



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1N32  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit bound to codon and near-cognate transfer RNA anticodon stem-loop mismatched at the first codon position at the a site with paromomycin  
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.  
Deposited on : 2002-10-25  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

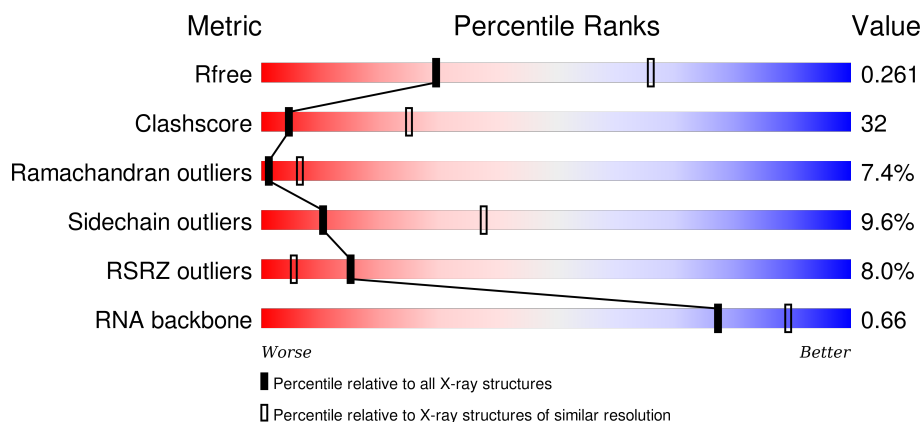
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>12%</div> <div>34%</div> <div>51%</div> <div>11%</div> <div>..</div> </div>
2	Y	17	<div> <div>29%</div> <div>53%</div> <div>6%</div> <div>12%</div> </div>
3	Z	6	<div> <div>17%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>
4	B	256	<div> <div>4%</div> <div>24%</div> <div>53%</div> <div>13%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	239	
6	D	208	
7	E	161	
8	F	101	
9	G	155	
10	H	138	
11	I	128	
12	J	104	
13	K	129	
14	L	135	
15	M	126	
16	N	60	
17	O	88	
18	P	88	
19	Q	104	
20	R	88	
21	S	92	
22	T	106	
23	V	26	

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	1561	-	-	-	X
25	MG	A	1572	-	-	-	X
25	MG	A	1600	-	-	-	X
25	MG	A	1601	-	-	-	X
25	MG	A	1615	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1624	-	-	-	X
25	MG	A	1626	-	-	-	X
25	MG	A	1632	-	-	-	X
25	MG	A	1636	-	-	-	X
25	MG	A	1644	-	-	-	X
25	MG	A	1650	-	-	-	X
25	MG	A	1659	-	-	-	X
25	MG	A	1665	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52275 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	1513	Total	C	N	O	P	0	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a RNA chain called ANTICODON STEM-LOOP OF LEU-2 TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	15	Total	C	N	O	P	0	0	0
			318	143	56	105	14			

- Molecule 3 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 4 is a protein called 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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 30S 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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	CONFLICT	UNP P24319
H	37	ARG	LYS	CONFLICT	UNP P24319
H	52	ASP	GLU	CONFLICT	UNP P24319
H	61	VAL	ILE	CONFLICT	UNP P24319
H	62	TYR	HIS	CONFLICT	UNP P24319
H	81	HIS	LYS	CONFLICT	UNP P24319
H	88	LYS	ARG	CONFLICT	UNP P24319
H	115	SER	PRO	CONFLICT	UNP P24319

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	118	Total	C	N	O	S		
			937	579	193	163	2	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 18 is a protein called 30S 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 30S 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			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	CONFLICT	UNP P24321
Q	53	LEU	VAL	CONFLICT	UNP P24321
Q	62	SER	ALA	CONFLICT	UNP P24321
Q	79	SER	GLU	CONFLICT	UNP P24321
Q	82	MET	LEU	CONFLICT	UNP P24321
Q	90	ILE	VAL	CONFLICT	UNP P24321
Q	96	GLN	ALA	CONFLICT	UNP P24321

- Molecule 20 is a protein called 30S 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 30S 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 30S RIBOSOMAL PROTEIN S20.

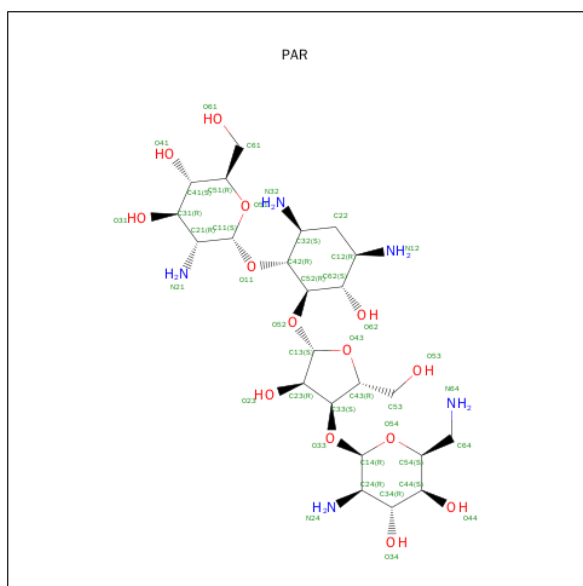
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 23 is a protein called 30S 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	J	1	Total	Mg	0	0
			1	1		
25	D	1	Total	Mg	0	0
			1	1		
25	E	1	Total	Mg	0	0
			1	1		
25	A	153	Total	Mg	0	0
			153	153		
25	Y	1	Total	Mg	0	0
			1	1		
25	M	1	Total	Mg	0	0
			1	1		

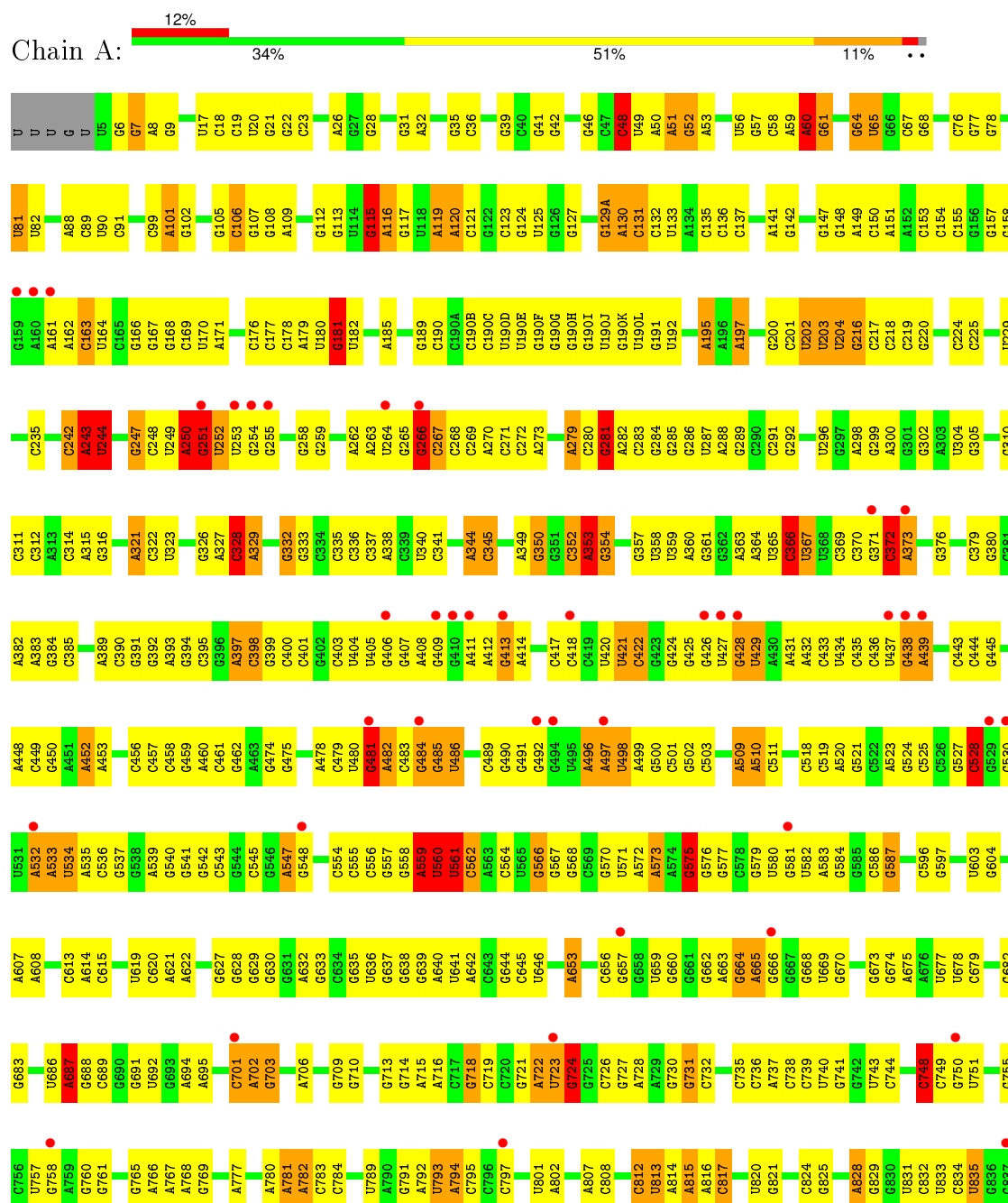
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

