O4'	2.17	0.45
1:A:423:G:H5''	1:A:424:G:H21	1.82	0.45
1:A:442:C:H2'	1:A:443:C:H6	1.81	0.45
1:A:601:C:O2'	1:A:602:A:H5'	2.17	0.45
1:A:624:C:H2'	1:A:625:G:H8	1.81	0.45
1:A:750:G:H1'	17:O:22:THR:OG1	2.17	0.45
1:A:865:A:H2'	1:A:866:C:C6	2.52	0.45
1:A:13:U:C5	1:A:916:G:O6	2.70	0.45
4:B:118:LEU:O	4:B:119:GLU:C	2.55	0.45
4:B:161:ALA:HB1	4:B:185:ILE:HD11	1.98	0.45
5:C:195:VAL:C	5:C:196:LEU:CD2	2.86	0.45
5:C:79:ARG:HH11	5:C:79:ARG:CB	2.30	0.45
7:E:89:ILE:HD13	7:E:90:VAL:H	1.81	0.45
14:L:27:LEU:HG	14:L:28:LYS:N	2.31	0.45
1:A:267:C:OP2	19:Q:67:LYS:HD2	2.16	0.45
20:R:47:THR:HA	20:R:83:GLU:HB2	1.98	0.45
22:T:72:LEU:O	22:T:73:HIS:C	2.55	0.45
1:A:1327:C:OP1	23:V:20:LYS:HB3	2.17	0.45
1:A:1038:C:H2'	1:A:1039:C:H6	1.81	0.45
1:A:1194:U:O2'	1:A:1195:C:H5'	2.17	0.45
1:A:1509:C:H2'	1:A:1510:U:O4'	2.17	0.45
1:A:410:G:O4'	1:A:431:A:N6	2.46	0.45
1:A:562:C:H1'	14:L:15:ARG:HB3	1.98	0.45
1:A:629:G:O2'	1:A:630:G:H5'	2.17	0.45
1:A:783:C:O2'	1:A:784:C:H5'	2.17	0.45
4:B:15:VAL:CG1	4:B:209:ARG:HG3	2.47	0.45
4:B:97:TRP:CE3	4:B:98:LEU:O	2.70	0.45
5:C:5:ILE:C	5:C:5:ILE:HD12	2.36	0.45
7:E:80:ILE:CG2	10:H:104:ARG:NH2	2.80	0.45
10:H:122:ARG:HG3	10:H:122:ARG:HH11	1.82	0.45
12:J:89:ASP:O	12:J:90:LEU:HD23	2.18	0.45
17:O:78:TYR:C	17:O:80:ALA:N	2.70	0.45
20:R:17:SER:HB2	20:R:54:ARG:CZ	2.47	0.45
22:T:56:MET:CE	22:T:88:VAL:HB	2.47	0.45
1:A:1118:C:C1'	1:A:1179:A:C4	3.00	0.44
1:A:131:C:H2'	1:A:132:C:H6	1.82	0.44
1:A:1329:A:O2'	1:A:1330:U:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:G:OP2	11:I:11:LYS:HE2	2.18	0.44
1:A:1505:G:H3'	1:A:1505:G:C8	2.52	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	1.99	0.44
4:B:212:GLN:O	4:B:216:SER:CB	2.65	0.44
5:C:22:TRP:CZ3	5:C:32:LEU:HD12	2.52	0.44
1:A:1250:A:C5'	11:I:68:GLY:H	2.29	0.44
12:J:29:ARG:CA	12:J:29:ARG:HH11	2.30	0.44
15:M:125:ARG:C	15:M:125:ARG:HD2	2.38	0.44
19:Q:59:ILE:HD13	19:Q:73:VAL:HA	1.99	0.44
1:A:1131:G:OP1	11:I:3:GLN:NE2	2.51	0.44
1:A:1328:C:O2'	1:A:1329:A:H5'	2.17	0.44
1:A:1417:G:H2'	1:A:1482:G:N2	2.33	0.44
1:A:254:G:O2'	1:A:255:G:H5'	2.16	0.44
1:A:532:A:C2'	1:A:533:A:OP1	2.65	0.44
4:B:132:LYS:HD3	4:B:135:GLN:CB	2.47	0.44
4:B:209:ARG:HD3	4:B:209:ARG:O	2.17	0.44
4:B:24:TRP:CG	4:B:25:ASN:N	2.80	0.44
5:C:134:ILE:CG2	5:C:168:ALA:HB3	2.47	0.44
6:D:163:GLU:O	6:D:165:MET:N	2.50	0.44
6:D:67:ILE:HG22	6:D:68:TYR:N	2.31	0.44
14:L:47:LYS:CB	14:L:48:PRO:CD	2.76	0.44
21:S:33:THR:CG2	21:S:34:TRP:N	2.80	0.44
21:S:71:LEU:H	21:S:71:LEU:CD1	2.30	0.44
22:T:96:GLY:O	22:T:97:ALA:CB	2.64	0.44
1:A:1060:C:H2'	1:A:1061:G:H8	1.83	0.44
1:A:1306:A:H2'	1:A:1307:U:O4'	2.16	0.44
1:A:1459:C:O2'	1:A:1460:A:H5'	2.17	0.44
1:A:1472:U:O2'	1:A:1473:A:H5'	2.17	0.44
1:A:1406:U:OP2	24:A:1545:PAR:N24	2.50	0.44
1:A:948:C:O2'	1:A:949:A:H5'	2.17	0.44
4:B:115:LEU:HD21	4:B:153:ARG:NH1	2.32	0.44
13:K:94:ALA:O	13:K:95:ILE:C	2.55	0.44
15:M:37:THR:O	15:M:37:THR:HG22	2.17	0.44
16:N:29:ARG:HH11	16:N:29:ARG:HG2	1.81	0.44
23:V:23:PRO:C	23:V:25:LYS:N	2.69	0.44
23:V:2:GLY:O	23:V:4:GLY:N	2.50	0.44
1:A:109:A:H5'	1:A:110:C:C5	2.51	0.44
1:A:1133:G:H2'	1:A:1134:G:C8	2.50	0.44
1:A:1196:U:H5''	1:A:1197:G:H5'	2.00	0.44
1:A:1286:A:H2'	1:A:1287:A:O5'	2.17	0.44
1:A:52:G:O2'	1:A:53:A:H5'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:H1'	1:A:622:A:H1'	1.98	0.44
1:A:924:C:H5'	1:A:1399:C:OP2	2.18	0.44
4:B:58:ILE:O	4:B:62:ALA:HB2	2.17	0.44
5:C:136:GLN:O	5:C:139:GLN:HB2	2.17	0.44
1:A:1060:C:N4	5:C:2:GLY:N	2.66	0.44
11:I:111:ARG:O	11:I:113:LYS:HD2	2.16	0.44
12:J:4:ILE:HA	12:J:100:THR:HA	1.99	0.44
13:K:74:ALA:C	13:K:76:GLY:N	2.70	0.44
14:L:43:VAL:CG1	14:L:44:THR:N	2.80	0.44
15:M:34:LEU:HD23	15:M:34:LEU:HA	1.84	0.44
17:O:70:LEU:HD12	17:O:78:TYR:CA	2.47	0.44
18:P:20:VAL:HG13	18:P:32:TYR:HB2	1.99	0.44
22:T:97:ALA:O	22:T:99:LEU:N	2.51	0.44
1:A:1112:C:O2	5:C:178:LEU:O	2.36	0.44
1:A:1148:U:O2'	1:A:1149:C:H5'	2.17	0.44
1:A:1427:U:H2'	1:A:1428:A:H8	1.82	0.44
1:A:1413:A:H2	1:A:1487:G:H22	1.64	0.44
1:A:188:C:N3	1:A:189:G:O2'	2.51	0.44
1:A:404:U:H2'	1:A:405:U:C6	2.52	0.44
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.44
1:A:476:G:H21	1:A:478:A:C5'	2.31	0.44
4:B:187:LEU:HD13	4:B:214:ILE:HG21	1.99	0.44
5:C:167:TRP:HB3	5:C:168:ALA:H	1.48	0.44
5:C:43:LEU:CD2	5:C:68:VAL:HG21	2.47	0.44
6:D:150:GLU:HA	6:D:153:ARG:HG2	2.00	0.44
11:I:43:ALA:O	11:I:44:VAL:C	2.56	0.44
13:K:33:THR:HG22	13:K:39:PRO:CA	2.41	0.44
15:M:60:VAL:CG1	15:M:66:LEU:HD11	2.48	0.44
17:O:56:LEU:HD12	17:O:56:LEU:O	2.18	0.44
18:P:18:ARG:NH1	18:P:32:TYR:OH	2.49	0.44
19:Q:75:ARG:HG3	19:Q:75:ARG:NH1	2.33	0.44
22:T:100:ILE:HG22	22:T:102:GLY:N	2.32	0.44
22:T:10:LEU:HD11	22:T:12:ALA:HB3	2.00	0.44
22:T:38:LYS:O	22:T:42:GLN:HB2	2.17	0.44
22:T:67:ALA:HB2	22:T:77:ALA:HB2	1.99	0.44
1:A:1039:C:H2'	1:A:1040:U:H6	1.82	0.44
1:A:156:G:O2'	1:A:157:G:H5'	2.17	0.44
1:A:338:A:H2	1:A:351:G:H22	1.64	0.44
1:A:407:G:H2'	1:A:431:A:P	2.58	0.44
1:A:603:U:H2'	1:A:604:G:H8	1.83	0.44
1:A:690:G:H2'	1:A:691:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:C:O2'	1:A:807:A:H5'	2.17	0.44
1:A:9:G:OP2	7:E:121:LYS:NZ	2.47	0.44
5:C:107:GLN:N	5:C:107:GLN:CD	2.68	0.44
5:C:83:ARG:HA	5:C:86:VAL:CG2	2.46	0.44
7:E:101:ILE:HD12	7:E:119:LEU:HD23	1.98	0.44
9:G:50:ILE:CG2	9:G:61:VAL:HG21	2.47	0.44
11:I:42:ARG:O	11:I:43:ALA:C	2.56	0.44
12:J:32:ALA:O	12:J:34:VAL:HG23	2.17	0.44
12:J:66:ARG:HB3	12:J:66:ARG:HE	1.61	0.44
13:K:29:ILE:C	13:K:29:ILE:CD1	2.81	0.44
15:M:39:ILE:CD1	15:M:52:GLU:HB3	2.47	0.44
20:R:27:GLY:O	20:R:29:PHE:HD2	2.00	0.44
1:A:190:C:OP1	1:A:190(K):G:C2	2.71	0.44
1:A:50:A:N6	1:A:361:G:H4'	2.33	0.44
1:A:920:U:H2'	1:A:921:U:C6	2.52	0.44
4:B:115:LEU:HD12	4:B:115:LEU:C	2.36	0.44
4:B:117:GLU:C	4:B:117:GLU:OE1	2.56	0.44
8:F:91:VAL:HG12	8:F:92:LYS:O	2.18	0.44
13:K:96:ARG:HB2	13:K:96:ARG:NH1	2.32	0.44
15:M:11:ARG:CG	15:M:12:ASN:H	2.31	0.44
16:N:34:TYR:N	16:N:34:TYR:CD1	2.85	0.44
20:R:52:PRO:O	20:R:56:THR:HG23	2.18	0.44
1:A:1182:G:H4'	1:A:1183:A:C5'	2.47	0.44
1:A:1221:G:O2'	1:A:1222:G:H5'	2.18	0.44
1:A:1431:C:C2'	1:A:1432:G:H5'	2.48	0.44
1:A:488:C:H6	1:A:488:C:O5'	2.01	0.44
1:A:791:G:C2'	1:A:792:A:C5'	2.96	0.44
1:A:91:C:H2'	1:A:92:C:H6	1.83	0.44
4:B:148:TYR:N	4:B:148:TYR:CD2	2.85	0.44
5:C:23:TYR:CG	5:C:24:ALA:N	2.86	0.44
9:G:18:TYR:HD2	9:G:59:LEU:HB2	1.79	0.44
10:H:116:LYS:HZ3	10:H:127:LEU:HB3	1.83	0.44
11:I:50:LEU:C	11:I:52:ALA:H	2.21	0.44
12:J:24:VAL:O	12:J:24:VAL:HG12	2.18	0.44
12:J:26:ALA:HA	12:J:29:ARG:NH2	2.33	0.44
12:J:91:PRO:HB2	12:J:94:VAL:CG2	2.48	0.44
13:K:95:ILE:CG2	13:K:108:ILE:HD13	2.48	0.44
14:L:115:LYS:O	14:L:117:ARG:N	2.49	0.44
20:R:43:PHE:CA	20:R:51:LEU:HD12	2.48	0.44
1:A:1137:C:C4'	1:A:1138:G:C2	2.99	0.44
1:A:149:A:H2'	1:A:150:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H1'	1:A:344:A:N7	2.32	0.44
1:A:17:U:H2'	1:A:18:C:H6	1.76	0.44
1:A:369:C:O2'	1:A:370:C:H5'	2.17	0.44
1:A:383:A:H2'	1:A:384:G:H5'	1.99	0.44
1:A:945:G:C2	1:A:946:A:C8	3.05	0.44
4:B:91:PRO:HG3	4:B:154:LEU:CB	2.29	0.44
5:C:50:ALA:O	5:C:70:VAL:HG12	2.17	0.44
7:E:60:TYR:O	7:E:64:ARG:HG2	2.18	0.44
8:F:14:LEU:HA	8:F:18:GLN:HE21	1.83	0.44
9:G:32:ARG:O	9:G:33:ASP:HB2	2.17	0.44
9:G:72:ARG:HG2	9:G:142:GLU:OE1	2.18	0.44
13:K:48:ILE:HG13	13:K:64:ALA:N	2.33	0.44
13:K:99:GLN:HA	13:K:105:VAL:CG2	2.48	0.44
14:L:73:GLU:OE2	14:L:73:GLU:HA	2.18	0.44
18:P:50:LYS:HG2	18:P:51:VAL:N	2.33	0.44
20:R:20:ALA:O	20:R:21:LYS:O	2.35	0.44
22:T:16:HIS:O	22:T:17:ARG:C	2.56	0.44
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.43
1:A:1349:A:H2'	1:A:1350:A:H8	1.83	0.43
1:A:1480:G:H2'	1:A:1481:U:C6	2.53	0.43
1:A:358:U:H2'	1:A:359:U:C6	2.53	0.43
1:A:978:A:C5	1:A:1319:A:C2	3.05	0.43
1:A:981:U:O5'	1:A:981:U:H6	2.00	0.43
4:B:90:MET:HE3	4:B:222:ILE:HD13	1.98	0.43
4:B:90:MET:CE	4:B:222:ILE:HD13	2.47	0.43
5:C:101:LEU:HD22	5:C:101:LEU:O	2.17	0.43
5:C:149:ALA:HA	5:C:201:TYR:O	2.18	0.43
1:A:1060:C:H41	5:C:2:GLY:N	2.15	0.43
6:D:111:ALA:HA	6:D:116:GLN:OE1	2.18	0.43
8:F:40:VAL:HG22	8:F:41:GLU:N	2.32	0.43
13:K:48:ILE:HD11	13:K:67:ASP:HB2	1.99	0.43
14:L:38:THR:HB	14:L:57:LYS:HB2	2.00	0.43
15:M:82:MET:CE	15:M:93:ARG:HG2	2.47	0.43
19:Q:13:ASP:H	19:Q:14:LYS:HD2	1.83	0.43
19:Q:95:TYR:O	19:Q:97:SER:O	2.36	0.43
1:A:1064:G:N2	1:A:1190:G:H2'	2.32	0.43
1:A:1397:C:O2'	1:A:1398:A:P	2.76	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.53	0.43
1:A:1428:A:H2'	1:A:1429:C:H6	1.82	0.43
1:A:200:G:H2'	1:A:201:C:O4'	2.18	0.43
1:A:538:G:OP2	14:L:115:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:C:H2'	1:A:757:U:O4'	2.17	0.43
1:A:826:C:H2'	1:A:827:U:C6	2.53	0.43
1:A:976:G:N7	1:A:1358:U:C2	2.86	0.43
4:B:34:ALA:O	4:B:41:ILE:N	2.42	0.43
4:B:83:MET:HG3	4:B:238:LEU:CD1	2.49	0.43
4:B:78:GLN:HG2	4:B:94:ASN:HB3	2.00	0.43
4:B:9:GLU:HB2	4:B:217:ARG:HH12	1.83	0.43
5:C:79:ARG:CB	5:C:79:ARG:NH1	2.80	0.43
5:C:91:LEU:HD23	5:C:92:ALA:HB2	2.00	0.43
10:H:48:TYR:CD1	10:H:48:TYR:C	2.89	0.43
13:K:110:ASP:OD2	20:R:88:LYS:NZ	2.51	0.43
14:L:65:GLU:CD	14:L:65:GLU:N	2.71	0.43
14:L:93:LEU:HD23	14:L:93:LEU:N	2.33	0.43
14:L:98:TYR:CD1	14:L:98:TYR:N	2.86	0.43
15:M:8:GLU:HG2	15:M:67:GLU:HG3	2.00	0.43
19:Q:13:ASP:O	19:Q:13:ASP:OD2	2.36	0.43
1:A:115:G:H1'	1:A:116:A:N7	2.34	0.43
1:A:1481:U:O2'	1:A:1482:G:H5'	2.18	0.43
1:A:619:U:O2	6:D:133:VAL:HA	2.18	0.43
1:A:833:U:H2'	1:A:834:C:C6	2.53	0.43
4:B:112:VAL:C	4:B:114:ARG:N	2.71	0.43
5:C:180:ALA:C	5:C:182:ILE:N	2.70	0.43
5:C:52:LEU:H	5:C:52:LEU:HD23	1.82	0.43
6:D:187:ARG:NH1	6:D:188:LEU:HD12	2.33	0.43
6:D:36:ARG:N	6:D:37:PRO:CD	2.51	0.43
10:H:61:VAL:O	10:H:63:LEU:HD22	2.18	0.43
13:K:108:ILE:HB	20:R:87:ARG:O	2.18	0.43
14:L:32:PHE:HB3	14:L:84:LEU:HD11	1.99	0.43
20:R:55:ARG:HB3	20:R:55:ARG:NH1	2.33	0.43
22:T:100:ILE:HG22	22:T:102:GLY:CA	2.48	0.43
22:T:13:LEU:HD12	22:T:14:LYS:N	2.34	0.43
1:A:1151:A:H5''	12:J:42:THR:OG1	2.18	0.43
1:A:1207:G:H2'	1:A:1208:C:H6	1.84	0.43
1:A:158:G:O2'	1:A:159:G:H5'	2.19	0.43
1:A:251:G:H4'	1:A:252:U:O5'	2.18	0.43
1:A:444:C:H2'	1:A:445:G:C8	2.47	0.43
1:A:585:G:N3	1:A:879:C:H4'	2.34	0.43
1:A:789:U:N3	1:A:792:A:OP2	2.44	0.43
4:B:15:VAL:HG11	4:B:210:SER:HA	1.99	0.43
4:B:236:TYR:CD2	4:B:239:VAL:HG21	2.53	0.43
5:C:193:TYR:CE1	5:C:196:LEU:HD21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:39:ILE:HG22	5:C:40:ARG:N	2.33	0.43
5:C:58:GLU:HB2	5:C:65:ALA:HB2	1.99	0.43
5:C:8:ILE:O	5:C:9:GLY:C	2.57	0.43
8:F:33:TYR:O	8:F:34:GLY:C	2.55	0.43
8:F:46:ARG:HB2	8:F:60:PHE:CE1	2.54	0.43
9:G:148:ASN:C	9:G:150:ALA:N	2.72	0.43
12:J:12:ASP:OD1	12:J:14:LYS:HB2	2.18	0.43
1:A:751:U:H4'	17:O:24:SER:HA	1.99	0.43
17:O:3:ILE:HD13	17:O:34:LEU:HD13	2.00	0.43
19:Q:59:ILE:HD13	19:Q:59:ILE:HA	1.77	0.43
21:S:41:VAL:HG22	21:S:44:MET:HE2	2.00	0.43
23:V:2:GLY:C	23:V:4:GLY:N	2.72	0.43
1:A:1120:G:O2'	1:A:1121:U:H5'	2.18	0.43
1:A:1153:C:H2'	1:A:1154:G:H8	1.84	0.43
1:A:1240:U:H4'	1:A:1241:G:OP2	2.18	0.43
1:A:21:G:H2'	1:A:22:G:C8	2.54	0.43
1:A:731:G:H5'	1:A:766:A:H4'	2.00	0.43
4:B:185:ILE:H	4:B:185:ILE:HD12	1.79	0.43
4:B:76:GLN:HG3	4:B:206:ASP:OD1	2.18	0.43
5:C:199:LYS:HB3	5:C:201:TYR:HE1	1.83	0.43
5:C:79:ARG:HG3	5:C:79:ARG:O	2.18	0.43
5:C:77:ILE:HD13	5:C:84:ILE:HD12	1.99	0.43
6:D:138:TYR:CD2	6:D:138:TYR:C	2.92	0.43
9:G:122:HIS:HD2	9:G:125:MET:HE3	1.82	0.43
14:L:47:LYS:CG	14:L:48:PRO:HD3	2.49	0.43
19:Q:60:ILE:HD13	19:Q:61:GLU:H	1.83	0.43
22:T:33:ILE:HD11	22:T:66:ALA:HB2	2.01	0.43
1:A:1039:C:O2'	1:A:1040:U:H5'	2.19	0.43
1:A:1168:A:C6	1:A:1169:A:C6	3.06	0.43
1:A:1185:G:H2'	1:A:1186:G:H8	1.83	0.43
1:A:1281:U:H3'	1:A:1281:U:C6	2.53	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.54	0.43
1:A:1288:A:H1'	1:A:1352:C:O2'	2.18	0.43
1:A:28:G:O2'	1:A:29:G:H5'	2.18	0.43
1:A:39:G:O2'	1:A:40:C:H5'	2.19	0.43
1:A:413:G:C4	1:A:416:G:H5'	2.53	0.43
1:A:539:A:OP2	14:L:115:LYS:HE3	2.18	0.43
4:B:154:LEU:O	4:B:155:LEU:C	2.55	0.43
9:G:46:ALA:HA	9:G:49:ILE:HD12	2.00	0.43
10:H:59:LEU:O	10:H:61:VAL:HG23	2.19	0.43
11:I:8:GLY:HA3	11:I:79:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:3:LYS:HB3	12:J:74:ILE:O	2.18	0.43
15:M:105:THR:HB	15:M:106:ASN:H	1.63	0.43
1:A:1048:G:OP1	16:N:3:ARG:HA	2.18	0.43
19:Q:4:LYS:HD2	19:Q:6:LEU:HD21	2.01	0.43
19:Q:85:VAL:O	19:Q:89:LEU:HG	2.19	0.43
21:S:39:THR:HA	21:S:70:LYS:HD2	2.01	0.43
21:S:11:VAL:HG21	21:S:41:VAL:HG13	1.99	0.43
1:A:1141:C:O2'	1:A:1142:G:H5'	2.18	0.43
1:A:1167:A:C6	1:A:1168:A:C6	3.06	0.43
1:A:243:A:C5'	1:A:244:U:H5'	2.47	0.43
1:A:674:G:H2'	1:A:675:A:H8	1.84	0.43
4:B:53:ARG:HH12	4:B:199:TYR:HD2	1.65	0.43
4:B:223:ILE:O	4:B:225:ALA:N	2.52	0.43
5:C:115:LEU:O	5:C:118:GLN:N	2.51	0.43
5:C:151:VAL:HG12	5:C:152:ILE:N	2.34	0.43
1:A:1056:U:C5'	5:C:163:ALA:HB2	2.48	0.43
6:D:138:TYR:CD2	6:D:139:ARG:N	2.87	0.43
1:A:429:U:C2'	6:D:25:ARG:HH12	2.31	0.43
9:G:61:VAL:O	9:G:64:GLN:HB3	2.18	0.43
10:H:59:LEU:O	10:H:60:ARG:C	2.55	0.43
11:I:16:ARG:CD	11:I:64:THR:HB	2.36	0.43