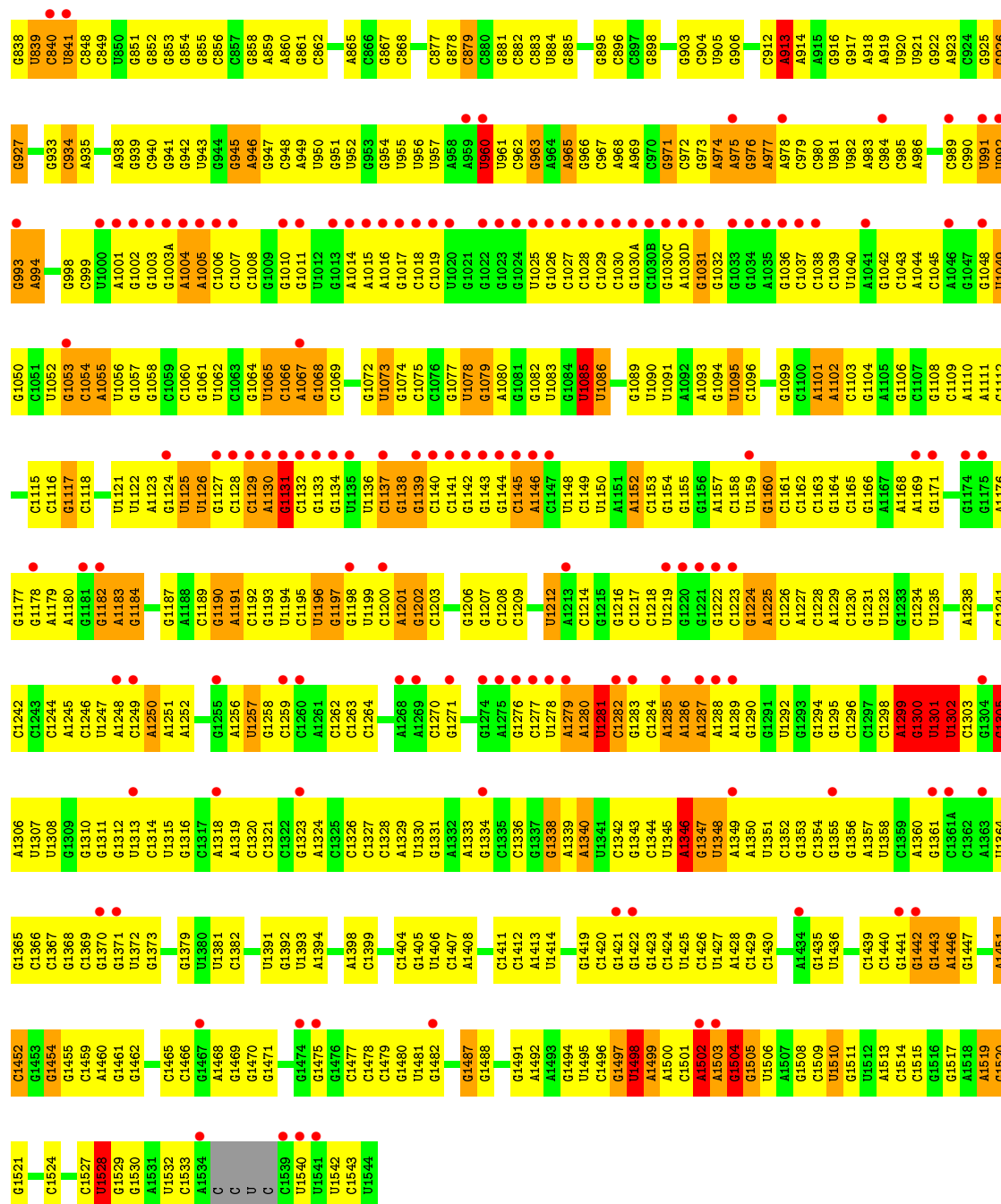
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

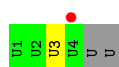
#### • Molecule 1: 16S RIBOSOMAL RNA



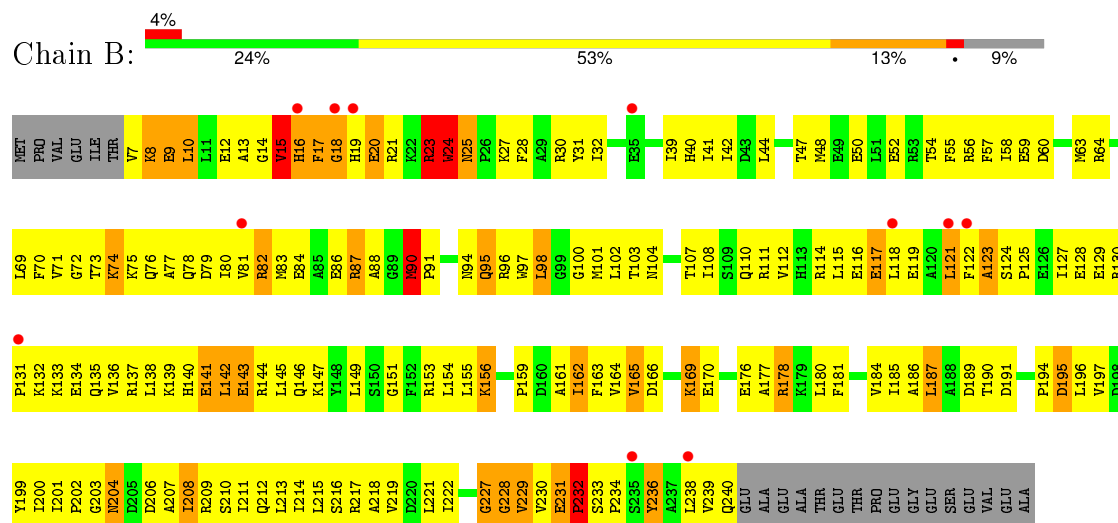


• Molecule 3: A-SITE MESSENGER RNA FRAGMENT

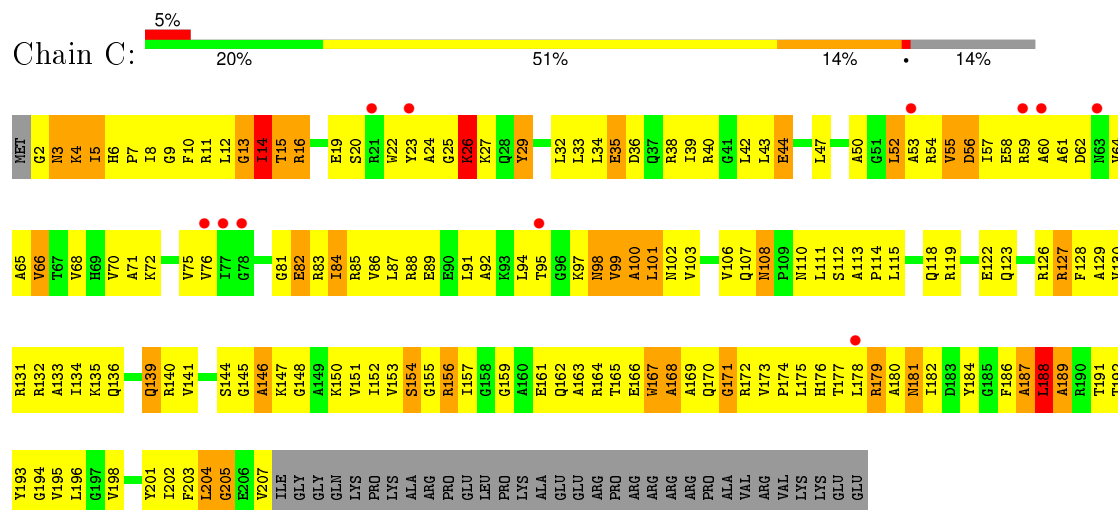




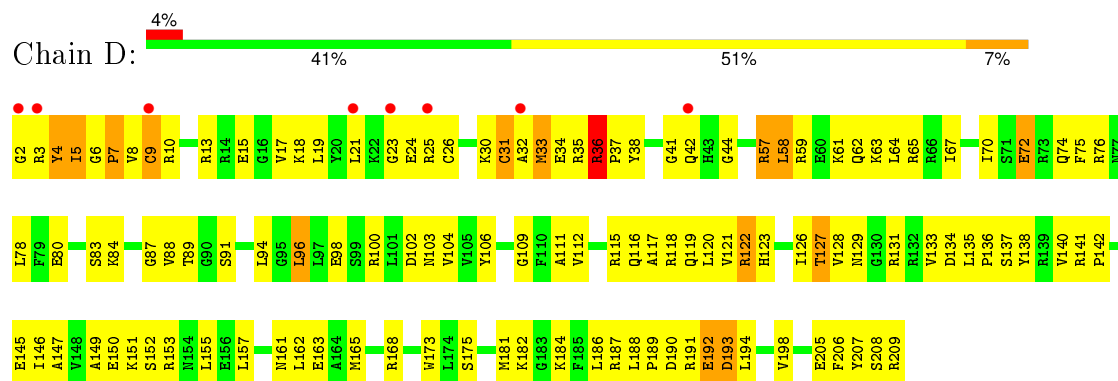
● Molecule 4: 30S RIBOSOMAL PROTEIN S2



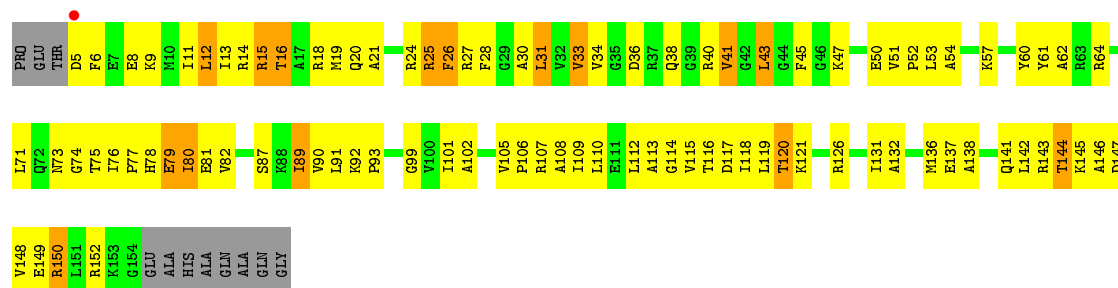
- Molecule 5: 30S RIBOSOMAL PROTEIN S3



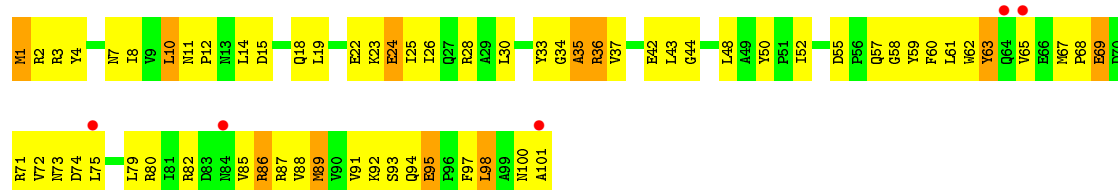
- Molecule 6: 30S RIBOSOMAL PROTEIN S4



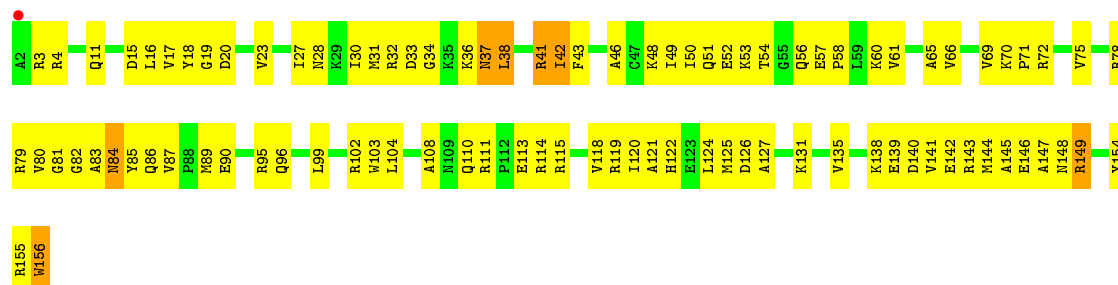
• Molecule 7: 30S RIBOSOMAL PROTEIN S5



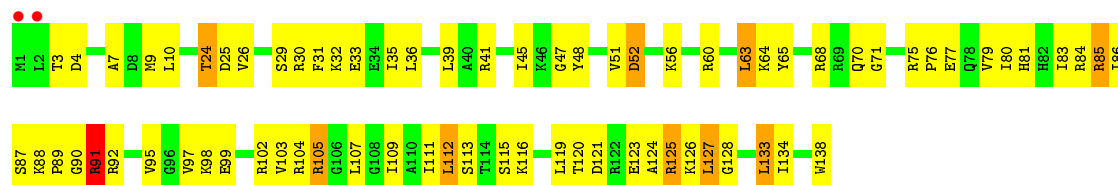
• Molecule 8: 30S RIBOSOMAL PROTEIN S6



• Molecule 9: 30S RIBOSOMAL PROTEIN S7

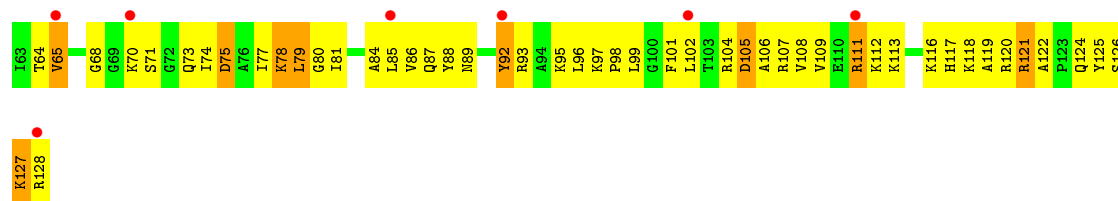


• Molecule 10: 30S RIBOSOMAL PROTEIN S8

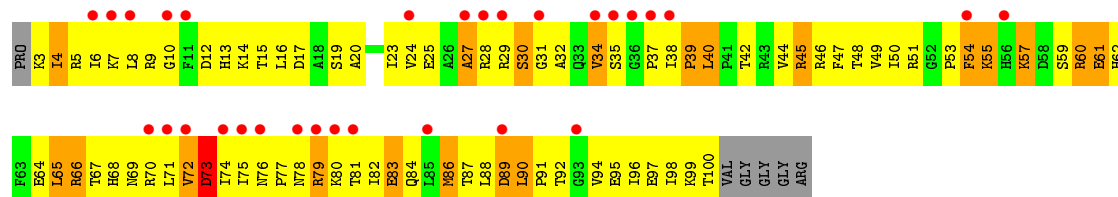
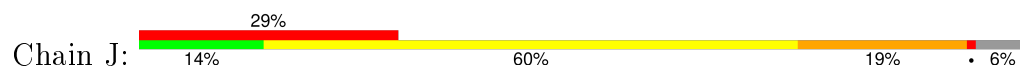


• Molecule 11: 30S RIBOSOMAL PROTEIN S9

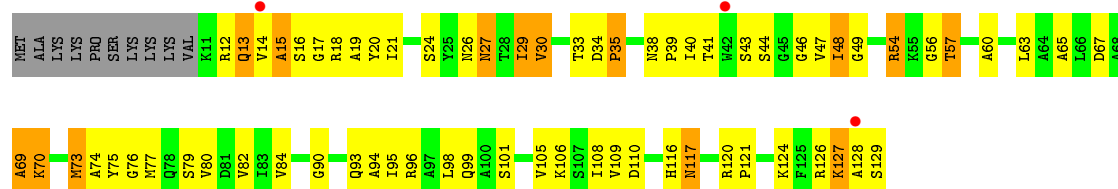




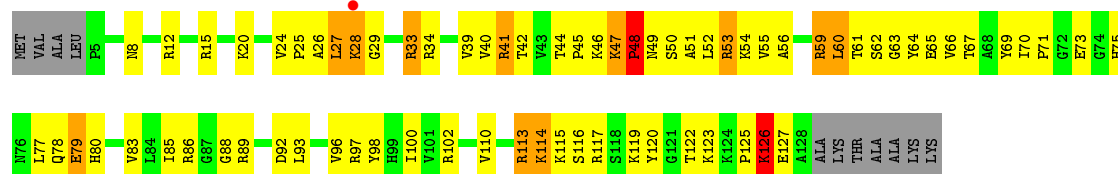
• Molecule 12: 30S RIBOSOMAL PROTEIN S10



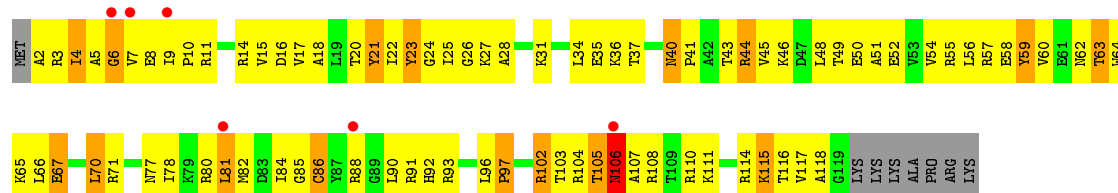
• Molecule 13: 30S RIBOSOMAL PROTEIN S11



• Molecule 14: 30S RIBOSOMAL PROTEIN S12

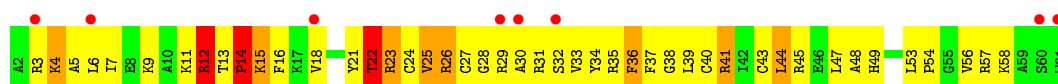


• Molecule 15: 30S RIBOSOMAL PROTEIN S13

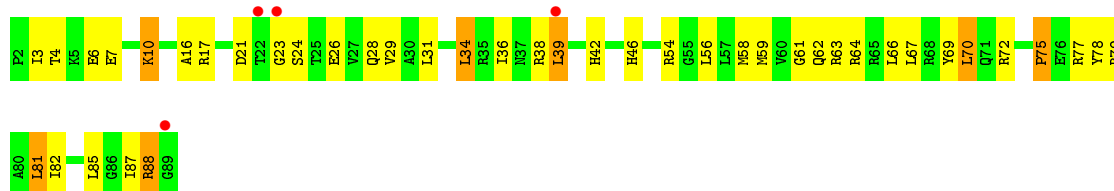


• Molecule 16: 30S RIBOSOMAL PROTEIN S14

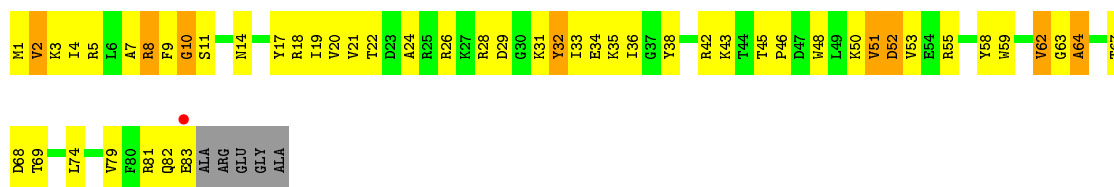




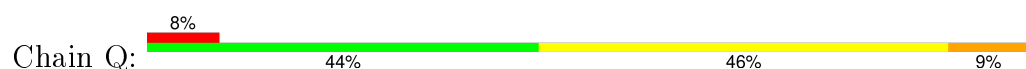
• Molecule 17: 30S RIBOSOMAL PROTEIN S15



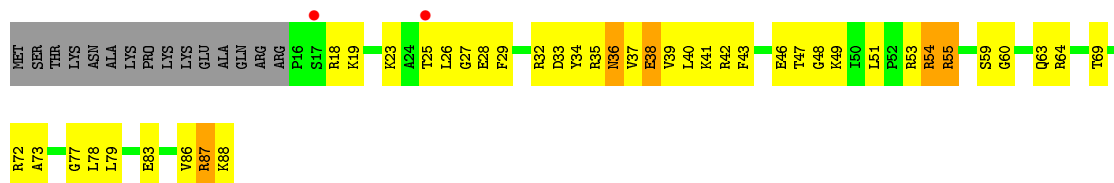
• Molecule 18: 30S RIBOSOMAL PROTEIN S16



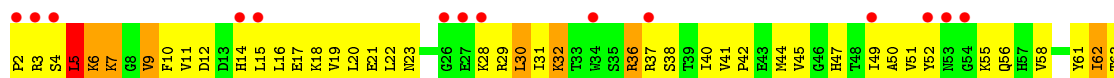
• Molecule 19: 30S RIBOSOMAL PROTEIN S17



• Molecule 20: 30S RIBOSOMAL PROTEIN S18



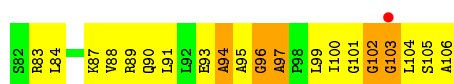
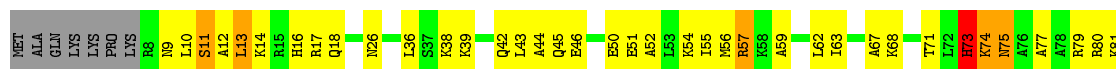
• Molecule 21: 30S RIBOSOMAL PROTEIN S19