11:I:84:ALA:C	11:I:86:VAL:H	2.22	0.43
16:N:11:LYS:C	16:N:13:THR:H	2.22	0.43
19:Q:14:LYS:NZ	19:Q:53:LEU:HD22	2.34	0.43
20:R:86:VAL:O	20:R:87:ARG:HB2	2.19	0.43
21:S:61:TYR:CD1	21:S:61:TYR:C	2.92	0.43
21:S:64:GLU:HA	21:S:67:VAL:CG2	2.49	0.43
1:A:1288:A:N1	1:A:1371:G:H1'	2.33	0.43
1:A:1367:C:N3	1:A:1368:G:C8	2.87	0.43
1:A:190(L):U:C2'	1:A:191:G:H5'	2.49	0.43
1:A:264:U:H4'	19:Q:63:ARG:HD3	2.00	0.43
1:A:409:G:H22	1:A:432:A:H3'	1.82	0.43
1:A:570:G:H2'	1:A:571:U:C6	2.54	0.43
1:A:910:C:P	14:L:97:ARG:HH22	2.42	0.43
1:A:934:C:N3	1:A:1345:U:C5	2.86	0.43
6:D:121:VAL:HG12	6:D:134:ASP:HA	2.01	0.43
7:E:144:THR:HG22	7:E:146:ALA:HB3	2.00	0.43
8:F:18:GLN:O	8:F:21:LEU:HB3	2.18	0.43
11:I:112:LYS:HD3	11:I:112:LYS:O	2.18	0.43
13:K:27:ASN:ND2	13:K:28:THR:N	2.66	0.43
17:O:4:THR:HB	17:O:6:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:69:LYS:C	19:Q:70:ARG:HD2	2.39	0.43
19:Q:86:GLU:O	19:Q:90:ILE:HG13	2.19	0.43
1:A:113:G:C2	1:A:315:A:C2	3.07	0.43
1:A:1290:G:H2'	1:A:1291:G:C8	2.53	0.43
1:A:1291:G:H4'	11:I:38:GLN:O	2.18	0.43
1:A:1303:C:N4	1:A:1304:G:C6	2.87	0.43
1:A:633:G:H2'	1:A:634:C:C6	2.54	0.43
4:B:127:ILE:HG13	4:B:128:GLU:OE2	2.19	0.43
6:D:163:GLU:C	6:D:165:MET:N	2.72	0.43
7:E:12:LEU:C	7:E:12:LEU:HD22	2.39	0.43
9:G:116:ALA:HA	9:G:119:ARG:CZ	2.49	0.43
10:H:20:TYR:HA	10:H:65:TYR:CZ	2.53	0.43
11:I:16:ARG:HG2	11:I:16:ARG:HH11	1.84	0.43
11:I:84:ALA:C	11:I:86:VAL:N	2.72	0.43
13:K:99:GLN:HA	13:K:105:VAL:HG23	2.00	0.43
17:O:87:ILE:O	17:O:88:ARG:CB	2.66	0.43
18:P:40:ASP:HB3	18:P:48:TRP:HB2	2.01	0.43
20:R:44:LEU:HD23	20:R:50:ILE:HA	2.01	0.43
22:T:13:LEU:HD12	22:T:13:LEU:H	1.84	0.43
22:T:87:LYS:O	22:T:91:LEU:HG	2.19	0.43
1:A:1055:A:C6	1:A:1206:G:C5	3.07	0.43
1:A:1318:A:O2'	21:S:37:ARG:HD2	2.19	0.43
1:A:253:U:H2'	1:A:254:G:C8	2.54	0.43
1:A:407:G:O2'	1:A:408:A:P	2.77	0.43
1:A:942:G:C2	1:A:943:U:C6	3.07	0.43
1:A:960:U:O2'	1:A:1223:C:H4'	2.18	0.43
1:A:967:C:OP1	1:A:969:A:H5'	2.19	0.43
4:B:132:LYS:C	4:B:134:GLU:N	2.70	0.43
5:C:95:THR:O	5:C:97:LYS:HG2	2.19	0.43
6:D:155:LEU:O	6:D:156:GLU:C	2.57	0.43
6:D:108:LEU:CD2	6:D:174:LEU:HD13	2.49	0.43
7:E:15:ARG:HG3	7:E:15:ARG:NH1	2.34	0.43
14:L:24:VAL:HG13	14:L:98:TYR:HE2	1.84	0.43
19:Q:15:MET:HE1	19:Q:43:LEU:HD22	2.00	0.43
21:S:63:THR:HG21	21:S:65:ASN:HD22	1.83	0.43
22:T:82:SER:O	22:T:86:ARG:HB2	2.19	0.43
22:T:94:ALA:O	22:T:95:ALA:HB3	2.19	0.43
1:A:1201:A:O2'	1:A:1202:G:OP2	2.32	0.42
1:A:976:G:C8	1:A:1358:U:O2	2.72	0.42
1:A:1511:G:C2'	1:A:1512:U:H5'	2.49	0.42
1:A:1520:G:O2'	1:A:1521:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H1'	1:A:344:A:C5	2.54	0.42
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.42
1:A:56:U:H2'	1:A:57:G:C8	2.54	0.42
4:B:130:ARG:HB3	4:B:131:PRO:HD2	2.01	0.42
5:C:54:ARG:NH1	5:C:54:ARG:HG2	2.34	0.42
7:E:11:ILE:HG21	7:E:31:LEU:HD12	2.00	0.42
9:G:73:MET:HB3	9:G:145:ALA:HB1	2.01	0.42
9:G:78:ARG:HD2	9:G:156:TRP:CE3	2.53	0.42
10:H:110:ALA:O	10:H:111:ILE:C	2.57	0.42
11:I:42:ARG:NH2	11:I:71:SER:OG	2.49	0.42
15:M:4:ILE:HG22	15:M:5:ALA:H	1.84	0.42
15:M:48:LEU:HD13	15:M:52:GLU:HB2	2.00	0.42
20:R:38:GLU:HA	20:R:41:LYS:HE2	2.01	0.42
1:A:1057:G:C2'	1:A:1058:G:H5'	2.48	0.42
1:A:1049:U:H1'	1:A:1201:A:N7	2.35	0.42
1:A:1454:G:H2'	1:A:1455:G:H8	1.85	0.42
1:A:410:G:C2	1:A:411:A:C8	3.06	0.42
1:A:767:A:H2'	1:A:768:A:C8	2.54	0.42
5:C:21:ARG:CD	5:C:21:ARG:N	2.72	0.42
6:D:127:THR:HG23	6:D:147:ALA:HB3	2.02	0.42
6:D:26:CYS:HA	6:D:31:CYS:HB2	2.01	0.42
6:D:16:GLY:C	6:D:33:MET:HE2	2.39	0.42
6:D:70:ILE:HD12	6:D:97:LEU:CD2	2.49	0.42
8:F:67:MET:HE2	8:F:72:VAL:H	1.84	0.42
8:F:68:PRO:HB2	8:F:71:ARG:HG2	2.01	0.42
11:I:32:ASP:O	11:I:35:GLU:N	2.52	0.42
13:K:127:LYS:HA	13:K:127:LYS:CE	2.49	0.42
18:P:12:LYS:O	18:P:13:HIS:HB2	2.18	0.42
18:P:4:ILE:CG1	18:P:64:ALA:HB1	2.48	0.42
20:R:28:GLU:CD	20:R:28:GLU:H	2.23	0.42
20:R:53:ARG:NH1	20:R:60:GLY:H	2.16	0.42
1:A:1097:C:H2'	1:A:1098:C:C6	2.53	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
1:A:1251:A:H1'	1:A:1369:C:O2'	2.19	0.42
1:A:1410:G:H2'	1:A:1411:C:H6	1.84	0.42
1:A:620:C:H2'	1:A:621:A:O4'	2.19	0.42
1:A:687:A:H2'	1:A:701:C:H41	1.84	0.42
1:A:743:U:H2'	1:A:744:C:C6	2.53	0.42
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.42
1:A:979:C:O2	16:N:19:ARG:HG2	2.20	0.42
1:A:983:A:H2	1:A:984:C:C6	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:208:ILE:C	4:B:210:SER:N	2.71	0.42
5:C:28:GLN:O	5:C:31:HIS:N	2.53	0.42
5:C:79:ARG:CZ	5:C:79:ARG:HB3	2.49	0.42
8:F:99:ALA:CB	20:R:31:LEU:HD12	2.49	0.42
10:H:60:ARG:NH1	10:H:60:ARG:HG3	2.34	0.42
11:I:27:THR:CG2	11:I:28:VAL:N	2.82	0.42
15:M:19:LEU:O	15:M:22:ILE:CD1	2.65	0.42
16:N:11:LYS:HG2	16:N:13:THR:H	1.82	0.42
18:P:51:VAL:O	18:P:53:VAL:N	2.51	0.42
19:Q:48:GLU:C	19:Q:50:LYS:N	2.71	0.42
19:Q:98:LEU:O	19:Q:99:SER:CB	2.65	0.42
23:V:6:ARG:CG	23:V:7:ARG:HD2	2.49	0.42
1:A:1085:U:H3'	1:A:1086:U:C5	2.54	0.42
1:A:344:A:O2'	1:A:345:C:OP1	2.37	0.42
1:A:941:G:O2'	1:A:942:G:H5'	2.19	0.42
4:B:130:ARG:HB3	4:B:134:GLU:OE1	2.18	0.42
4:B:137:ARG:HG2	4:B:137:ARG:NH1	2.34	0.42
6:D:121:VAL:O	6:D:134:ASP:HA	2.19	0.42
6:D:173:TRP:CE3	6:D:189:PRO:HB3	2.55	0.42
7:E:150:ARG:CG	7:E:150:ARG:HH11	2.27	0.42
7:E:31:LEU:HA	7:E:31:LEU:HD23	1.90	0.42
10:H:31:PHE:CZ	10:H:134:ILE:CD1	3.02	0.42
10:H:4:ASP:OD2	10:H:7:ALA:HB2	2.19	0.42
11:I:43:ALA:O	11:I:45:ALA:N	2.53	0.42
12:J:16:LEU:O	12:J:17:ASP:C	2.55	0.42
12:J:49:VAL:HG13	12:J:49:VAL:O	2.19	0.42
15:M:2:ALA:O	15:M:3:ARG:C	2.57	0.42
15:M:3:ARG:HB2	15:M:9:ILE:HG13	2.01	0.42
16:N:22:THR:O	16:N:23:ARG:HG3	2.19	0.42
16:N:59:ALA:HB1	16:N:61:TRP:HZ3	1.85	0.42
18:P:81:ARG:HD3	18:P:83:GLU:HB3	2.01	0.42
20:R:53:ARG:C	20:R:55:ARG:H	2.21	0.42
20:R:54:ARG:H	20:R:54:ARG:HG3	1.62	0.42
21:S:17:GLU:CA	21:S:20:LEU:HG	2.46	0.42
21:S:52:TYR:CD1	21:S:56:GLN:O	2.73	0.42
1:A:1193:G:N2	1:A:1194:U:C2	2.88	0.42
1:A:479:C:C5	1:A:480:U:C4	3.08	0.42
4:B:23:ARG:HH12	4:B:191:ASP:HA	1.84	0.42
4:B:55:PHE:O	4:B:56:ARG:C	2.57	0.42
5:C:150:LYS:HB2	5:C:169:ALA:HB1	2.01	0.42
10:H:122:ARG:HG3	10:H:122:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:39:LEU:HA	10:H:39:LEU:HD13	1.80	0.42
11:I:88:TYR:CD2	11:I:89:ASN:N	2.88	0.42
12:J:28:ARG:HH11	12:J:28:ARG:HG2	1.84	0.42
12:J:46:ARG:NH1	12:J:64:GLU:HB3	2.35	0.42
15:M:126:LYS:HB2	15:M:126:LYS:NZ	2.35	0.42
15:M:13:LYS:O	15:M:44:ARG:NE	2.52	0.42
17:O:88:ARG:NE	17:O:88:ARG:HA	2.34	0.42
18:P:67:THR:HG22	18:P:69:THR:H	1.84	0.42
18:P:75:ARG:O	18:P:78:GLY:N	2.50	0.42
21:S:11:VAL:HG22	21:S:39:THR:O	2.19	0.42
1:A:1321:C:O2'	21:S:77:THR:HG21	2.20	0.42
21:S:7:LYS:CG	21:S:7:LYS:O	2.67	0.42
1:A:1137:C:H5'	1:A:1138:G:C6	2.54	0.42
1:A:1153:C:C2	1:A:1154:G:C8	3.07	0.42
1:A:1465:C:O2'	1:A:1466:C:H5'	2.19	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.42
1:A:300:A:H2'	1:A:301:G:O4'	2.19	0.42
1:A:356:A:O2'	1:A:357:G:H5'	2.18	0.42
4:B:144:ARG:HG3	4:B:145:LEU:H	1.84	0.42
4:B:26:PRO:O	4:B:28:PHE:N	2.47	0.42
5:C:178:LEU:O	5:C:179:ARG:HB2	2.19	0.42
9:G:15:ASP:OD2	9:G:44:TYR:OH	2.35	0.42
9:G:50:ILE:HG21	9:G:61:VAL:HG21	2.00	0.42
13:K:95:ILE:HG21	13:K:108:ILE:HD13	2.00	0.42
14:L:55:VAL:CG1	14:L:56:ALA:H	2.29	0.42
15:M:48:LEU:HA	15:M:48:LEU:HD22	1.89	0.42
22:T:36:LEU:HD12	22:T:62:LEU:CD1	2.47	0.42
22:T:71:THR:O	22:T:72:LEU:HD23	2.19	0.42
1:A:129(A):G:O2'	1:A:190(E):U:C6	2.71	0.42
1:A:409:G:C3'	1:A:431:A:N7	2.83	0.42
4:B:134:GLU:C	4:B:136:VAL:N	2.72	0.42
5:C:109:PRO:HA	5:C:115:LEU:HD12	2.02	0.42
5:C:61:ALA:C	5:C:63:ASN:H	2.23	0.42
6:D:170:VAL:O	6:D:171:GLY:C	2.57	0.42
8:F:11:ASN:O	8:F:14:LEU:HG	2.19	0.42
9:G:15:ASP:OD2	9:G:16:LEU:N	2.53	0.42
10:H:104:ARG:HD2	10:H:138:TRP:CD2	2.54	0.42
11:I:90:PRO:O	11:I:93:ARG:HG3	2.19	0.42
14:L:28:LYS:O	14:L:30:ALA:N	2.51	0.42
14:L:24:VAL:HG13	14:L:98:TYR:CE2	2.54	0.42
15:M:119:GLY:O	15:M:120:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:27:CYS:SG	16:N:29:ARG:CB	3.04	0.42
1:A:1018:C:O5'	1:A:1018:C:H6	2.02	0.42
1:A:145:G:O2'	1:A:146:G:H5'	2.20	0.42
1:A:560:U:O2'	1:A:561:U:OP2	2.26	0.42
1:A:723:U:C2'	1:A:723:U:O2	2.67	0.42
1:A:741:G:H5''	17:O:39:LEU:HD12	2.00	0.42
4:B:107:THR:C	4:B:109:SER:H	2.23	0.42
4:B:12:GLU:HA	4:B:12:GLU:OE1	2.19	0.42
4:B:136:VAL:HG12	4:B:140:HIS:CE1	2.55	0.42
4:B:206:ASP:O	4:B:207:ALA:CB	2.66	0.42
4:B:16:HIS:NE2	4:B:214:ILE:CG1	2.83	0.42
4:B:87:ARG:HH11	4:B:234:PRO:HD2	1.84	0.42
5:C:108:ASN:C	5:C:110:ASN:H	2.23	0.42
5:C:114:PRO:HD3	5:C:183:ASP:OD1	2.20	0.42
9:G:17:VAL:HG12	9:G:18:TYR:N	2.35	0.42
10:H:117:GLY:O	10:H:119:LEU:CD2	2.67	0.42
14:L:101:VAL:O	14:L:101:VAL:CG1	2.67	0.42
17:O:87:ILE:HG22	17:O:88:ARG:H	1.84	0.42
19:Q:82:MET:O	19:Q:83:ASP:C	2.58	0.42
1:A:1207:G:O2'	1:A:1208:C:H5'	2.20	0.42
1:A:1256:A:OP1	5:C:26:LYS:HE3	2.20	0.42
1:A:190(C):C:H1'	1:A:190(G):G:N2	2.34	0.42
1:A:707:C:O2'	1:A:708:C:H5'	2.20	0.42
1:A:838:G:H2'	1:A:839:U:C5'	2.39	0.42
1:A:92:C:O2'	1:A:93:G:H5'	2.20	0.42
1:A:930:C:C2'	1:A:931:C:H5'	2.50	0.42
4:B:129:GLU:O	4:B:135:GLN:NE2	2.49	0.42
4:B:223:ILE:C	4:B:225:ALA:N	2.71	0.42
4:B:25:ASN:HD21	4:B:27:LYS:H	1.66	0.42
5:C:120:VAL:O	5:C:124:ILE:HG13	2.20	0.42
5:C:131:ARG:HD3	5:C:166:GLU:OE2	2.20	0.42
5:C:3:ASN:O	5:C:4:LYS:CB	2.67	0.42
12:J:9:ARG:HB2	12:J:9:ARG:HH11	1.84	0.42
9:G:151:TYR:OH	13:K:54:ARG:NE	2.53	0.42
21:S:45:VAL:HA	21:S:62:ILE:CG1	2.50	0.42
1:A:994:A:N7	1:A:1216:G:H4'	2.35	0.42
1:A:1238:A:C2	1:A:1241:G:N3	2.88	0.42
1:A:16:A:H2'	1:A:17:U:H5'	2.01	0.42
1:A:192:U:H1'	22:T:103:GLY:CA	2.50	0.42
1:A:283:C:O2'	1:A:284:G:H5'	2.20	0.42
1:A:428:G:O4'	1:A:430:A:C8	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:U:O2	1:A:791:G:C8	2.72	0.42
4:B:23:ARG:HD3	4:B:23:ARG:H	1.85	0.42
4:B:7:VAL:C	4:B:8:LYS:HG3	2.40	0.42
5:C:101:LEU:CD2	5:C:101:LEU:O	2.68	0.42
6:D:106:TYR:CD2	6:D:106:TYR:C	2.93	0.42
6:D:187:ARG:HD2	6:D:188:LEU:N	2.33	0.42
9:G:18:TYR:HE2	9:G:58:PRO:HG2	1.85	0.42
12:J:89:ASP:CB	12:J:91:PRO:HD2	2.50	0.42
1:A:267:C:P	19:Q:67:LYS:HB2	2.60	0.42
1:A:109:A:H5'	1:A:110:C:H5	1.85	0.41
1:A:1203:C:OP1	16:N:2:ALA:HB3	2.20	0.41
1:A:1220:G:O2'	1:A:1221:G:H5'	2.19	0.41
1:A:1270:C:H4'	1:A:1314:C:H5'	2.02	0.41
1:A:1431:C:H2'	1:A:1432:G:H5'	2.01	0.41
1:A:1521:G:O2'	1:A:1522:U:H5'	2.20	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.55	0.41
1:A:32:A:H2'	1:A:33:A:C8	2.55	0.41
1:A:459:G:C3'	1:A:460:A:H5''	2.50	0.41
1:A:480:U:H5'	1:A:481:G:OP2	2.19	0.41
1:A:603:U:H2'	1:A:604:G:C8	2.55	0.41
1:A:747:C:H2'	1:A:748:C:H1'	2.02	0.41
1:A:974:A:H8	1:A:974:A:OP1	2.03	0.41
1:A:975:A:O2'	1:A:976:G:OP2	2.31	0.41
4:B:118:LEU:O	4:B:122:PHE:N	2.53	0.41
5:C:22:TRP:HB2	5:C:59:ARG:HB2	2.02	0.41
6:D:205:GLU:O	6:D:208:SER:HB2	2.19	0.41
10:H:113:SER:O	10:H:131:GLY:HA3	2.20	0.41
10:H:18:ARG:HE	10:H:18:ARG:HA	1.85	0.41
11:I:53:VAL:CG2	11:I:85:LEU:HD21	2.42	0.41
12:J:28:ARG:C	12:J:29:ARG:HD3	2.40	0.41
17:O:41:GLU:O	17:O:44:LYS:HB3	2.19	0.41
18:P:75:ARG:NH1	18:P:75:ARG:HG3	2.35	0.41
19:Q:33:GLY:O	19:Q:34:LYS:C	2.57	0.41
1:A:1021:G:O2'	1:A:1022:G:H5'	2.21	0.41
1:A:1152:A:O2'	1:A:1153:C:H5'	2.19	0.41
1:A:1176:A:H2'	1:A:1177:G:C8	2.55	0.41
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.56	0.41
1:A:1300:G:O2'	1:A:1301:U:H6	2.03	0.41
1:A:37:U:O2'	1:A:38:G:H5'	2.20	0.41
1:A:562:C:N3	14:L:16:GLU:HG2	2.35	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:112:VAL:HG22	4:B:149:LEU:HD13	2.02	0.41
4:B:67:THR:N	4:B:160:ASP:OD2	2.52	0.41
4:B:237:ALA:C	4:B:239:VAL:H	2.21	0.41
4:B:33:TYR:HB3	4:B:41:ILE:O	2.20	0.41
8:F:99:ALA:O	8:F:100:ASN:HB3	2.20	0.41
8:F:99:ALA:HB2	20:R:31:LEU:HD12	2.01	0.41
12:J:89:ASP:HB2	12:J:91:PRO:CD	2.50	0.41
13:K:48:ILE:HA	13:K:48:ILE:HD13	1.91	0.41
13:K:76:GLY:O	13:K:78:GLN:HG3	2.19	0.41
1:A:981:U:H5'	16:N:21:TYR:CE1	2.55	0.41
19:Q:66:SER:OG	19:Q:69:LYS:CB	2.68	0.41
21:S:13:ASP:O	21:S:16:LEU:N	2.53	0.41
1:A:134:A:H1'	1:A:325:A:C5	2.55	0.41
1:A:190:C:OP1	1:A:190(K):G:N2	2.53	0.41
1:A:6:G:H4'	1:A:298:A:H4'	2.03	0.41
1:A:412:A:C2'	1:A:413:G:H5'	2.51	0.41
1:A:499:A:H4'	1:A:500:G:OP1	2.20	0.41
1:A:600:C:O2'	1:A:601:C:H5'	2.20	0.41
1:A:757:U:O2'	1:A:879:C:H1'	2.21	0.41
4:B:16:HIS:NE2	4:B:214:ILE:HG12	2.36	0.41
4:B:59:GLU:HA	4:B:62:ALA:HB3	2.01	0.41
5:C:12:LEU:HD23	5:C:12:LEU:HA	1.71	0.41
5:C:91:LEU:HD21	5:C:99:VAL:CG2	2.48	0.41
7:E:105:VAL:HB	7:E:106:PRO:HD3	2.01	0.41
7:E:150:ARG:CG	7:E:150:ARG:NH1	2.82	0.41
7:E:150:ARG:HG3	7:E:150:ARG:NH1	2.31	0.41
9:G:78:ARG:O	9:G:84:ASN:HA	2.20	0.41
7:E:143:ARG:NH1	10:H:77:GLU:OE2	2.53	0.41
12:J:27:ALA:HB2	12:J:85:LEU:CD2	2.50	0.41
15:M:19:LEU:CA	15:M:22:ILE:HD13	2.51	0.41
21:S:12:ASP:HB2	21:S:35:SER:OG	2.21	0.41
1:A:1051:C:O2'	1:A:1052:U:H5'	2.20	0.41
1:A:1196:U:H5''	1:A:1197:G:C5'	2.50	0.41
1:A:1372:U:H2'	1:A:1373:G:O4'	2.20	0.41
1:A:1504:G:H3'	1:A:1504:G:OP2	2.20	0.41
1:A:182:U:OP2	1:A:183:G:C8	2.72	0.41
1:A:262:A:C6	1:A:263:A:C6	3.08	0.41