- Molecule 22: 30S RIBOSOMAL PROTEIN S20



- Molecule 23: 30S RIBOSOMAL PROTEIN THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.30Å 400.30Å 175.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.00 131.95 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.9 (141.42-3.00) 91.1 (131.95-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.270 0.219 , 0.261	Depositor DCC
$R_{free}$ test set	13154 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 86.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 259445 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	52275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.46	0/36387	0.74	39/56789 (0.1%)
2	Y	0.41	0/333	0.71	0/518
3	Z	0.49	0/84	0.82	0/128
4	B	0.32	0/1935	0.64	0/2609
5	C	0.35	0/1636	0.62	0/2205
6	D	0.38	0/1733	0.67	0/2318
7	E	0.44	0/1162	0.71	0/1564
8	F	0.31	0/856	0.60	0/1154
9	G	0.36	0/1276	0.59	0/1709
10	H	0.44	0/1136	0.77	0/1527
11	I	0.35	0/1029	0.64	0/1378
12	J	0.36	0/805	0.64	0/1082
13	K	0.39	0/900	0.73	0/1213
14	L	0.43	0/986	0.77	0/1320
15	M	0.33	0/947	0.65	0/1270
16	N	0.41	0/501	0.68	0/664
17	O	0.36	0/745	0.58	0/992
18	P	0.45	0/716	0.73	0/963
19	Q	0.44	0/870	0.75	0/1159
20	R	0.33	0/603	0.62	0/799
21	S	0.32	0/661	0.64	0/890
22	T	0.39	0/765	0.71	0/1007
23	V	0.44	0/212	0.76	0/277
All	All	0.44	0/56278	0.72	39/83535 (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	4	35
18	P	0	1
All	All	4	36

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	C	C2'-C3'-O3'	11.02	133.74	109.50
1	A	1498	U	C2'-C3'-O3'	10.16	131.86	109.50
1	A	243	A	C2'-C3'-O3'	9.62	130.66	109.50
1	A	281	G	C2'-C3'-O3'	9.39	130.16	109.50
1	A	115	G	C2'-C3'-O3'	9.27	129.88	109.50
1	A	1302	U	C2'-C3'-O3'	9.24	129.82	109.50
1	A	328	C	C2'-C3'-O3'	8.65	128.54	109.50
1	A	575	G	C2'-C3'-O3'	8.59	128.40	109.50
1	A	1528	U	C2'-C3'-O3'	8.57	128.35	109.50
1	A	687	A	C2'-C3'-O3'	8.17	127.48	109.50
1	A	1503	A	C2'-C3'-O3'	7.62	126.27	109.50
1	A	1502	A	N9-C1'-C2'	7.62	123.90	114.00
1	A	181	G	C2'-C3'-O3'	7.60	126.22	109.50
1	A	60	A	C2'-C3'-O3'	7.59	126.19	109.50
1	A	913	A	C2'-C3'-O3'	7.41	125.81	109.50
1	A	965	A	C2'-C3'-O3'	7.35	125.67	109.50
1	A	266	G	C2'-C3'-O3'	7.21	125.35	109.50
1	A	1504	G	C2'-C3'-O3'	7.16	125.26	109.50
1	A	372	C	C2'-C3'-O3'	7.10	125.12	109.50
1	A	509	A	C2'-C3'-O3'	7.07	125.05	109.50
1	A	1299	A	N9-C1'-C2'	6.68	122.68	114.00
1	A	366	C	C2'-C3'-O3'	6.45	124.02	113.70
1	A	1346	A	C2'-C3'-O3'	6.37	123.90	113.70
1	A	748	C	N1-C1'-C2'	5.87	121.64	114.00
1	A	1085	U	C2'-C3'-O3'	5.86	123.08	113.70
1	A	353	A	C5'-C4'-O4'	-5.79	102.15	109.10
1	A	559	A	C2'-C3'-O3'	5.76	122.91	113.70
1	A	960	U	N1-C1'-C2'	5.70	121.41	114.00
1	A	244	U	C5'-C4'-C3'	-5.68	106.90	116.00
1	A	1528	U	C4'-C3'-O3'	5.52	124.04	113.00
1	A	7	G	C2'-C3'-O3'	5.43	122.39	113.70
1	A	460	A	N9-C1'-C2'	5.31	120.90	114.00
1	A	694	A	C5'-C4'-C3'	-5.25	107.60	116.00
1	A	1305	G	N9-C1'-C2'	5.21	120.78	114.00
1	A	1301	U	C2'-C3'-O3'	5.16	121.96	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C4'-C3'-O3'	5.14	123.27	113.00
1	A	528	C	C5'-C4'-C3'	5.14	124.22	116.00
1	A	560	U	C2'-C3'-O3'	5.10	121.86	113.70
1	A	1281	U	C2'-C3'-O3'	5.08	121.83	113.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	48	C	C3'
1	A	243	A	C3'
1	A	281	G	C3'
1	A	1528	U	C3'

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	1073	U	Sidechain
1	A	1077	G	Sidechain
1	A	1078	U	Sidechain
1	A	1079	G	Sidechain
1	A	1131	G	Sidechain
1	A	1299	A	Sidechain
1	A	1300	G	Sidechain
1	A	1301	U	Sidechain
1	A	1340	A	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	1510	U	Sidechain
1	A	1519	A	Sidechain
1	A	229	U	Sidechain
1	A	242	C	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	481	G	Sidechain
1	A	528	C	Sidechain
1	A	561	U	Sidechain
1	A	566	G	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	664	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	835	U	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	905	U	Sidechain
1	A	946	A	Sidechain
1	A	960	U	Sidechain
1	A	963	G	Sidechain
18	P	32	TYR	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	32508	0	16413	1088	0
2	Y	318	0	162	14	0
3	Z	77	0	42	1	0
4	B	1900	0	1951	255	0
5	C	1612	0	1677	229	0
6	D	1703	0	1763	134	0
7	E	1146	0	1207	105	0
8	F	843	0	857	95	0
9	G	1257	0	1296	107	0
10	H	1116	0	1177	80	0
11	I	1011	0	1043	124	0
12	J	792	0	835	131	0
13	K	885	0	904	75	0
14	L	970	0	1057	101	0
15	M	937	0	995	110	0
16	N	492	0	530	71	0
17	O	734	0	771	41	0
18	P	700	0	720	56	0
19	Q	857	0	930	69	0
20	R	597	0	668	63	0
21	S	647	0	673	86	0
22	T	763	0	861	79	0
23	V	208	0	221	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	42	0	45	2	0
25	A	153	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	J	1	0	0	0	0
25	M	1	0	0	0	0
25	Y	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52275	0	36798	2844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (2844) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:36:ARG:H	6:D:37:PRO:HD3	1.02	1.18
15:M:10:PRO:HB2	15:M:18:ALA:HB1	1.29	1.14
7:E:15:ARG:HD3	7:E:26:PHE:HD2	1.13	1.11
1:A:975:A:H4'	1:A:976:G:H5''	1.31	1.11
1:A:1532:U:H2'	1:A:1533:C:H5''	1.19	1.09
1:A:723:U:H2'	1:A:724:G:H5'	1.33	1.07
1:A:760:G:H1	19:Q:105:ALA:HB2	1.19	1.07
5:C:108:ASN:HD22	5:C:111:LEU:HG	1.09	1.07
13:K:48:ILE:HG22	13:K:49:GLY:H	1.10	1.06
9:G:90:GLU:HG3	9:G:155:ARG:HH22	1.19	1.06
13:K:40:ILE:HG22	13:K:41:THR:HG23	1.38	1.05
4:B:77:ALA:HB2	4:B:211:ILE:HD13	1.36	1.05
12:J:4:ILE:HD12	12:J:74:ILE:HB	1.33	1.04
12:J:38:ILE:HB	12:J:71:LEU:HB2	1.38	1.03
1:A:243:A:H4'	1:A:244:U:H5'	1.36	1.03
1:A:737:A:H1'	8:F:73:ASN:HD21	1.22	1.03
21:S:28:LYS:HG2	21:S:29:ARG:H	1.25	1.01
1:A:349:A:H2'	1:A:350:G:H5''	1.43	1.01
1:A:1443:G:H5''	1:A:1446:A:H5'	1.03	1.00
1:A:877:C:O2	10:H:3:THR:HG21	1.60	0.99
12:J:45:ARG:HH11	12:J:45:ARG:HB3	1.22	0.99
1:A:1250:A:H4'	11:I:68:GLY:H	1.28	0.98
1:A:1502:A:H2	1:A:1505:G:H1	0.97	0.97
17:O:3:ILE:HD13	17:O:34:LEU:HD13	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:C5'	1:A:1446:A:H5'	1.95	0.97
1:A:1305:G:O2'	1:A:1306:A:H8	1.48	0.96
22:T:13:LEU:HD12	22:T:13:LEU:H	1.30	0.96
7:E:15:ARG:HD3	7:E:26:PHE:CD2	2.00	0.96
1:A:371:G:O2'	1:A:372:C:H5'	1.66	0.96
7:E:80:ILE:CD1	7:E:91:LEU:HB2	1.95	0.96
8:F:33:TYR:HB2	8:F:75:LEU:HD23	1.47	0.96
1:A:579:G:H5'	1:A:728:A:H1'	1.48	0.96
7:E:79:GLU:HG3	7:E:93:PRO:HD2	1.46	0.95
1:A:1101:A:H4'	1:A:1102:A:O5'	1.63	0.95
6:D:151:LYS:H	6:D:151:LYS:HD2	1.33	0.94
5:C:14:ILE:H	5:C:14:ILE:HD13	1.32	0.94
1:A:266:G:H5''	1:A:268:C:H41	1.31	0.94
22:T:57:ARG:NE	22:T:102:GLY:HA3	1.81	0.93
1:A:1532:U:C2'	1:A:1533:C:H5''	1.98	0.93
6:D:36:ARG:N	6:D:37:PRO:HD3	1.83	0.93
1:A:1127:G:H21	1:A:1146:A:H62	1.18	0.92
7:E:81:GLU:HG2	7:E:90:VAL:HG22	1.49	0.92
4:B:102:LEU:HD21	4:B:162:ILE:HD11	1.52	0.92
12:J:34:VAL:HG22	12:J:74:ILE:HG23	1.51	0.92
5:C:108:ASN:ND2	5:C:111:LEU:HG	1.83	0.92
20:R:47:THR:HA	20:R:83:GLU:HB2	1.51	0.92
10:H:121:ASP:HB2	10:H:125:ARG:HH21	1.32	0.91
12:J:51:ARG:HG2	12:J:60:ARG:O	1.69	0.91
11:I:93:ARG:HD3	11:I:97:LYS:HZ1	1.34	0.91
5:C:191:THR:HB	5:C:194:GLY:O	1.70	0.91
11:I:8:GLY:HA2	11:I:79:LEU:HD13	1.52	0.91
1:A:1057:G:H5''	5:C:154:SER:HB2	1.53	0.91
6:D:8:VAL:HG13	6:D:21:LEU:HD12	1.53	0.90
8:F:100:ASN:HD22	20:R:23:LYS:HG2	1.35	0.90
8:F:87:ARG:HH11	8:F:87:ARG:HG3	1.35	0.90
1:A:664:G:H22	1:A:741:G:H1	1.18	0.90
1:A:1443:G:H5''	1:A:1446:A:C5'	1.97	0.90
14:L:47:LYS:HB3	14:L:48:PRO:CD	2.03	0.89
1:A:1502:A:H2	1:A:1505:G:N1	1.71	0.89
1:A:838:G:H2'	1:A:839:U:H5''	1.51	0.89
1:A:723:U:H2'	1:A:724:G:C5'	2.03	0.89
5:C:91:LEU:HD21	5:C:99:VAL:HG13	1.55	0.89
1:A:972:C:H4'	12:J:57:LYS:HG2	1.53	0.89
19:Q:93:GLN:O	19:Q:96:GLN:HB2	1.71	0.89
5:C:7:PRO:O	5:C:11:ARG:HD2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:132:LYS:HA	4:B:135:GLN:HB3	1.55	0.88
14:L:47:LYS:HB3	14:L:48:PRO:HD3	1.52	0.88
1:A:1305:G:HO2'	1:A:1306:A:H8	0.90	0.88
1:A:1195:C:H3'	1:A:1196:U:H5''	1.53	0.88
13:K:48:ILE:HG22	13:K:49:GLY:N	1.85	0.88
4:B:116:GLU:HG2	4:B:153:ARG:HH12	1.35	0.88
1:A:1319:A:H4'	21:S:37:ARG:NH1	1.88	0.88
5:C:50:ALA:HB1	5:C:70:VAL:HG11	1.54	0.88
1:A:975:A:H5'	1:A:975:A:H8	1.38	0.87
1:A:760:G:N1	19:Q:105:ALA:HB2	1.88	0.87
5:C:64:VAL:HB	5:C:99:VAL:HB	1.54	0.87
1:A:1127:G:N2	1:A:1146:A:H62	1.73	0.87
12:J:12:ASP:HB3	12:J:15:THR:HG22	1.55	0.87
17:O:4:THR:OG1	17:O:7:GLU:HB2	1.75	0.87
15:M:8:GLU:HG3	15:M:22:ILE:HG12	1.58	0.86
6:D:70:ILE:HD11	6:D:100:ARG:HD2	1.56	0.86
1:A:1137:C:H4'	1:A:1138:G:C2	2.10	0.86
4:B:84:GLU:HB3	4:B:219:VAL:HG21	1.56	0.86
22:T:57:ARG:HG2	22:T:102:GLY:O	1.73	0.86
6:D:8:VAL:HG21	6:D:115:ARG:NH1	1.90	0.86
1:A:1086:U:H3	1:A:1099:G:H22	1.20	0.86
1:A:204:U:H4'	1:A:216:G:O5'	1.73	0.85
2:Y:33:U:H5'	2:Y:34:G:OP2	1.76	0.85
15:M:34:LEU:HD13	15:M:41:PRO:HA	1.57	0.85
6:D:190:ASP:HB3	6:D:193:ASP:OD1	1.76	0.85
1:A:975:A:H4'	1:A:976:G:C5'	2.05	0.85
4:B:77:ALA:HB2	4:B:211:ILE:CD1	2.06	0.85
22:T:54:LYS:HE3	22:T:100:ILE:HD11	1.57	0.85
5:C:26:LYS:H	5:C:26:LYS:HD3	1.40	0.85
23:V:6:ARG:HD2	23:V:15:ARG:HH12	1.42	0.85
11:I:16:ARG:HG3	11:I:64:THR:HB	1.57	0.84
6:D:57:ARG:H	6:D:57:ARG:HD3	1.42	0.84
6:D:127:THR:HG23	6:D:147:ALA:HB3	1.57	0.84
1:A:1152:A:H5''	12:J:13:HIS:CD2	2.12	0.84
22:T:12:ALA:H	22:T:13:LEU:HD12	1.43	0.84
1:A:1238:A:H5'	1:A:1336:C:H41	1.41	0.84
1:A:1367:C:H5'	12:J:60:ARG:NH1	1.91	0.84
5:C:35:GLU:HG2	5:C:59:ARG:HH22	1.43	0.84
15:M:4:ILE:HG22	15:M:5:ALA:N	1.93	0.83
8:F:28:ARG:NH1	8:F:28:ARG:HB2	1.92	0.83
4:B:231:GLU:HB2	4:B:232:PRO:HD2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.78	0.83
1:A:1124:G:H5''	12:J:35:SER:O	1.78	0.83
22:T:50:GLU:HB2	22:T:99:LEU:HD12	1.58	0.83
6:D:36:ARG:H	6:D:37:PRO:CD	1.90	0.83
5:C:34:LEU:HD12	16:N:25:VAL:HG21	1.59	0.83