1:A:293:G:C6	1:A:294:U:C4	3.08	0.41
1:A:443:C:H2'	1:A:444:C:H6	1.85	0.41
1:A:501:C:O2'	1:A:502:G:H5'	2.19	0.41
1:A:824:C:H2'	1:A:825:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:U:OP2	14:L:97:ARG:NH2	2.53	0.41
1:A:939:G:H5''	9:G:102:ARG:CZ	2.49	0.41
4:B:239:VAL:HG12	4:B:239:VAL:O	2.20	0.41
4:B:75:LYS:HA	4:B:78:GLN:HB2	2.03	0.41
5:C:155:GLY:CA	5:C:164:ARG:H	2.34	0.41
5:C:173:VAL:HG12	5:C:175:LEU:CD2	2.50	0.41
6:D:198:VAL:CG1	6:D:199:ASN:N	2.83	0.41
7:E:37:ARG:HG3	7:E:112:LEU:HA	2.02	0.41
9:G:115:ARG:CB	9:G:118:VAL:HG23	2.49	0.41
9:G:20:ASP:OD2	9:G:63:LYS:NZ	2.49	0.41
9:G:95:ARG:HG3	9:G:95:ARG:NH1	2.35	0.41
7:E:80:ILE:CG2	10:H:104:ARG:HH22	2.33	0.41
12:J:6:ILE:O	12:J:71:LEU:O	2.38	0.41
17:O:17:ARG:CG	17:O:17:ARG:NH1	2.83	0.41
17:O:88:ARG:NE	17:O:88:ARG:CA	2.83	0.41
17:O:82:ILE:HD13	17:O:88:ARG:CG	2.50	0.41
19:Q:7:THR:O	19:Q:23:VAL:HG22	2.20	0.41
20:R:88:LYS:CG	20:R:88:LYS:OXT	2.64	0.41
22:T:39:LYS:HD3	22:T:55:ILE:HD13	2.01	0.41
22:T:56:MET:HG3	22:T:84:LEU:HD13	2.01	0.41
1:A:1305:G:H2'	1:A:1331:G:H22	1.85	0.41
1:A:102:G:O2'	1:A:151:A:N3	2.43	0.41
1:A:242:C:H2'	1:A:243:A:H5'	2.02	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.55	0.41
1:A:737:A:H2'	1:A:738:C:C6	2.55	0.41
1:A:800:G:O5'	1:A:800:G:H8	2.03	0.41
1:A:900:A:H2'	1:A:901:A:C8	2.54	0.41
1:A:979:C:H2'	1:A:980:C:H5'	2.03	0.41
1:A:977:A:O2'	1:A:979:C:OP2	2.38	0.41
1:A:994:A:N3	1:A:994:A:H2'	2.34	0.41
1:A:996:A:H2	1:A:1045:C:O2'	2.03	0.41
4:B:122:PHE:HA	4:B:127:ILE:HG21	2.03	0.41
4:B:20:GLU:HG3	4:B:191:ASP:HB3	2.03	0.41
4:B:20:GLU:O	4:B:39:ILE:HG23	2.20	0.41
4:B:95:GLN:HG3	4:B:148:TYR:CD2	2.54	0.41
5:C:139:GLN:O	5:C:140:ARG:C	2.59	0.41
7:E:152:ARG:HA	10:H:64:LYS:HZ1	1.84	0.41
11:I:55:ALA:O	11:I:56:LEU:HB3	2.19	0.41
14:L:82:VAL:O	14:L:106:ASP:HB2	2.20	0.41
16:N:59:ALA:O	16:N:60:SER:CB	2.67	0.41
18:P:81:ARG:C	18:P:81:ARG:HE	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:86:GLU:O	19:Q:87:LYS:C	2.59	0.41
20:R:47:THR:HG23	20:R:83:GLU:O	2.20	0.41
1:A:103:C:OP2	22:T:17:ARG:NH1	2.52	0.41
22:T:68:LYS:HA	22:T:68:LYS:HD2	1.86	0.41
1:A:1234:C:C2'	1:A:1235:U:H5'	2.51	0.41
1:A:1286:A:H2'	1:A:1287:A:H4'	2.01	0.41
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.41
1:A:328:C:H1'	1:A:329:A:OP2	2.20	0.41
1:A:47:C:H5''	1:A:365:U:C6	2.56	0.41
1:A:397:A:N3	1:A:397:A:H3'	2.35	0.41
1:A:409:G:H22	1:A:432:A:C2'	2.32	0.41
4:B:168:THR:OG1	4:B:192:SER:HB3	2.19	0.41
5:C:137:ALA:HA	5:C:140:ARG:HE	1.86	0.41
5:C:180:ALA:O	5:C:182:ILE:N	2.53	0.41
5:C:46:GLU:C	5:C:48:TYR:H	2.23	0.41
5:C:67:THR:O	5:C:69:HIS:CD2	2.73	0.41
5:C:55:VAL:HG22	5:C:68:VAL:HG22	2.02	0.41
10:H:34:GLU:OE2	10:H:34:GLU:HA	2.21	0.41
10:H:90:GLY:O	10:H:91:ARG:CB	2.65	0.41
1:A:1150:U:O3'	12:J:41:PRO:HA	2.20	0.41
17:O:76:GLU:CA	17:O:79:ARG:HH21	2.33	0.41
1:A:1350:A:C2	1:A:1351:U:C2	3.09	0.41
1:A:1420:C:H2'	1:A:1421:G:H8	1.86	0.41
1:A:411:A:O2'	1:A:417:C:O2'	2.33	0.41
1:A:421:U:O2'	1:A:422:C:H5'	2.20	0.41
1:A:446:G:C2'	1:A:447:G:H5'	2.51	0.41
1:A:474:G:H5'	1:A:475:G:N7	2.35	0.41
1:A:53:A:N6	1:A:54:C:C4	2.88	0.41
4:B:91:PRO:CG	4:B:155:LEU:HG	2.46	0.41
5:C:95:THR:O	5:C:97:LYS:N	2.53	0.41
7:E:30:ALA:O	7:E:45:PHE:HA	2.21	0.41
7:E:72:GLN:O	7:E:73:ASN:HB3	2.20	0.41
7:E:81:GLU:OE1	7:E:88:LYS:HE2	2.21	0.41
1:A:933:G:OP2	9:G:3:ARG:HB3	2.19	0.41
12:J:62:HIS:HB3	16:N:59:ALA:HB3	2.01	0.41
14:L:110:VAL:O	14:L:122:THR:HG22	2.20	0.41
14:L:89:ARG:NH2	14:L:97:ARG:HD3	2.35	0.41
15:M:49:THR:CG2	15:M:51:ALA:HB3	2.50	0.41
16:N:6:LEU:C	16:N:8:GLU:H	2.22	0.41
20:R:53:ARG:NH1	20:R:60:GLY:N	2.69	0.41
21:S:38:SER:OG	21:S:71:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:A:H5''	9:G:4:ARG:CZ	2.51	0.41
1:A:1144:G:H21	1:A:1146:A:H62	1.68	0.41
1:A:1145:C:O2'	1:A:1146:A:O5'	2.34	0.41
1:A:1368:G:OP2	11:I:112:LYS:CD	2.68	0.41
1:A:1381:U:C2'	1:A:1382:C:H5'	2.50	0.41
1:A:1392:G:O2'	1:A:1393:U:H5'	2.20	0.41
1:A:41:G:H2'	1:A:42:G:H8	1.83	0.41
4:B:102:LEU:HB3	4:B:180:LEU:HD12	2.03	0.41
5:C:136:GLN:O	5:C:139:GLN:N	2.54	0.41
6:D:60:GLU:HG2	6:D:202:LEU:HB2	2.03	0.41
6:D:36:ARG:HG2	6:D:36:ARG:NH1	2.34	0.41
8:F:68:PRO:HB2	8:F:71:ARG:CG	2.50	0.41
9:G:136:LYS:O	9:G:137:LYS:C	2.57	0.41
10:H:82:HIS:O	10:H:83:ILE:CB	2.69	0.41
11:I:117:HIS:O	11:I:118:LYS:HG3	2.21	0.41
11:I:28:VAL:HG23	11:I:28:VAL:O	2.21	0.41
14:L:30:ALA:HA	14:L:31:PRO:HD3	1.88	0.41
1:A:103:C:P	22:T:17:ARG:HH11	2.44	0.41
22:T:23:ARG:HG2	22:T:23:ARG:NH1	2.36	0.41
22:T:49:ALA:CB	22:T:99:LEU:HG	2.47	0.41
1:A:1384:C:H2'	1:A:1385:G:C8	2.56	0.41
1:A:1420:C:H2'	1:A:1421:G:C8	2.56	0.41
1:A:1468:A:H2'	1:A:1469:G:O4'	2.21	0.41
1:A:192:U:H2'	1:A:193:C:O4'	2.21	0.41
1:A:253:U:H2'	1:A:254:G:H8	1.84	0.41
1:A:356:A:H1'	1:A:368:U:O2'	2.21	0.41
1:A:384:G:O2'	1:A:385:C:H5'	2.21	0.41
1:A:460:A:N6	1:A:463:A:C5	2.88	0.41
1:A:477:G:H2'	1:A:478:A:H4'	2.01	0.41
1:A:622:A:C8	1:A:623:C:C5	3.09	0.41
1:A:972:C:H4'	12:J:57:LYS:CD	2.51	0.41
5:C:48:TYR:O	5:C:51:GLY:N	2.52	0.41
5:C:3:ASN:HB2	5:C:4:LYS:H	1.68	0.41
6:D:98:GLU:HG2	6:D:189:PRO:HG3	2.02	0.41
6:D:80:GLU:HA	6:D:80:GLU:OE2	2.21	0.41
1:A:1298:C:C2'	9:G:114:ARG:HH12	2.33	0.41
9:G:155:ARG:O	9:G:156:TRP:CB	2.68	0.41
9:G:43:PHE:O	9:G:46:ALA:HB3	2.21	0.41
9:G:70:LYS:HB3	9:G:96:GLN:HG2	2.02	0.41
10:H:85:ARG:C	10:H:85:ARG:HD3	2.41	0.41
11:I:76:ALA:O	11:I:79:LEU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:70:LEU:HD11	17:O:77:ARG:HB2	2.03	0.41
19:Q:78:GLU:OE2	19:Q:81:ARG:NH1	2.50	0.41
22:T:20:LEU:HD23	22:T:20:LEU:HA	1.93	0.41
22:T:62:LEU:HD23	22:T:62:LEU:HA	1.86	0.41
1:A:1060:C:H5''	12:J:51:ARG:HB3	2.01	0.41
1:A:1358:U:H3'	1:A:1359:C:C6	2.56	0.41
1:A:1386:G:O2'	1:A:1387:G:H5'	2.21	0.41
1:A:308:C:H2'	1:A:309:G:C8	2.55	0.41
1:A:358:U:H2'	1:A:359:U:H6	1.85	0.41
1:A:411:A:C2	1:A:418:C:OP2	2.74	0.41
1:A:579:G:H2'	1:A:580:U:C6	2.55	0.41
1:A:668:G:O2'	17:O:46:HIS:CD2	2.74	0.41
4:B:23:ARG:HH12	4:B:191:ASP:CB	2.33	0.41
6:D:120:LEU:HD23	6:D:120:LEU:HA	1.91	0.41
6:D:98:GLU:OE2	6:D:103:ASN:ND2	2.52	0.41
10:H:64:LYS:HB3	10:H:64:LYS:HE2	1.87	0.41
11:I:108:VAL:HG12	11:I:109:VAL:N	2.35	0.41
1:A:1173:G:O2'	1:A:1174:G:H5'	2.21	0.41
1:A:1212:U:O2'	1:A:1213:A:P	2.78	0.41
1:A:1470:G:O2'	1:A:1471:G:H5'	2.20	0.41
1:A:1511:G:H2'	1:A:1512:U:O4'	2.21	0.41
1:A:162:A:H2'	1:A:163:C:O4'	2.21	0.41
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.21	0.41
1:A:232:G:H1'	1:A:262:A:N1	2.35	0.41
1:A:953:G:H2'	1:A:954:G:O4'	2.20	0.41
4:B:122:PHE:HA	4:B:127:ILE:CG2	2.51	0.41
4:B:178:ARG:NE	4:B:196:LEU:O	2.54	0.41
4:B:209:ARG:NH2	4:B:239:VAL:HG11	2.36	0.41
4:B:75:LYS:C	4:B:77:ALA:N	2.74	0.41
5:C:157:ILE:HG21	5:C:164:ARG:NH2	2.36	0.41
5:C:72:LYS:HD3	5:C:75:VAL:CG2	2.51	0.41
6:D:3:ARG:CD	6:D:3:ARG:N	2.71	0.41
7:E:34:VAL:O	7:E:34:VAL:HG13	2.21	0.41
10:H:104:ARG:O	10:H:105:ARG:C	2.59	0.41
10:H:116:LYS:HD3	10:H:127:LEU:HD12	2.04	0.41
10:H:69:ARG:HG3	10:H:69:ARG:HH11	1.86	0.41
13:K:97:ALA:O	13:K:98:LEU:C	2.59	0.41
17:O:26:GLU:OE1	17:O:77:ARG:HD2	2.20	0.41
22:T:13:LEU:CD1	22:T:13:LEU:C	2.89	0.41
1:A:252:U:H2'	1:A:253:U:C5	2.56	0.40
1:A:363:A:OP1	14:L:33:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:H1'	13:K:115:PRO:HB3	2.03	0.40
1:A:709:G:O2'	1:A:710:G:H5'	2.21	0.40
4:B:122:PHE:CA	4:B:127:ILE:HG21	2.52	0.40
4:B:184:VAL:HG12	4:B:197:VAL:CG1	2.50	0.40
4:B:209:ARG:CZ	4:B:239:VAL:HG11	2.51	0.40
4:B:51:LEU:HD22	4:B:55:PHE:CE1	2.55	0.40
5:C:151:VAL:HA	5:C:199:LYS:O	2.20	0.40
5:C:50:ALA:CB	5:C:70:VAL:HG11	2.51	0.40
6:D:153:ARG:HH11	6:D:153:ARG:HG3	1.85	0.40
8:F:67:MET:CE	8:F:71:ARG:HB2	2.51	0.40
10:H:104:ARG:CZ	10:H:138:TRP:CH2	3.04	0.40
10:H:4:ASP:OD2	10:H:85:ARG:NH1	2.51	0.40
11:I:96:LEU:CD1	11:I:96:LEU:N	2.85	0.40
12:J:18:ALA:O	12:J:21:GLN:HB3	2.21	0.40
12:J:21:GLN:HE21	12:J:25:GLU:CG	2.34	0.40
12:J:71:LEU:HD23	12:J:71:LEU:HA	1.85	0.40
15:M:79:LYS:O	15:M:82:MET:N	2.51	0.40
22:T:53:LEU:O	22:T:54:LYS:C	2.59	0.40
1:A:1036:G:O2'	1:A:1037:C:H5'	2.21	0.40
1:A:1104:G:O2'	1:A:1105:A:H5'	2.21	0.40
1:A:116:A:H2'	1:A:117:G:H8	1.86	0.40
1:A:1225:A:H5'	1:A:1226:C:OP2	2.21	0.40
1:A:1230:C:HO2'	1:A:1231:G:H5'	1.86	0.40
1:A:1394:A:C5	1:A:1501:C:H4'	2.56	0.40
1:A:259:G:O2'	1:A:260:G:H5'	2.20	0.40
1:A:113:G:C1'	1:A:354:G:C5'	2.99	0.40
1:A:363:A:O2'	1:A:364:A:H5'	2.21	0.40
1:A:397:A:H5'	1:A:398:C:P	2.62	0.40
1:A:425:G:H2'	1:A:426:G:O4'	2.21	0.40
1:A:409:G:N1	1:A:433:C:OP1	2.50	0.40
1:A:443:C:H2'	1:A:444:C:C6	2.56	0.40
1:A:448:A:O2'	1:A:449:C:H5'	2.21	0.40
1:A:632:A:C2'	1:A:633:G:H5'	2.51	0.40
1:A:974:A:P	16:N:29:ARG:HH22	2.44	0.40
4:B:187:LEU:HD12	4:B:201:ILE:O	2.21	0.40
5:C:110:ASN:ND2	5:C:140:ARG:HB3	2.37	0.40
5:C:39:ILE:C	5:C:41:GLY:N	2.73	0.40
6:D:208:SER:O	6:D:209:ARG:C	2.60	0.40
7:E:78:HIS:CD2	10:H:107:LEU:HD12	2.44	0.40
11:I:19:LEU:HB3	11:I:59:PHE:CD2	2.56	0.40
12:J:16:LEU:HD23	12:J:94:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:38:ILE:HD12	12:J:71:LEU:HD13	2.03	0.40
14:L:50:SER:O	14:L:51:ALA:CB	2.68	0.40
19:Q:68:ARG:HE	19:Q:68:ARG:HB2	1.65	0.40
1:A:1152:A:H5''	12:J:13:HIS:CB	2.52	0.40
1:A:103:C:O2'	1:A:172:A:N1	2.47	0.40
1:A:273:A:N6	1:A:274:A:C6	2.89	0.40
1:A:485:G:O2'	1:A:486:U:C5	2.74	0.40
1:A:522:C:O2'	1:A:523:A:H5'	2.21	0.40
1:A:836:G:C6	1:A:851:G:C6	3.10	0.40
1:A:925:G:C6	1:A:927:G:N7	2.89	0.40
4:B:16:HIS:CE1	4:B:214:ILE:HG12	2.56	0.40
5:C:133:ALA:O	5:C:134:ILE:C	2.60	0.40
5:C:135:LYS:HA	5:C:135:LYS:HD2	1.87	0.40
5:C:15:THR:O	5:C:16:ARG:CB	2.62	0.40
5:C:73:PRO:O	5:C:74:GLY:C	2.60	0.40
10:H:38:ILE:N	10:H:38:ILE:CD1	2.84	0.40
10:H:86:ILE:HG22	10:H:87:SER:N	2.35	0.40
15:M:66:LEU:O	15:M:67:GLU:C	2.59	0.40
16:N:34:TYR:HD1	16:N:34:TYR:N	2.19	0.40
12:J:61:GLU:OE2	16:N:58:LYS:HE2	2.21	0.40
19:Q:40:LYS:HD3	19:Q:42:TYR:OH	2.21	0.40
1:A:1063:C:H3'	1:A:1064:G:H2'	2.04	0.40
1:A:961:U:O2	1:A:1201:A:N1	2.54	0.40
1:A:1250:A:H5''	11:I:68:GLY:N	2.35	0.40
1:A:1481:U:H2'	1:A:1482:G:O4'	2.21	0.40
1:A:419:C:C5	1:A:424:G:C4	3.10	0.40
1:A:426:G:O2'	1:A:427:U:H5'	2.21	0.40
1:A:435:C:H2'	1:A:435:C:O2	2.21	0.40
1:A:485:G:O2'	1:A:486:U:H5	2.04	0.40
1:A:662:G:O2'	1:A:836:G:H5''	2.22	0.40
1:A:760:G:H1	19:Q:105:ALA:CB	2.34	0.40
4:B:36:ARG:HE	4:B:41:ILE:HD12	1.86	0.40
5:C:58:GLU:O	5:C:59:ARG:CG	2.69	0.40
1:A:620:C:C2	6:D:135:LEU:HD13	2.57	0.40
9:G:79:ARG:HD3	9:G:79:ARG:C	2.41	0.40
11:I:19:LEU:HB3	11:I:59:PHE:HD2	1.86	0.40
12:J:89:ASP:CG	12:J:91:PRO:HD2	2.41	0.40
15:M:56:LEU:O	15:M:56:LEU:HD23	2.22	0.40
20:R:18:ARG:HA	20:R:18:ARG:NE	2.37	0.40
21:S:28:LYS:CG	21:S:29:ARG:N	2.82	0.40
1:A:1226:C:O2'	1:A:1227:A:O5'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:A:O2'	1:A:1281:U:OP2	2.28	0.40
1:A:197:A:N1	1:A:220:G:O2'	2.39	0.40
1:A:382:A:H2'	1:A:383:A:H8	1.84	0.40
1:A:742:G:H2'	1:A:743:U:O4'	2.22	0.40
1:A:828:A:H2'	1:A:829:G:O5'	2.22	0.40
4:B:115:LEU:CG	4:B:116:GLU:N	2.83	0.40
4:B:186:ALA:HB3	4:B:197:VAL:HG11	2.03	0.40
6:D:190:ASP:O	6:D:191:ARG:C	2.59	0.40
1:A:8:A:N6	6:D:209:ARG:HB2	2.36	0.40
7:E:121:LYS:HD2	7:E:122:GLU:N	2.37	0.40
9:G:116:ALA:HA	9:G:119:ARG:NH2	2.36	0.40
9:G:22:LEU:HD12	9:G:101:LEU:HD11	2.02	0.40
10:H:11:THR:O	10:H:12:ARG:C	2.59	0.40
10:H:38:ILE:H	10:H:38:ILE:CD1	2.30	0.40
11:I:45:ALA:O	11:I:46:ALA:C	2.60	0.40
11:I:69:GLY:O	11:I:73:GLN:HG3	2.22	0.40
12:J:15:THR:O	12:J:19:SER:HB3	2.20	0.40
16:N:26:ARG:CZ	16:N:47:LEU:HD21	2.51	0.40
17:O:38:ARG:NH1	17:O:38:ARG:HG3	2.37	0.40
18:P:67:THR:HG22	18:P:69:THR:N	2.36	0.40
19:Q:98:LEU:N	19:Q:98:LEU:HD12	2.37	0.40
19:Q:9:VAL:HG21	19:Q:84:LEU:CD1	2.47	0.40
21:S:33:THR:CG2	21:S:34:TRP:H	2.30	0.40
23:V:6:ARG:HG3	23:V:7:ARG:H	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:79:ARG:NE	12:J:79:ARG:NE[8_665]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	232/256 (91%)	154 (66%)	52 (22%)	26 (11%)	0	2
5	C	204/239 (85%)	132 (65%)	48 (24%)	24 (12%)	0	1
6	D	206/209 (99%)	160 (78%)	37 (18%)	9 (4%)	2	12
7	E	148/162 (91%)	125 (84%)	17 (12%)	6 (4%)	3	14
8	F	99/101 (98%)	75 (76%)	19 (19%)	5 (5%)	2	10
9	G	153/156 (98%)	120 (78%)	27 (18%)	6 (4%)	3	15
10	H	136/138 (99%)	113 (83%)	18 (13%)	5 (4%)	3	16
11	I	125/128 (98%)	88 (70%)	23 (18%)	14 (11%)	0	2
12	J	96/105 (91%)	61 (64%)	23 (24%)	12 (12%)	0	1
13	K	117/129 (91%)	90 (77%)	22 (19%)	5 (4%)	2	13
14	L	122/135 (90%)	92 (75%)	18 (15%)	12 (10%)	0	2
15	M	123/126 (98%)	88 (72%)	21 (17%)	14 (11%)	0	1
16	N	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2	10
17	O	86/89 (97%)	70 (81%)	11 (13%)	5 (6%)	1	8
18	P	81/88 (92%)	61 (75%)	16 (20%)	4 (5%)	2	11
19	Q	102/105 (97%)	80 (78%)	15 (15%)	7 (7%)	1	5
20	R	71/88 (81%)	53 (75%)	13 (18%)	5 (7%)	1	5
21	S	78/93 (84%)	50 (64%)	22 (28%)	6 (8%)	1	4
22	T	97/106 (92%)	71 (73%)	17 (18%)	9 (9%)	0	3
23	V	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	12
All	All	2356/2541 (93%)	1737 (74%)	441 (19%)	178 (8%)	1	4

All (178) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	20	GLU
4	B	21	ARG
4	B	24	TRP
4	B	77	ALA
4	B	88	ALA
4	B	95	GLN
4	B	211	ILE
4	B	229	VAL

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Mol	Chain	Res	Type
5	C	15	THR
5	C	16	ARG
5	C	47	LEU
5	C	55	VAL
5	C	61	ALA
5	C	96	GLY
5	C	100	ALA
5	C	101	LEU
5	C	179	ARG
6	D	36	ARG
8	F	34	GLY
8	F	72	VAL
9	G	7	ALA
9	G	147	ALA
10	H	83	ILE
10	H	91	ARG
11	I	38	GLN
11	I	41	VAL
11	I	127	LYS
12	J	27	ALA
12	J	61	GLU
12	J	72	VAL
13	K	127	LYS
14	L	27	LEU
14	L	28	LYS
14	L	30	ALA
14	L	41	ARG
14	L	47	LYS
14	L	48	PRO
14	L	80	HIS
15	M	7	VAL
15	M	27	LYS
15	M	67	GLU
15	M	86	CYS
15	M	122	LYS
18	P	47	ASP
18	P	81	ARG
19	Q	69	LYS
19	Q	81	ARG
19	Q	99	SER
20	R	21	LYS
21	S	25	LYS