21:S:41:VAL:HG12	21:S:42:PRO:HD2	1.60	0.83
20:R:55:ARG:HB3	20:R:55:ARG:HH11	1.44	0.83
2:Y:29:A:H2'	2:Y:30:C:C6	2.14	0.83
1:A:31:G:N1	1:A:48:C:H5''	1.94	0.83
1:A:1125:U:H3	12:J:5:ARG:HH21	1.26	0.82
10:H:24:THR:HG22	10:H:63:LEU:HD21	1.61	0.82
4:B:59:GLU:HB3	4:B:221:LEU:HD11	1.62	0.82
1:A:250:A:H4'	1:A:251:G:O5'	1.78	0.82
17:O:16:ALA:HB1	17:O:21:ASP:HB3	1.59	0.82
1:A:1366:C:H2'	1:A:1367:C:H6	1.41	0.82
1:A:1250:A:H4'	11:I:68:GLY:N	1.94	0.82
15:M:102:ARG:HH11	15:M:102:ARG:HB2	1.44	0.82
12:J:7:LYS:HE3	12:J:40:LEU:HD11	1.61	0.82
1:A:1352:C:H2'	1:A:1353:G:C8	2.14	0.82
1:A:1106:G:H5''	5:C:172:ARG:HG2	1.62	0.82
13:K:48:ILE:CG2	13:K:49:GLY:H	1.92	0.82
5:C:35:GLU:HG2	5:C:59:ARG:NH2	1.93	0.82
12:J:10:GLY:HA3	12:J:16:LEU:HD21	1.62	0.81
1:A:1128:C:H4'	11:I:16:ARG:NH2	1.95	0.81
10:H:113:SER:HB2	10:H:134:ILE:HD11	1.63	0.81
7:E:144:THR:HG22	7:E:147:ASP:H	1.42	0.81
1:A:1190:G:OP1	5:C:4:LYS:HA	1.80	0.81
9:G:54:THR:HG22	9:G:56:GLN:H	1.46	0.81
4:B:124:SER:HB2	4:B:125:PRO:HD2	1.62	0.81
1:A:1425:U:H2'	1:A:1426:C:C6	2.17	0.80
5:C:24:ALA:HB2	5:C:32:LEU:HD12	1.62	0.80
5:C:180:ALA:O	5:C:181:ASN:HB3	1.78	0.80
1:A:1223:C:P	21:S:78:ARG:HH12	2.05	0.80
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.64	0.80
5:C:191:THR:HG22	5:C:193:TYR:H	1.45	0.80
4:B:84:GLU:OE1	4:B:216:SER:HA	1.81	0.80
21:S:28:LYS:HG2	21:S:29:ARG:N	1.96	0.80
8:F:2:ARG:HD2	8:F:69:GLU:HB3	1.64	0.80
1:A:192:U:H4'	22:T:102:GLY:O	1.82	0.80
10:H:121:ASP:HB2	10:H:125:ARG:NH2	1.96	0.79
4:B:134:GLU:HA	4:B:137:ARG:HH12	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:102:ARG:HG2	10:H:125:ARG:HH12	1.46	0.79
1:A:1208:C:H2'	1:A:1209:C:C6	2.17	0.79
1:A:656:C:H4'	17:O:62:GLN:HE22	1.47	0.79
13:K:84:VAL:HG23	13:K:110:ASP:HA	1.64	0.79
7:E:51:VAL:HB	7:E:52:PRO:HD3	1.63	0.79
1:A:349:A:C2'	1:A:350:G:H5''	2.12	0.79
1:A:390:C:H2'	1:A:391:G:C8	2.18	0.79
9:G:90:GLU:HG3	9:G:155:ARG:NH2	1.98	0.78
14:L:55:VAL:HG12	14:L:56:ALA:H	1.49	0.78
1:A:132:C:O3'	22:T:74:LYS:HE3	1.83	0.78
13:K:84:VAL:HG21	20:R:88:LYS:HD3	1.63	0.78
1:A:438:G:H4'	1:A:439:A:OP1	1.83	0.78
1:A:946:A:H2'	1:A:947:G:C8	2.18	0.78
7:E:105:VAL:HB	7:E:106:PRO:HD3	1.66	0.78
6:D:104:VAL:HG11	6:D:146:ILE:HG12	1.64	0.78
1:A:1208:C:H2'	1:A:1209:C:H6	1.49	0.78
11:I:43:ALA:HA	11:I:74:ILE:HD13	1.66	0.78
1:A:1065:U:H4'	1:A:1066:C:O5'	1.84	0.78
15:M:8:GLU:O	15:M:9:ILE:HG23	1.83	0.77
7:E:80:ILE:HD12	7:E:91:LEU:HB2	1.65	0.77
20:R:86:VAL:O	20:R:87:ARG:HB2	1.81	0.77
4:B:80:ILE:HD11	4:B:208:ILE:HG23	1.65	0.77
11:I:10:ARG:HD2	11:I:75:ASP:CB	2.13	0.77
1:A:344:A:H4'	1:A:345:C:OP2	1.84	0.77
7:E:8:GLU:HG2	7:E:34:VAL:HG22	1.67	0.77
1:A:1285:A:H4'	1:A:1286:A:O5'	1.84	0.77
4:B:77:ALA:CB	4:B:211:ILE:HD13	2.11	0.77
5:C:191:THR:HG21	5:C:193:TYR:CE1	2.20	0.77
1:A:243:A:C4'	1:A:244:U:H5'	2.15	0.76
9:G:50:ILE:HG21	9:G:61:VAL:HG21	1.65	0.76
11:I:93:ARG:HB2	11:I:97:LYS:HE3	1.66	0.76
4:B:134:GLU:HA	4:B:137:ARG:NH1	1.98	0.76
12:J:31:GLY:HA2	12:J:78:ASN:HD22	1.49	0.76
12:J:49:VAL:HG13	16:N:41:ARG:HD2	1.67	0.76
1:A:812:C:HO2'	1:A:813:U:P	2.08	0.76
12:J:49:VAL:HG11	16:N:41:ARG:O	1.85	0.76
14:L:47:LYS:CB	14:L:48:PRO:HD3	2.15	0.76
1:A:328:C:O2	1:A:328:C:H2'	1.84	0.76
6:D:23:GLY:HA3	6:D:112:VAL:HG12	1.68	0.76
12:J:53:PRO:HA	16:N:41:ARG:HH21	1.49	0.76
4:B:87:ARG:O	4:B:87:ARG:HD2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:30:SER:HB3	12:J:84:GLN:NE2	2.01	0.76
1:A:556:C:OP2	14:L:20:LYS:HE3	1.85	0.76
14:L:114:LYS:HE3	14:L:114:LYS:HA	1.67	0.76
1:A:975:A:H5'	1:A:975:A:C8	2.19	0.75
21:S:16:LEU:O	21:S:19:VAL:HG12	1.85	0.75
16:N:14:PRO:O	16:N:15:LYS:HB2	1.85	0.75
1:A:722:A:H4'	1:A:723:U:OP1	1.85	0.75
12:J:45:ARG:NH1	12:J:45:ARG:HB3	2.01	0.75
1:A:1367:C:H5'	12:J:60:ARG:HH12	1.50	0.75
8:F:10:LEU:HD12	8:F:59:TYR:HB3	1.69	0.75
4:B:218:ALA:O	4:B:222:ILE:HG13	1.85	0.75
15:M:49:THR:HG22	15:M:51:ALA:H	1.51	0.75
1:A:838:G:C2'	1:A:839:U:H5''	2.14	0.75
19:Q:97:SER:H	19:Q:103:GLY:HA2	1.50	0.75
9:G:50:ILE:O	9:G:54:THR:HB	1.86	0.75
17:O:17:ARG:HH11	17:O:17:ARG:HG3	1.51	0.75
14:L:89:ARG:HG2	14:L:97:ARG:HA	1.68	0.75
1:A:530:G:O6	3:Z:3:U:H1'	1.87	0.75
1:A:1250:A:C4'	11:I:68:GLY:H	1.98	0.74
22:T:54:LYS:HE3	22:T:100:ILE:CD1	2.16	0.74
15:M:50:GLU:O	15:M:54:VAL:HG23	1.87	0.74
1:A:1222:G:OP1	21:S:77:THR:HG21	1.87	0.74
18:P:20:VAL:HG11	18:P:32:TYR:CB	2.16	0.74
8:F:28:ARG:HB2	8:F:28:ARG:HH11	1.49	0.74
21:S:42:PRO:HA	21:S:45:VAL:HG23	1.68	0.74
20:R:25:THR:CG2	20:R:42:ARG:HH22	2.00	0.74
10:H:116:LYS:HD3	10:H:127:LEU:HD12	1.68	0.74
1:A:939:G:H5''	9:G:102:ARG:NH2	2.02	0.74
1:A:1250:A:H2'	1:A:1251:A:C8	2.22	0.74
11:I:106:ALA:O	11:I:108:VAL:HG23	1.88	0.74
1:A:1343:G:H2'	1:A:1344:C:C6	2.23	0.74
5:C:119:ARG:O	5:C:122:GLU:HB2	1.86	0.74
8:F:4:TYR:CZ	8:F:72:VAL:HG21	2.23	0.74
5:C:174:PRO:HB2	5:C:177:THR:HG22	1.69	0.74
4:B:116:GLU:HG2	4:B:153:ARG:NH1	2.02	0.74
7:E:76:ILE:HG23	7:E:77:PRO:HD2	1.68	0.74
1:A:839:U:H5'	1:A:840:C:C5	2.23	0.74
7:E:144:THR:O	7:E:148:VAL:HG23	1.88	0.74
15:M:49:THR:HB	15:M:52:GLU:HG3	1.67	0.74
1:A:31:G:H1	1:A:48:C:H5''	1.51	0.73
7:E:110:LEU:HD13	7:E:118:ILE:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:C:H2'	1:A:1116:C:H6	1.52	0.73
1:A:1168:A:H2'	1:A:1169:A:C8	2.23	0.73
1:A:269:C:H2'	1:A:270:A:C8	2.23	0.73
1:A:1281:U:H5'	1:A:1282:C:H5	1.51	0.73
4:B:178:ARG:HG3	4:B:178:ARG:HH11	1.53	0.73
4:B:15:VAL:HG21	4:B:209:ARG:HG3	1.68	0.73
1:A:1251:A:H2'	1:A:1252:A:C8	2.24	0.73
5:C:64:VAL:HB	5:C:99:VAL:CB	2.19	0.73
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.73
1:A:1038:C:H2'	1:A:1039:C:H6	1.53	0.73
1:A:1381:U:O2'	1:A:1382:C:H5'	1.88	0.73
14:L:71:PRO:O	14:L:102:ARG:HD2	1.89	0.73
1:A:1368:G:O2'	1:A:1369:C:H5'	1.87	0.73
1:A:1005:A:H2'	1:A:1006:C:H5'	1.71	0.73
1:A:371:G:C2'	1:A:372:C:H5'	2.18	0.72
22:T:73:HIS:O	22:T:74:LYS:HB2	1.88	0.72
1:A:706:A:O4'	13:K:29:ILE:HD11	1.89	0.72
1:A:923:A:OP1	7:E:21:ALA:HB2	1.89	0.72
1:A:662:G:H2'	1:A:663:A:C8	2.24	0.72
1:A:112:G:H21	1:A:354:G:H5'	1.53	0.72
1:A:1356:G:H2'	1:A:1357:A:C8	2.23	0.72
17:O:39:LEU:HD13	17:O:56:LEU:HB2	1.70	0.72
9:G:72:ARG:HH12	9:G:138:LYS:NZ	1.88	0.72
9:G:37:ASN:ND2	11:I:41:VAL:HG23	2.04	0.72
1:A:163:C:O2'	1:A:164:U:H5'	1.90	0.72
1:A:1095:U:H2'	1:A:1096:C:C6	2.25	0.72
1:A:539:A:H2'	1:A:540:G:C8	2.25	0.72
13:K:106:LYS:HE2	13:K:106:LYS:HA	1.70	0.72
4:B:16:HIS:HA	4:B:204:ASN:HB2	1.72	0.72
1:A:1128:C:H4'	11:I:16:ARG:HH22	1.53	0.72
11:I:47:LEU:C	11:I:49:PRO:HD2	2.10	0.72