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Mol	Chain	Res	Type
4	B	9	GLU
4	B	17	PHE
4	B	18	GLY
4	B	27	LYS
4	B	60	ASP
4	B	115	LEU
4	B	224	GLN
5	C	91	LEU
5	C	98	ASN
5	C	108	ASN
5	C	154	SER
6	D	25	ARG
7	E	140	ARG
7	E	153	LYS
9	G	17	VAL
10	H	134	ILE
11	I	39	GLY
11	I	55	ALA
11	I	88	TYR
11	I	121	ARG
12	J	34	VAL
12	J	57	LYS
13	K	12	ARG
13	K	126	ARG
14	L	91	LYS
14	L	102	ARG
15	M	12	ASN
15	M	28	ALA
15	M	63	THR
15	M	68	GLY
15	M	100	GLY
15	M	106	ASN
15	M	120	LYS
16	N	15	LYS
16	N	60	SER
18	P	10	GLY
18	P	82	GLN
19	Q	49	GLU
19	Q	80	GLY
20	R	20	ALA
21	S	27	GLU
21	S	47	HIS

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Mol	Chain	Res	Type
22	T	50	GLU
22	T	73	HIS
22	T	74	LYS
22	T	96	GLY
22	T	102	GLY
4	B	15	VAL
4	B	76	GLN
4	B	134	GLU
4	B	155	LEU
5	C	26	LYS
5	C	127	ARG
5	C	189	ALA
6	D	164	ALA
7	E	16	THR
7	E	71	LEU
8	F	64	GLN
9	G	52	GLU
9	G	155	ARG
10	H	81	HIS
11	I	31	GLN
11	I	43	ALA
11	I	46	ALA
11	I	56	LEU
11	I	119	ALA
12	J	73	ASP
12	J	86	MET
12	J	90	LEU
13	K	75	TYR
16	N	17	LYS
17	O	88	ARG
22	T	86	ARG
22	T	98	PRO
4	B	22	LYS
4	B	119	GLU
4	B	154	LEU
5	C	60	ALA
5	C	62	ASP
6	D	4	TYR
12	J	35	SER
13	K	70	LYS
14	L	51	ALA
14	L	105	TYR