8:F:12:PRO:HG3	8:F:57:GLN:O	1.90	0.72
18:P:74:LEU:O	18:P:79:VAL:HG23	1.89	0.72
1:A:202:U:H5''	1:A:203:U:OP2	1.89	0.71
15:M:40:ASN:HD22	15:M:41:PRO:CD	2.03	0.71
8:F:14:LEU:HA	8:F:18:GLN:NE2	2.04	0.71
10:H:112:LEU:HD23	10:H:112:LEU:H	1.55	0.71
12:J:57:LYS:O	12:J:57:LYS:HD2	1.90	0.71
16:N:27:CYS:SG	16:N:29:ARG:HB2	2.30	0.71
11:I:31:GLN:HE21	11:I:35:GLU:HG3	1.55	0.71
11:I:10:ARG:HD2	11:I:75:ASP:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.20	0.71
21:S:4:SER:O	21:S:5:LEU:HB2	1.89	0.71
1:A:384:G:H2'	1:A:385:C:H6	1.55	0.71
12:J:7:LYS:HE3	12:J:40:LEU:CD1	2.21	0.71
5:C:6:HIS:HD2	5:C:8:ILE:H	1.37	0.71
4:B:95:GLN:O	4:B:96:ARG:HD2	1.89	0.71
5:C:58:GLU:HB3	12:J:92:THR:HG21	1.73	0.71
1:A:437:U:H5''	6:D:155:LEU:HD22	1.72	0.71
1:A:1201:A:H4'	1:A:1202:G:O5'	1.91	0.71
1:A:1256:A:H5'	1:A:1258:G:C1'	2.20	0.71
1:A:113:G:H1'	1:A:354:G:H5'	1.72	0.71
14:L:110:VAL:O	14:L:122:THR:HG21	1.90	0.71
1:A:1106:G:OP1	5:C:172:ARG:HD3	1.91	0.70
1:A:1425:U:H3	1:A:1475:G:H1	1.36	0.70
1:A:824:C:H2'	1:A:825:G:H8	1.56	0.70
21:S:55:LYS:HG2	21:S:56:GLN:HE21	1.56	0.70
16:N:45:ARG:HH11	16:N:45:ARG:HG3	1.56	0.70
14:L:53:ARG:HG2	14:L:69:TYR:HE1	1.56	0.70
1:A:781:A:H2'	1:A:782:A:H5'	1.72	0.70
1:A:1123:A:H4'	12:J:37:PRO:HD2	1.73	0.70
1:A:1061:G:O2'	1:A:1062:U:H5'	1.92	0.70
1:A:524:G:H2'	1:A:525:C:C6	2.26	0.70
1:A:393:A:O2'	1:A:394:G:H5'	1.90	0.70
1:A:853:G:O2'	1:A:854:G:H5'	1.91	0.70
21:S:45:VAL:HA	21:S:62:ILE:CG2	2.20	0.70
1:A:1499:A:H1'	1:A:1520:G:H5'	1.73	0.70
11:I:81:ILE:O	11:I:85:LEU:HB2	1.92	0.70
15:M:81:LEU:O	15:M:86:CYS:HB3	1.92	0.70
4:B:231:GLU:HB2	4:B:232:PRO:CD	2.22	0.70
1:A:1427:U:H2'	1:A:1428:A:C8	2.26	0.70
1:A:64:G:H4'	1:A:65:U:O5'	1.92	0.70
1:A:35:G:H2'	1:A:36:C:C6	2.25	0.70
1:A:1314:C:H3'	21:S:6:LYS:NZ	2.06	0.70
1:A:835:U:OP1	20:R:64:ARG:NH2	2.24	0.70
5:C:70:VAL:HG12	5:C:71:ALA:H	1.57	0.70
1:A:1278:U:H4'	1:A:1279:A:C5'	2.22	0.70
1:A:1207:G:O2'	1:A:1208:C:H5'	1.92	0.70
17:O:4:THR:HG1	17:O:7:GLU:HB2	1.56	0.70
9:G:50:ILE:CG2	9:G:61:VAL:HG21	2.22	0.70
1:A:1263:C:H2'	1:A:1264:C:C6	2.27	0.70
8:F:8:ILE:HD11	8:F:79:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:43:LEU:HD13	22:T:51:GLU:HG3	1.73	0.70
1:A:1054:C:H3'	1:A:1054:C:O2	1.91	0.70
8:F:94:GLN:NE2	20:R:32:ARG:HD3	2.06	0.70
1:A:639:G:O2'	1:A:640:A:H5'	1.92	0.70
14:L:83:VAL:HG13	14:L:100:ILE:HG23	1.72	0.70
4:B:209:ARG:HH12	4:B:236:TYR:HE2	1.40	0.69
5:C:14:ILE:O	5:C:16:ARG:N	2.24	0.69
1:A:1152:A:H2'	1:A:1153:C:C6	2.27	0.69
1:A:478:A:O2'	1:A:479:C:H5'	1.91	0.69
1:A:1191:A:P	5:C:3:ASN:ND2	2.65	0.69
1:A:780:A:O2'	1:A:781:A:H5''	1.91	0.69
15:M:84:ILE:HG22	21:S:65:ASN:HD22	1.56	0.69
16:N:57:ARG:HG2	16:N:58:LYS:H	1.57	0.69
6:D:8:VAL:CG1	6:D:21:LEU:HD12	2.23	0.69
5:C:83:ARG:HA	5:C:86:VAL:HG23	1.73	0.69
1:A:1319:A:H4'	21:S:37:ARG:HH12	1.53	0.69
1:A:556:C:O2'	1:A:557:G:H5'	1.92	0.69
10:H:112:LEU:HD23	10:H:112:LEU:N	2.08	0.69
18:P:22:THR:HA	18:P:33:ILE:HG13	1.73	0.69
5:C:52:LEU:H	5:C:52:LEU:HD23	1.56	0.69
1:A:1057:G:H5''	5:C:154:SER:CB	2.23	0.69
13:K:34:ASP:OD2	13:K:38:ASN:HB2	1.92	0.69
9:G:38:LEU:O	9:G:42:ILE:HG13	1.91	0.69
12:J:4:ILE:HD11	12:J:77:PRO:HB3	1.74	0.69
6:D:57:ARG:HB3	6:D:206:PHE:HB2	1.75	0.69
1:A:1116:C:H2'	1:A:1117:G:H5''	1.75	0.69
14:L:70:ILE:HD13	14:L:77:LEU:HD12	1.73	0.69
1:A:677:U:H3	1:A:713:G:H22	1.38	0.69
5:C:94:LEU:HD22	5:C:95:THR:HG23	1.74	0.69
22:T:89:ARG:HG3	22:T:104:LEU:HD13	1.73	0.69
4:B:208:ILE:HA	4:B:211:ILE:HD12	1.74	0.69
21:S:28:LYS:CG	21:S:29:ARG:H	2.03	0.69
13:K:93:GLN:HE21	13:K:96:ARG:HH21	1.38	0.69
8:F:10:LEU:CD1	8:F:59:TYR:HB3	2.22	0.69
1:A:1305:G:H5'	23:V:4:GLY:HA3	1.75	0.69
1:A:1195:C:H3'	1:A:1196:U:C5'	2.22	0.69
17:O:26:GLU:OE1	17:O:77:ARG:HD2	1.92	0.69
1:A:1279:A:H5''	1:A:1280:A:OP1	1.93	0.68
12:J:3:LYS:N	12:J:75:ILE:HA	2.08	0.68
1:A:1086:U:H3	1:A:1099:G:N2	1.91	0.68
1:A:656:C:H4'	17:O:62:GLN:NE2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H2'	1:A:391:G:H8	1.55	0.68
6:D:187:ARG:HA	6:D:187:ARG:HE	1.59	0.68
1:A:443:C:H2'	1:A:444:C:H6	1.58	0.68
13:K:30:VAL:HG21	13:K:65:ALA:HA	1.75	0.68
1:A:1391:U:H2'	1:A:1392:G:C8	2.27	0.68
5:C:179:ARG:HD3	5:C:207:VAL:HA	1.74	0.68
4:B:15:VAL:HG11	4:B:209:ARG:HB3	1.73	0.68
22:T:54:LYS:HG3	22:T:100:ILE:HD12	1.75	0.68
1:A:627:G:O2'	1:A:628:G:H5'	1.93	0.68
6:D:6:GLY:O	6:D:8:VAL:HG23	1.94	0.68
5:C:91:LEU:HD23	5:C:92:ALA:N	2.08	0.68
1:A:1320:C:O2	21:S:72:GLY:HA3	1.93	0.68
4:B:219:VAL:HA	4:B:222:ILE:HD12	1.74	0.68
14:L:56:ALA:O	14:L:67:THR:HA	1.93	0.68
1:A:539:A:H2'	1:A:540:G:H8	1.59	0.68
1:A:191:G:C4	22:T:105:SER:HB3	2.28	0.68
1:A:1191:A:P	5:C:3:ASN:HD21	2.17	0.68
1:A:1404:C:H2'	1:A:1405:G:C8	2.29	0.68
14:L:25:PRO:C	14:L:27:LEU:H	1.95	0.68
1:A:877:C:H1'	10:H:3:THR:CG2	2.24	0.68
15:M:23:TYR:O	15:M:25:ILE:N	2.26	0.68
20:R:55:ARG:HB3	20:R:55:ARG:NH1	2.07	0.68
14:L:27:LEU:O	14:L:29:GLY:N	2.27	0.68
14:L:27:LEU:C	14:L:29:GLY:H	1.97	0.68
1:A:501:C:H2'	1:A:502:G:H8	1.58	0.68
9:G:126:ASP:OD1	9:G:131:LYS:HE3	1.94	0.68
11:I:70:LYS:O	11:I:74:ILE:HG13	1.94	0.67
1:A:357:G:O2'	1:A:358:U:H5'	1.95	0.67
12:J:46:ARG:NH1	12:J:64:GLU:HB3	2.09	0.67
1:A:41:G:H2'	1:A:42:G:H8	1.59	0.67
15:M:62:ASN:O	15:M:63:THR:HB	1.94	0.67
4:B:197:VAL:HB	4:B:200:ILE:HG12	1.75	0.67
1:A:266:G:C8	1:A:266:G:H5'	2.29	0.67
1:A:839:U:H5'	1:A:840:C:H5	1.59	0.67
19:Q:63:ARG:O	19:Q:65:ILE:HD12	1.94	0.67
1:A:580:U:H2'	1:A:581:G:O4'	1.95	0.67
7:E:92:LYS:HB3	7:E:119:LEU:HB2	1.76	0.67
1:A:1016:A:H2'	1:A:1017:G:O4'	1.94	0.67
6:D:8:VAL:C	6:D:10:ARG:H	1.98	0.67
1:A:1343:G:H2'	1:A:1344:C:H6	1.59	0.67
1:A:384:G:H2'	1:A:385:C:C6	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:2:ARG:HH11	8:F:69:GLU:HB3	1.58	0.67
14:L:75:HIS:HD2	14:L:77:LEU:H	1.42	0.67
1:A:1310:G:N7	21:S:2:PRO:HD3	2.09	0.67
1:A:1497:G:C2'	1:A:1498:U:H5'	2.25	0.67
4:B:10:LEU:HD22	4:B:48:MET:CE	2.24	0.67
1:A:192:U:H4'	22:T:102:GLY:C	2.14	0.67
16:N:26:ARG:HH11	16:N:43:CYS:HB3	1.58	0.67
1:A:1306:A:N6	1:A:1331:G:H1'	2.09	0.67
4:B:135:GLN:O	4:B:139:LYS:HG2	1.94	0.67
15:M:40:ASN:HD22	15:M:41:PRO:HD2	1.60	0.67
12:J:4:ILE:HA	12:J:100:THR:CB	2.25	0.67
1:A:1330:U:OP1	15:M:23:TYR:O	2.12	0.67
21:S:41:VAL:CG1	21:S:42:PRO:HD2	2.25	0.67
1:A:939:G:H2'	1:A:940:C:C6	2.30	0.66
14:L:41:ARG:HG2	14:L:42:THR:N	2.09	0.66
10:H:90:GLY:O	10:H:91:ARG:HB2	1.94	0.66
1:A:975:A:C4'	1:A:976:G:H5''	2.18	0.66
4:B:19:HIS:CE1	4:B:206:ASP:HB3	2.30	0.66
1:A:737:A:H1'	8:F:73:ASN:ND2	2.03	0.66