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Mol	Chain	Res	Type
17	O	73	GLU
17	O	86	GLY
19	Q	98	LEU
20	R	19	LYS
22	T	9	ASN
22	T	97	ALA
23	V	3	LYS
4	B	227	GLY
5	C	51	GLY
5	C	146	ALA
5	C	168	ALA
6	D	156	GLU
7	E	107	ARG
8	F	17	SER
10	H	24	THR
12	J	40	LEU
20	R	87	ARG
21	S	28	LYS
4	B	202	PRO
5	C	134	ILE
5	C	205	GLY
6	D	5	ILE
6	D	171	GLY
7	E	128	PRO
8	F	97	PHE
11	I	101	PHE
12	J	41	PRO
15	M	85	GLY
17	O	46	HIS
5	C	84	ILE
15	M	4	ILE
4	B	131	PRO
11	I	44	VAL
21	S	31	ILE
6	D	88	VAL
12	J	76	ASN
20	R	60	GLY
6	D	39	PRO
9	G	42	ILE
14	L	121	GLY
17	O	82	ILE
19	Q	102	GLY

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Mol	Chain	Res	Type
21	S	45	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	202/220 (92%)	178 (88%)	24 (12%)	5	18
5	C	160/188 (85%)	144 (90%)	16 (10%)	7	25
6	D	180/181 (99%)	166 (92%)	14 (8%)	12	37
7	E	115/123 (94%)	99 (86%)	16 (14%)	3	13
8	F	90/90 (100%)	88 (98%)	2 (2%)	52	76
9	G	126/127 (99%)	121 (96%)	5 (4%)	31	62
10	H	119/119 (100%)	109 (92%)	10 (8%)	11	34
11	I	98/99 (99%)	82 (84%)	16 (16%)	2	9
12	J	87/92 (95%)	78 (90%)	9 (10%)	7	24
13	K	90/99 (91%)	85 (94%)	5 (6%)	21	49
14	L	104/111 (94%)	98 (94%)	6 (6%)	20	48
15	M	100/101 (99%)	89 (89%)	11 (11%)	6	22
16	N	49/50 (98%)	44 (90%)	5 (10%)	7	24
17	O	79/80 (99%)	72 (91%)	7 (9%)	9	31
18	P	72/74 (97%)	68 (94%)	4 (6%)	21	49
19	Q	96/97 (99%)	88 (92%)	8 (8%)	11	35
20	R	64/77 (83%)	60 (94%)	4 (6%)	18	45
21	S	71/80 (89%)	67 (94%)	4 (6%)	21	49
22	T	75/82 (92%)	68 (91%)	7 (9%)	9	29
23	V	19/22 (86%)	18 (95%)	1 (5%)	22	51
All	All	1996/2112 (94%)	1822 (91%)	174 (9%)	10	33

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	9	GLU
4	B	17	PHE
4	B	21	ARG
4	B	23	ARG
4	B	24	TRP
4	B	25	ASN
4	B	33	TYR
4	B	76	GLN
4	B	98	LEU
4	B	114	ARG
4	B	117	GLU
4	B	129	GLU
4	B	144	ARG
4	B	162	ILE
4	B	170	GLU
4	B	178	ARG
4	B	184	VAL
4	B	191	ASP
4	B	195	ASP
4	B	215	LEU
4	B	221	LEU
4	B	231	GLU
4	B	236	TYR
5	C	3	ASN
5	C	21	ARG
5	C	38	ARG
5	C	52	LEU
5	C	70	VAL
5	C	72	LYS
5	C	82	GLU
5	C	93	LYS
5	C	102	ASN
5	C	107	GLN
5	C	139	GLN
5	C	156	ARG
5	C	167	TRP
5	C	188	LEU
5	C	196	LEU
5	C	204	LEU
6	D	3	ARG
6	D	9	CYS
6	D	15	GLU

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Mol	Chain	Res	Type
6	D	58	LEU
6	D	85	LYS
6	D	105	VAL
6	D	106	TYR
6	D	122	ARG
6	D	156	GLU
6	D	170	VAL
6	D	177	ASP
6	D	199	ASN
6	D	200	GLU
6	D	201	GLN
7	E	12	LEU
7	E	15	ARG
7	E	16	THR
7	E	24	ARG
7	E	31	LEU
7	E	41	VAL
7	E	43	LEU
7	E	80	ILE
7	E	89	ILE
7	E	116	THR
7	E	120	THR
7	E	126	ARG
7	E	144	THR
7	E	147	ASP
7	E	150	ARG
7	E	151	LEU
8	F	10	LEU
8	F	82	ARG
9	G	8	GLU
9	G	79	ARG
9	G	126	ASP
9	G	140	ASP
9	G	155	ARG
10	H	18	ARG
10	H	26	VAL
10	H	39	LEU
10	H	52	ASP
10	H	83	ILE
10	H	85	ARG
10	H	91	ARG
10	H	92	ARG

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Mol	Chain	Res	Type
10	H	119	LEU
10	H	133	LEU
11	I	2	GLU
11	I	5	TYR
11	I	10	ARG
11	I	12	GLU
11	I	16	ARG
11	I	23	ASN
11	I	38	GLN
11	I	42	ARG
11	I	47	LEU
11	I	78	LYS
11	I	79	LEU
11	I	92	TYR
11	I	104	ARG
11	I	111	ARG
11	I	121	ARG
11	I	127	LYS
12	J	12	ASP
12	J	29	ARG
12	J	33	GLN
12	J	45	ARG
12	J	57	LYS
12	J	60	ARG
12	J	73	ASP
12	J	83	GLU
12	J	86	MET
13	K	29	ILE
13	K	51	LYS
13	K	84	VAL
13	K	96	ARG
13	K	127	LYS
14	L	33	ARG
14	L	48	PRO
14	L	54	LYS
14	L	83	VAL
14	L	93	LEU
14	L	126	LYS
15	M	12	ASN
15	M	40	ASN
15	M	48	LEU
15	M	70	LEU

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Mol	Chain	Res	Type
15	M	88	ARG
15	M	102	ARG
15	M	105	THR
15	M	110	ARG
15	M	115	LYS
15	M	125	ARG
15	M	126	LYS
16	N	8	GLU
16	N	12	ARG
16	N	34	TYR
16	N	41	ARG
16	N	44	LEU
17	O	4	THR
17	O	7	GLU
17	O	9	GLN
17	O	31	LEU
17	O	34	LEU
17	O	70	LEU
17	O	81	LEU
18	P	2	VAL
18	P	53	VAL
18	P	80	PHE
18	P	82	GLN
19	Q	38	ARG
19	Q	48	GLU
19	Q	60	ILE
19	Q	68	ARG
19	Q	74	LEU
19	Q	78	GLU
19	Q	99	SER
19	Q	100	LYS
20	R	36	ASN
20	R	42	ARG
20	R	54	ARG
20	R	80	PRO
21	S	6	LYS
21	S	61	TYR
21	S	77	THR
21	S	81	ARG
22	T	9	ASN
22	T	13	LEU
22	T	42	GLN

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Mol	Chain	Res	Type
22	T	45	GLN
22	T	57	ARG
22	T	75	ASN
22	T	84	LEU
23	V	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	25	ASN
4	B	40	HIS
4	B	94	ASN
4	B	140	HIS
4	B	212	GLN
4	B	240	GLN
5	C	3	ASN
5	C	6	HIS
5	C	31	HIS
5	C	37	GLN
5	C	102	ASN
5	C	107	GLN
5	C	110	ASN
5	C	123	GLN
5	C	139	GLN
5	C	170	GLN
5	C	176	HIS
5	C	181	ASN
6	D	42	GLN
6	D	45	GLN
6	D	62	GLN
6	D	74	GLN
6	D	119	GLN
6	D	123	HIS
6	D	161	ASN
6	D	199	ASN
7	E	73	ASN
7	E	78	HIS
8	F	18	GLN
8	F	27	GLN
8	F	32	ASN
8	F	100	ASN
9	G	28	ASN

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Mol	Chain	Res	Type
9	G	37	ASN
9	G	86	GLN
9	G	96	GLN
9	G	106	GLN
9	G	122	HIS
11	I	23	ASN
11	I	73	GLN
12	J	21	GLN
12	J	33	GLN
12	J	84	GLN
13	K	13	GLN
13	K	38	ASN
13	K	117	ASN
14	L	49	ASN
14	L	75	HIS
15	M	40	ASN
15	M	62	ASN
15	M	77	ASN
17	O	13	GLN
17	O	37	ASN
18	P	82	GLN
20	R	36	ASN
21	S	14	HIS
21	S	23	ASN
21	S	56	GLN
21	S	65	ASN
22	T	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	226 (15%)	73 (4%)
2	X	10/11 (90%)	0	0
3	W	3/4 (75%)	0	0
All	All	1519/1537 (98%)	226 (14%)	73 (4%)

All (226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A

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Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	189	G
1	A	190	C
1	A	190(A)	C
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C

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Mol	Chain	Res	Type
1	A	350	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	407	G
1	A	408	A
1	A	409	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	416	G
1	A	417	C
1	A	418	C
1	A	422	C
1	A	423	G
1	A	425	G
1	A	429	U
1	A	430	A
1	A	434	U
1	A	435	C
1	A	439	A
1	A	448	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	474	G
1	A	475	G
1	A	476	G
1	A	478	A
1	A	480	U
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U

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Mol	Chain	Res	Type
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	588	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	748	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	812	C
1	A	813	U
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C

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Mol	Chain	Res	Type
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	945	G
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1002	G
1	A	1005	A
1	A	1026	G
1	A	1029	C
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1125	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G

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Mol	Chain	Res	Type
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1152	A
1	A	1159	U
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1257	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1319	A
1	A	1320	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1361	G
1	A	1362	C
1	A	1363	A
1	A	1398	A
1	A	1443	G
1	A	1446	A
1	A	1447	G

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Mol	Chain	Res	Type
1	A	1452	C
1	A	1492	A
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
1	A	1539	C

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	188	C
1	A	190	C
1	A	203	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	328	C
1	A	344	A
1	A	350	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	407	G
1	A	428	G

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Mol	Chain	Res	Type
1	A	429	U
1	A	434	U
1	A	463	A
1	A	484	G
1	A	496	A
1	A	518	C
1	A	532	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	945	G
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1182	G
1	A	1183	A
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1224	G
1	A	1226	C
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1319	A
1	A	1346	A
1	A	1347	G
1	A	1397	C

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Mol	Chain	Res	Type
1	A	1451	A
1	A	1498	U
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 109 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	$\# Z  > 2$
24	PAR	A	1545	-	45,45,45	1.55	8 (17%)	64,67,67	1.18	7 (10%)

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
24	PAR	A	1545	-	-	4/18/94/94	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C64-C54	4.76	1.58	1.52
24	A	1545	PAR	O54-C14	3.63	1.51	1.41
24	A	1545	PAR	C11-C21	2.67	1.57	1.52
24	A	1545	PAR	O51-C11	2.61	1.48	1.41
24	A	1545	PAR	C31-C21	2.54	1.56	1.53
24	A	1545	PAR	C52-C42	2.32	1.57	1.52
24	A	1545	PAR	O33-C14	2.09	1.47	1.41
24	A	1545	PAR	C44-C34	2.03	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O54-C54-C64	3.52	112.56	106.01
24	A	1545	PAR	O33-C14-C24	3.37	114.02	108.22
24	A	1545	PAR	C14-O54-C54	2.93	119.44	113.69
24	A	1545	PAR	O52-C13-C23	2.91	113.99	107.96
24	A	1545	PAR	O52-C13-O43	-2.27	108.97	111.43
24	A	1545	PAR	C11-O51-C51	2.09	117.80	113.69
24	A	1545	PAR	O11-C11-C21	2.05	111.74	108.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	C44-C54-C64-N64
24	A	1545	PAR	O54-C54-C64-N64
24	A	1545	PAR	C52-C42-O11-C11
24	A	1545	PAR	C23-C33-O33-C14

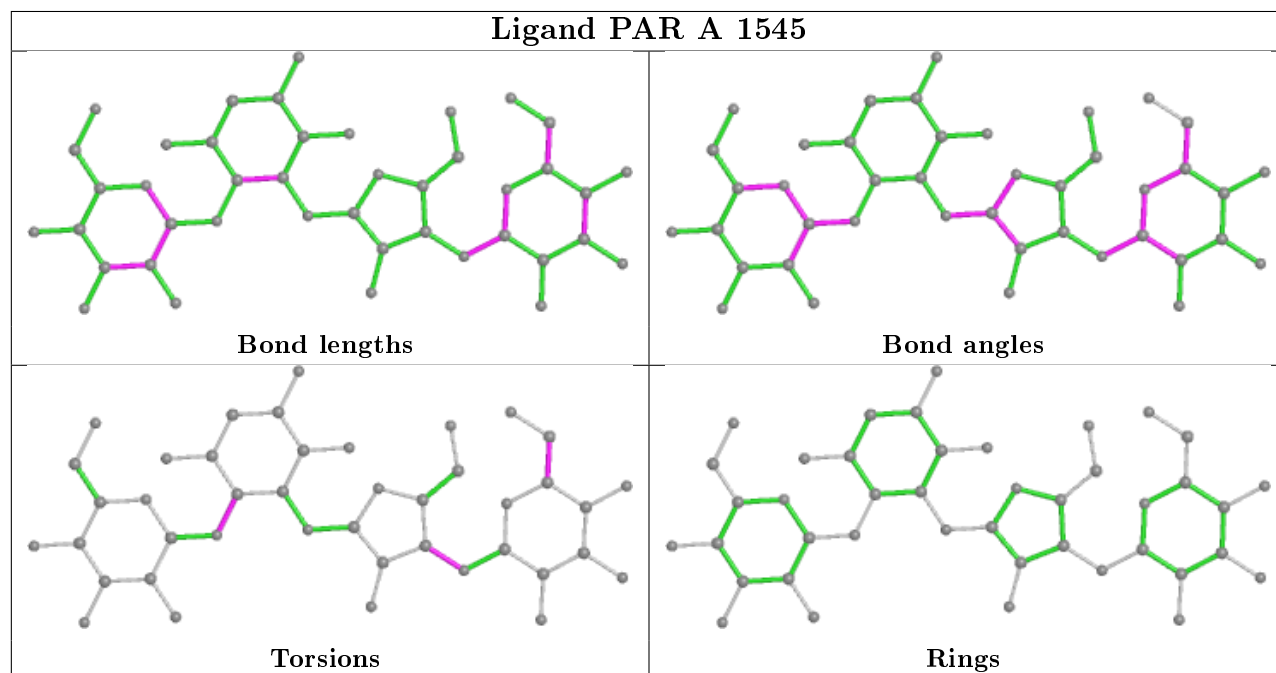
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1507/1522 (99%)	0.97	74 (4%) 29 13	31, 65, 156, 200	0
2	X	10/11 (90%)	0.22	0 100 100	79, 120, 147, 149	0
3	W	4/4 (100%)	0.73	0 100 100	63, 68, 79, 134	0
4	B	234/256 (91%)	0.29	6 (2%) 56 30	45, 102, 162, 200	0
5	C	206/239 (86%)	0.32	3 (1%) 73 51	44, 92, 150, 185	0
6	D	208/209 (99%)	0.49	11 (5%) 26 11	40, 73, 128, 164	0
7	E	150/162 (92%)	0.30	1 (0%) 87 72	35, 59, 110, 151	0
8	F	101/101 (100%)	0.10	0 100 100	54, 95, 138, 162	0
9	G	155/156 (99%)	0.21	4 (2%) 56 30	46, 80, 138, 172	0
10	H	138/138 (100%)	0.36	3 (2%) 62 38	32, 57, 101, 130	0
11	I	127/128 (99%)	0.69	8 (6%) 20 8	45, 93, 141, 168	0
12	J	98/105 (93%)	0.78	7 (7%) 16 6	49, 116, 172, 189	0
13	K	119/129 (92%)	0.54	3 (2%) 57 32	38, 67, 123, 173	0
14	L	124/135 (91%)	0.52	4 (3%) 47 24	30, 69, 120, 189	0
15	M	125/126 (99%)	0.84	14 (11%) 5 1	51, 85, 149, 181	0
16	N	60/61 (98%)	0.94	11 (18%) 1 0	53, 81, 126, 188	0
17	O	88/89 (98%)	0.34	1 (1%) 80 60	39, 72, 131, 191	0
18	P	83/88 (94%)	0.54	2 (2%) 59 34	37, 54, 89, 146	0
19	Q	104/105 (99%)	0.91	6 (5%) 23 9	33, 57, 124, 200	0
20	R	73/88 (82%)	0.37	3 (4%) 37 18	48, 79, 153, 193	0
21	S	80/93 (86%)	0.82	9 (11%) 5 1	65, 110, 155, 178	0
22	T	99/106 (93%)	0.41	1 (1%) 82 63	35, 61, 118, 160	0
23	V	24/27 (88%)	0.84	3 (12%) 3 1	45, 70, 135, 147	0
All	All	3917/4078 (96%)	0.67	174 (4%) 34 16	30, 73, 150, 200	0



All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Q	103	GLY	18.3
19	Q	102	GLY	13.3
15	M	126	LYS	13.1
15	M	124	PRO	12.7
19	Q	105	ALA	11.7
13	K	129	SER	10.6
1	A	423	G	9.4
1	A	407	G	9.0
15	M	123	ALA	9.0
1	A	190	C	8.7
1	A	1534	A	8.6
11	I	128	ARG	8.5
21	S	3	ARG	8.3
1	A	1129	C	8.3
15	M	125	ARG	8.2
1	A	422	C	8.0
1	A	1533	C	7.7
1	A	1540	U	7.5
15	M	120	LYS	7.2
19	Q	104	LYS	7.0
21	S	2	PRO	5.6
1	A	432	A	5.6
12	J	10	GLY	5.5
1	A	1539	C	5.5
19	Q	101	ARG	5.5
1	A	412	A	5.4
16	N	30	ALA	5.2
16	N	3	ARG	5.2
23	V	6	ARG	5.1
1	A	1446	A	4.9
15	M	121	LYS	4.8
10	H	1	MET	4.7
1	A	421	U	4.7
1	A	413	G	4.7
1	A	417	C	4.6
1	A	1031	G	4.5
21	S	37	ARG	4.4
1	A	416	G	4.4
1	A	993	G	4.4
21	S	54	GLY	4.3
14	L	28	LYS	4.3
20	R	16	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
11	I	105	ASP	4.1
6	D	3	ARG	4.0
16	N	2	ALA	4.0
20	R	17	SER	4.0
1	A	1006	C	4.0
1	A	478	A	4.0
6	D	21	LEU	3.9
16	N	6	LEU	3.9
1	A	424	G	3.9
9	G	5	ARG	3.9
6	D	209	ARG	3.8
16	N	29	ARG	3.7
1	A	1035	A	3.7
1	A	202	U	3.6
18	P	41	PRO	3.5
6	D	23	GLY	3.5
9	G	2	ALA	3.4
13	K	128	ALA	3.4
1	A	1004	A	3.4
1	A	1017	G	3.4
1	A	373	A	3.3
15	M	102	ARG	3.3
23	V	2	GLY	3.3
4	B	230	VAL	3.3
15	M	106	ASN	3.2
1	A	1030	C	3.2
1	A	1220	G	3.2
1	A	1361	G	3.2
12	J	43	ARG	3.1
1	A	1443	G	3.1
4	B	16	HIS	3.1
12	J	54	PHE	3.1
1	A	1038	C	3.1
6	D	22	LYS	3.0
1	A	189	G	3.0
1	A	1442	G	3.0
11	I	65	VAL	3.0
1	A	1259	C	2.9
7	E	17	ALA	2.9
1	A	414	A	2.9
5	C	2	GLY	2.9
1	A	1200	C	2.9

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Mol	Chain	Res	Type	RSRZ
15	M	122	LYS	2.8
1	A	1124	G	2.8
12	J	9	ARG	2.8
11	I	102	LEU	2.8
1	A	984	C	2.8
12	J	57	LYS	2.8
15	M	27	LYS	2.8
1	A	1002	G	2.7
6	D	2	GLY	2.7
15	M	88	ARG	2.7
4	B	238	LEU	2.7
1	A	462	G	2.7
11	I	7	THR	2.7
1	A	1026	G	2.7
6	D	42	GLN	2.7
10	H	2	LEU	2.7
1	A	1003	G	2.7
12	J	52	GLY	2.7
6	D	9	CYS	2.6
19	Q	98	LEU	2.6
1	A	1300	G	2.5
22	T	68	LYS	2.5
14	L	89	ARG	2.5
14	L	115	LYS	2.5
15	M	7	VAL	2.5
1	A	1053	G	2.5
4	B	222	ILE	2.5
4	B	148	TYR	2.5
9	G	156	TRP	2.5
15	M	104	ARG	2.5
18	P	13	HIS	2.4
21	S	34	TRP	2.4
1	A	1001	A	2.4
1	A	975	A	2.4
1	A	408	A	2.4
1	A	1221	G	2.4
12	J	7	LYS	2.4
6	D	158	ILE	2.3
21	S	52	TYR	2.3
1	A	433	C	2.3
1	A	415	A	2.3
1	A	1362	C	2.3

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Mol	Chain	Res	Type	RSRZ
16	N	18	VAL	2.3
11	I	19	LEU	2.3
16	N	21	TYR	2.3
20	R	76	LEU	2.3
21	S	71	LEU	2.2
1	A	1048	G	2.2
1	A	463	A	2.2
1	A	1224	G	2.2
1	A	1521	G	2.2
16	N	60	SER	2.2
11	I	15	ALA	2.2
14	L	60	LEU	2.2
17	O	89	GLY	2.2
1	A	379	C	2.2
1	A	1036	G	2.2
5	C	76	VAL	2.2
6	D	5	ILE	2.2
1	A	108	G	2.2
1	A	991	U	2.2
1	A	1279	A	2.2
4	B	108	ILE	2.2
5	C	161	GLU	2.2
1	A	1018	C	2.1
6	D	33	MET	2.1
1	A	1025	U	2.1
16	N	61	TRP	2.1
1	A	482	A	2.1
1	A	1304	G	2.1
16	N	39	LEU	2.1
21	S	4	SER	2.1
15	M	103	THR	2.1
21	S	51	VAL	2.1
1	A	530	G	2.1
1	A	1039	C	2.1
1	A	1127	G	2.1
9	G	33	ASP	2.1
1	A	532	A	2.1
1	A	547	A	2.1
1	A	548	G	2.1
1	A	961	U	2.1
16	N	32	SER	2.0
10	H	3	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	581	G	2.0
1	A	1505	G	2.0
11	I	119	ALA	2.0
23	V	24	ARG	2.0
1	A	1027	C	2.0
13	K	54	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	MG	X	502	1/1	0.19	1.74	67,67,67,67	1
25	MG	A	1607	1/1	0.33	0.34	67,67,67,67	1
25	MG	A	1575	1/1	0.38	0.54	67,67,67,67	1
25	MG	A	1594	1/1	0.58	1.02	67,67,67,67	1
25	MG	A	1630	1/1	0.66	0.33	67,67,67,67	0
25	MG	A	1621	1/1	0.67	0.32	67,67,67,67	0
25	MG	A	1565	1/1	0.69	0.32	67,67,67,67	0
25	MG	A	1598	1/1	0.72	0.16	67,67,67,67	0
25	MG	A	467	1/1	0.72	0.79	67,67,67,67	0
25	MG	A	1573	1/1	0.72	0.37	67,67,67,67	0
25	MG	A	1562	1/1	0.73	0.26	67,67,67,67	0
25	MG	A	441	1/1	0.74	0.26	67,67,67,67	0
25	MG	A	470	1/1	0.74	0.26	67,67,67,67	0
25	MG	A	1568	1/1	0.76	0.31	67,67,67,67	0
25	MG	A	1586	1/1	0.76	0.33	67,67,67,67	0
25	MG	A	1613	1/1	0.76	0.31	67,67,67,67	0
25	MG	A	1592	1/1	0.77	0.38	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	214	1/1	0.78	0.16	67,67,67,67	0
25	MG	A	1571	1/1	0.79	0.31	67,67,67,67	0
25	MG	A	1585	1/1	0.80	0.30	67,67,67,67	0
25	MG	A	1601	1/1	0.80	0.14	67,67,67,67	0
25	MG	J	449	1/1	0.80	0.30	67,67,67,67	0
25	MG	A	466	1/1	0.80	0.23	67,67,67,67	0
25	MG	A	210	1/1	0.80	0.15	67,67,67,67	0
25	MG	A	1627	1/1	0.81	0.28	67,67,67,67	0
25	MG	A	1633	1/1	0.81	0.19	67,67,67,67	0
25	MG	A	1628	1/1	0.82	0.28	67,67,67,67	0
25	MG	A	1603	1/1	0.83	0.24	67,67,67,67	0
25	MG	A	1634	1/1	0.83	0.33	67,67,67,67	0
25	MG	A	211	1/1	0.84	0.33	67,67,67,67	0
25	MG	A	1619	1/1	0.84	0.17	67,67,67,67	0
25	MG	A	1616	1/1	0.84	0.27	67,67,67,67	0
25	MG	A	1597	1/1	0.84	0.11	67,67,67,67	0
25	MG	A	87	1/1	0.85	0.34	67,67,67,67	0
25	MG	A	1583	1/1	0.85	0.34	67,67,67,67	0
25	MG	A	1610	1/1	0.85	0.54	67,67,67,67	1
25	MG	A	493	1/1	0.85	0.30	67,67,67,67	1
25	MG	A	1632	1/1	0.86	0.28	67,67,67,67	0
25	MG	A	1626	1/1	0.86	0.12	67,67,67,67	0
25	MG	A	1620	1/1	0.86	0.19	67,67,67,67	0
25	MG	A	86	1/1	0.86	0.32	67,67,67,67	0
25	MG	A	1590	1/1	0.87	0.35	67,67,67,67	0
25	MG	A	1574	1/1	0.87	0.39	67,67,67,67	0
25	MG	A	1608	1/1	0.88	0.29	67,67,67,67	0
25	MG	A	1577	1/1	0.88	0.31	67,67,67,67	0
25	MG	A	1576	1/1	0.88	0.43	67,67,67,67	0
25	MG	A	1548	1/1	0.88	0.25	67,67,67,67	0
25	MG	A	1602	1/1	0.88	0.23	67,67,67,67	0
25	MG	A	471	1/1	0.88	0.23	67,67,67,67	0
25	MG	A	1559	1/1	0.89	0.55	67,67,67,67	0
25	MG	A	1604	1/1	0.89	0.37	67,67,67,67	0
25	MG	A	1605	1/1	0.89	0.27	67,67,67,67	0
25	MG	A	1622	1/1	0.89	0.38	67,67,67,67	0
25	MG	A	1558	1/1	0.89	0.33	67,67,67,67	0
25	MG	A	1617	1/1	0.89	0.25	67,67,67,67	0
25	MG	A	1611	1/1	0.89	0.24	67,67,67,67	0
25	MG	A	1624	1/1	0.89	0.35	67,67,67,67	0
25	MG	A	1566	1/1	0.90	0.41	67,67,67,67	0
25	MG	A	1587	1/1	0.90	0.42	67,67,67,67	0

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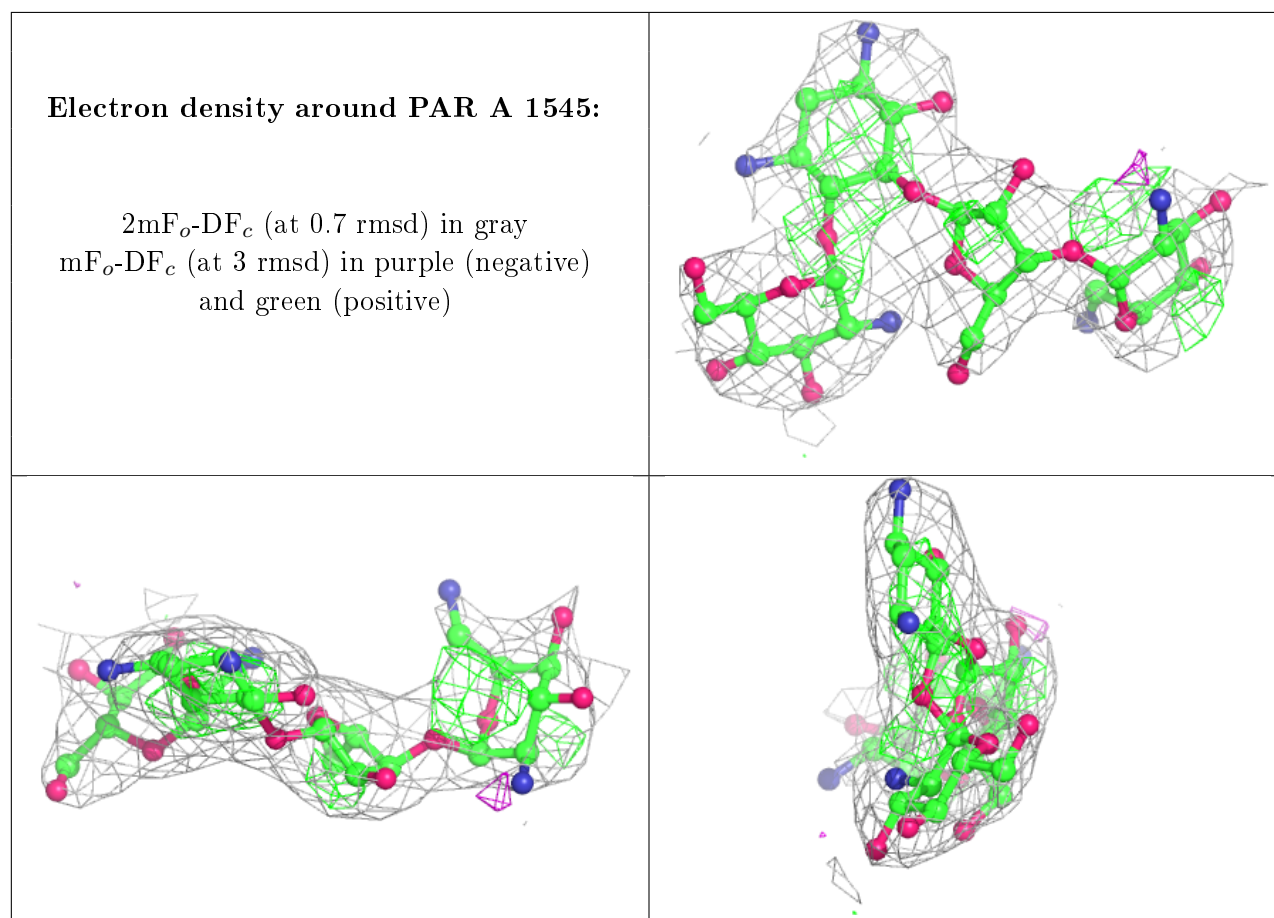
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1600	1/1	0.90	0.23	67,67,67,67	0
25	MG	X	500	1/1	0.90	0.86	67,67,67,67	1
25	MG	A	1581	1/1	0.90	0.47	67,67,67,67	0
25	MG	A	1615	1/1	0.90	0.25	67,67,67,67	0
25	MG	A	1547	1/1	0.90	0.40	67,67,67,67	0
25	MG	A	1570	1/1	0.91	0.40	67,67,67,67	0
25	MG	A	1623	1/1	0.91	0.17	67,67,67,67	0
25	MG	A	1572	1/1	0.91	0.24	67,67,67,67	0
25	MG	A	1561	1/1	0.91	0.21	67,67,67,67	0
25	MG	A	1606	1/1	0.91	0.35	67,67,67,67	0
25	MG	A	1629	1/1	0.91	0.33	67,67,67,67	0
25	MG	A	1555	1/1	0.91	0.41	67,67,67,67	0
25	MG	A	1567	1/1	0.92	0.42	67,67,67,67	0
25	MG	A	1595	1/1	0.92	0.14	67,67,67,67	0
25	MG	A	1596	1/1	0.92	0.29	67,67,67,67	0
25	MG	A	1582	1/1	0.92	0.27	67,67,67,67	0
24	PAR	A	1545	42/42	0.92	0.34	67,67,67,67	0
25	MG	A	1578	1/1	0.93	0.29	67,67,67,67	0
25	MG	A	1584	1/1	0.93	0.34	67,67,67,67	0
25	MG	A	1564	1/1	0.93	0.48	67,67,67,67	0
25	MG	A	1609	1/1	0.93	0.30	67,67,67,67	0
25	MG	A	71	1/1	0.93	0.39	67,67,67,67	0
25	MG	A	1614	1/1	0.94	0.16	67,67,67,67	0
25	MG	A	1550	1/1	0.94	0.35	67,67,67,67	0
25	MG	A	1549	1/1	0.94	0.48	67,67,67,67	0
25	MG	A	1554	1/1	0.94	0.33	67,67,67,67	0
25	MG	A	1560	1/1	0.95	0.46	67,67,67,67	0
25	MG	A	1612	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	1557	1/1	0.95	0.40	67,67,67,67	0
25	MG	A	1569	1/1	0.95	0.40	67,67,67,67	0
25	MG	A	1553	1/1	0.95	0.51	67,67,67,67	0
25	MG	A	1618	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	1593	1/1	0.95	0.33	67,67,67,67	0
25	MG	A	469	1/1	0.95	0.13	67,67,67,67	1
25	MG	A	1556	1/1	0.96	0.53	67,67,67,67	0
25	MG	A	1579	1/1	0.96	0.32	67,67,67,67	0
25	MG	A	1625	1/1	0.96	0.17	67,67,67,67	0
25	MG	A	1552	1/1	0.96	0.47	67,67,67,67	0
25	MG	A	1635	1/1	0.96	0.26	67,67,67,67	1
25	MG	A	1546	1/1	0.96	0.33	67,67,67,67	0
25	MG	A	1591	1/1	0.96	0.22	67,67,67,67	0
25	MG	A	1563	1/1	0.97	0.36	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1580	1/1	0.97	0.33	67,67,67,67	0
25	MG	A	1589	1/1	0.97	0.51	67,67,67,67	0
25	MG	A	1631	1/1	0.97	0.08	67,67,67,67	0
25	MG	A	1588	1/1	0.97	0.47	67,67,67,67	0
25	MG	A	1551	1/1	0.97	0.47	67,67,67,67	0
25	MG	A	1599	1/1	0.97	0.24	67,67,67,67	0
25	MG	A	473	1/1	0.99	0.09	67,67,67,67	1
26	ZN	D	306	1/1	0.99	0.43	67,67,67,67	0
26	ZN	N	307	1/1	0.99	0.23	67,67,67,67	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.