5:C:76:VAL:HG11	5:C:103:VAL:HG21	1.77	0.66
14:L:89:ARG:NH2	14:L:97:ARG:HH21	1.91	0.66
1:A:443:C:H2'	1:A:444:C:C6	2.31	0.66
1:A:41:G:H2'	1:A:42:G:C8	2.30	0.66
5:C:111:LEU:HD21	5:C:144:SER:O	1.94	0.66
21:S:31:ILE:HG22	21:S:32:LYS:H	1.59	0.66
1:A:1125:U:H3	12:J:5:ARG:NH2	1.93	0.66
6:D:70:ILE:HD11	6:D:100:ARG:CD	2.26	0.66
1:A:1280:A:H5'	12:J:40:LEU:HD22	1.77	0.66
1:A:912:C:O2'	1:A:913:A:H5'	1.94	0.66
5:C:64:VAL:HB	5:C:99:VAL:CG2	2.26	0.66
1:A:1154:G:H2'	1:A:1155:G:H8	1.60	0.66
5:C:10:PHE:CE2	5:C:178:LEU:HD13	2.31	0.66
1:A:149:A:H2'	1:A:150:C:C6	2.31	0.66
1:A:421:U:H5'	1:A:422:C:OP2	1.94	0.66
15:M:37:THR:HG23	15:M:55:ARG:HD2	1.76	0.66
1:A:1366:C:H2'	1:A:1367:C:C6	2.27	0.66
4:B:87:ARG:HH22	4:B:233:SER:HB2	1.59	0.66
1:A:940:C:H2'	1:A:941:G:H8	1.59	0.66
5:C:15:THR:O	5:C:16:ARG:HB2	1.96	0.66
11:I:97:LYS:HG2	11:I:102:LEU:HD12	1.76	0.66
1:A:1056:U:H5'	5:C:163:ALA:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:C:H2'	1:A:1116:C:C6	2.31	0.66
4:B:12:GLU:C	4:B:14:GLY:H	1.98	0.66
12:J:8:LEU:HD23	12:J:96:ILE:HG12	1.78	0.66
12:J:12:ASP:HB3	12:J:15:THR:CG2	2.24	0.66
1:A:1189:C:P	12:J:51:ARG:HH22	2.19	0.65
15:M:54:VAL:O	15:M:58:GLU:HG2	1.96	0.65
5:C:52:LEU:H	5:C:52:LEU:CD2	2.09	0.65
12:J:61:GLU:OE1	16:N:45:ARG:NH1	2.29	0.65
11:I:8:GLY:HA2	11:I:79:LEU:CD1	2.25	0.65
6:D:7:PRO:HB2	6:D:10:ARG:HD2	1.78	0.65
20:R:26:LEU:HD11	20:R:29:PHE:CD2	2.31	0.65
1:A:337:C:H2'	1:A:338:A:H8	1.61	0.65
7:E:71:LEU:HD11	7:E:114:GLY:HA3	1.76	0.65
6:D:151:LYS:H	6:D:151:LYS:CD	2.08	0.65
4:B:213:LEU:O	4:B:217:ARG:HG2	1.97	0.65
6:D:61:LYS:HD2	6:D:207:TYR:OH	1.97	0.65
20:R:87:ARG:HG2	20:R:87:ARG:HH11	1.62	0.65
1:A:112:G:H4'	1:A:389:A:H5''	1.77	0.65
19:Q:66:SER:OG	19:Q:69:LYS:HB3	1.95	0.65
1:A:1225:A:H5'	1:A:1226:C:OP2	1.96	0.65
8:F:33:TYR:HA	8:F:71:ARG:NH2	2.10	0.65
11:I:40:LEU:O	11:I:42:ARG:N	2.29	0.65
22:T:51:GLU:HA	22:T:54:LYS:HB2	1.78	0.65
1:A:1527:C:O2'	1:A:1528:U:H5'	1.95	0.65
13:K:110:ASP:HB2	20:R:88:LYS:HD2	1.78	0.65
18:P:18:ARG:O	18:P:20:VAL:HG23	1.95	0.65
1:A:1014:A:C2	1:A:1219:U:H1'	2.31	0.65
19:Q:80:GLY:O	19:Q:81:ARG:HB3	1.97	0.65
13:K:48:ILE:HD13	13:K:63:LEU:HB3	1.78	0.65
1:A:1141:C:O2'	1:A:1142:G:H5'	1.97	0.65
1:A:1262:C:O2'	1:A:1263:C:H5'	1.97	0.65
4:B:7:VAL:HG11	4:B:221:LEU:HD23	1.79	0.65
12:J:30:SER:HB3	12:J:84:GLN:HE22	1.61	0.65
18:P:3:LYS:O	18:P:21:VAL:HA	1.97	0.65
18:P:20:VAL:CG1	18:P:32:TYR:HB2	2.26	0.65
7:E:75:THR:HG23	7:E:76:ILE:N	2.11	0.65
22:T:96:GLY:O	22:T:97:ALA:HB3	1.96	0.65
1:A:413:G:H2'	1:A:428:G:N2	2.11	0.65
18:P:19:ILE:HG22	18:P:36:ILE:HG13	1.78	0.65
6:D:111:ALA:HA	6:D:161:ASN:ND2	2.11	0.65
1:A:1314:C:C6	21:S:6:LYS:HE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:G:H2'	1:A:1134:G:H8	1.59	0.65
1:A:1372:U:OP1	11:I:71:SER:HB3	1.97	0.65
4:B:239:VAL:HG12	4:B:239:VAL:O	1.97	0.65
7:E:76:ILE:HG22	7:E:78:HIS:H	1.62	0.65
1:A:1003:G:H22	1:A:1039:C:H1'	1.61	0.65
11:I:10:ARG:HD2	11:I:75:ASP:HB2	1.77	0.64
15:M:4:ILE:HG22	15:M:5:ALA:H	1.62	0.64
9:G:37:ASN:HD21	11:I:41:VAL:HG23	1.60	0.64
1:A:1241:G:H2'	1:A:1242:C:C6	2.32	0.64
22:T:11:SER:HA	22:T:13:LEU:CD1	2.27	0.64
4:B:86:GLU:C	4:B:88:ALA:H	2.00	0.64
1:A:991:U:O4	1:A:1212:U:H1'	1.97	0.64
9:G:65:ALA:O	9:G:69:VAL:HG23	1.97	0.64
19:Q:27:PHE:HB2	19:Q:28:PRO:HD2	1.79	0.64
1:A:1116:C:C2'	1:A:1117:G:H5''	2.27	0.64
1:A:353:A:H5'	1:A:353:A:H8	1.63	0.64
1:A:1305:G:H22	1:A:1331:G:H2'	1.61	0.64
13:K:110:ASP:OD2	20:R:88:LYS:NZ	2.30	0.64
1:A:812:C:O2'	1:A:813:U:P	2.55	0.64
16:N:26:ARG:NH1	16:N:47:LEU:HG	2.13	0.64
12:J:44:VAL:HG22	12:J:66:ARG:HB3	1.78	0.64
5:C:129:ALA:HB3	5:C:132:ARG:HH12	1.62	0.64
5:C:155:GLY:O	5:C:156:ARG:HB2	1.96	0.64
5:C:34:LEU:HD23	5:C:34:LEU:C	2.18	0.64
21:S:77:THR:HG22	21:S:78:ARG:HG3	1.79	0.64
1:A:1292:U:P	9:G:41:ARG:HH22	2.21	0.64
19:Q:68:ARG:HG2	19:Q:68:ARG:HH11	1.61	0.64
10:H:85:ARG:NE	10:H:87:SER:O	2.30	0.64
21:S:22:LEU:HD22	21:S:28:LYS:HD2	1.79	0.64
12:J:50:ILE:HA	12:J:60:ARG:HA	1.79	0.64
1:A:985:C:H2'	1:A:986:A:C8	2.33	0.64
21:S:14:HIS:O	21:S:18:LYS:HE3	1.98	0.64
5:C:129:ALA:HB3	5:C:132:ARG:NH1	2.13	0.64
5:C:177:THR:HG23	5:C:180:ALA:HB2	1.80	0.64
9:G:146:GLU:O	9:G:149:ARG:HG2	1.98	0.64
10:H:51:VAL:HG12	10:H:52:ASP:N	2.13	0.64
1:A:403:C:O2'	1:A:404:U:H5'	1.98	0.64
1:A:950:U:H5	15:M:102:ARG:HE	1.45	0.64
1:A:1039:C:H2'	1:A:1040:U:C6	2.33	0.64
1:A:954:G:H2'	1:A:955:U:C6	2.33	0.64
1:A:107:G:C2'	1:A:108:G:H5'	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:78:ASN:O	12:J:80:LYS:N	2.31	0.63
1:A:1281:U:H5'	1:A:1282:C:C5	2.31	0.63
5:C:186:PHE:CG	5:C:187:ALA:N	2.65	0.63
4:B:16:HIS:NE2	4:B:214:ILE:HD11	2.13	0.63
4:B:15:VAL:CG2	4:B:209:ARG:HG3	2.28	0.63
11:I:42:ARG:NH2	11:I:71:SER:OG	2.31	0.63
19:Q:97:SER:O	19:Q:99:SER:N	2.25	0.63
8:F:15:ASP:H	8:F:18:GLN:NE2	1.96	0.63
9:G:69:VAL:HG21	9:G:104:LEU:HD21	1.81	0.63
1:A:750:G:N3	17:O:23:GLY:HA3	2.13	0.63
5:C:204:LEU:O	5:C:204:LEU:HD12	1.97	0.63
17:O:78:TYR:CZ	17:O:82:ILE:HD11	2.32	0.63
1:A:807:A:H2'	1:A:808:C:C6	2.33	0.63
15:M:31:LYS:O	15:M:35:GLU:HB2	1.98	0.63
4:B:211:ILE:O	4:B:215:LEU:HB2	1.98	0.63
1:A:411:A:C4	1:A:413:G:H1'	2.33	0.63
5:C:150:LYS:HE2	5:C:152:ILE:HD11	1.79	0.63
5:C:54:ARG:HG2	5:C:55:VAL:N	2.14	0.63
4:B:9:GLU:HB3	4:B:12:GLU:OE2	1.99	0.63
8:F:35:ALA:O	8:F:36:ARG:HB2	1.99	0.63
6:D:146:ILE:HD12	6:D:146:ILE:N	2.13	0.63
20:R:38:GLU:HA	20:R:41:LYS:HE2	1.81	0.63
1:A:1142:G:H2'	1:A:1143:G:O4'	1.99	0.63
8:F:100:ASN:ND2	20:R:23:LYS:HG2	2.11	0.63
1:A:328:C:O2	1:A:328:C:C2'	2.47	0.63
22:T:83:ARG:O	22:T:87:LYS:HG3	1.99	0.63
11:I:4:TYR:CD2	11:I:88:TYR:HA	2.33	0.63
1:A:877:C:H1'	10:H:3:THR:HG21	1.81	0.63
5:C:83:ARG:C	5:C:85:ARG:H	2.02	0.63
1:A:701:C:H5''	1:A:703:G:O4'	1.98	0.63
10:H:120:THR:OG1	10:H:123:GLU:HG3	1.99	0.63
1:A:1305:G:C5'	23:V:4:GLY:HA3	2.27	0.63
1:A:1127:G:H21	1:A:1146:A:N6	1.92	0.63
15:M:102:ARG:NH1	15:M:102:ARG:HB2	2.14	0.63
10:H:111:ILE:O	10:H:134:ILE:HB	1.99	0.63
9:G:15:ASP:HB3	9:G:20:ASP:H	1.64	0.63
13:K:57:THR:CG2	13:K:60:ALA:H	2.11	0.63
4:B:181:PHE:CD2	10:H:70:GLN:HB3	2.33	0.63
2:Y:34:G:H2'	2:Y:35:A:H8	1.63	0.63
5:C:83:ARG:HE	5:C:87:LEU:HD11	1.63	0.63
6:D:57:ARG:N	6:D:57:ARG:HD3	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:15:ALA:O	13:K:77:MET:HG3	1.98	0.63
1:A:180:U:H2'	1:A:181:G:H5'	1.80	0.63
1:A:112:G:O2'	1:A:113:G:H5'	1.98	0.62
1:A:1031:G:H2'	1:A:1032:G:H8	1.64	0.62
8:F:100:ASN:HD22	20:R:23:LYS:CG	2.12	0.62
14:L:27:LEU:HG	14:L:28:LYS:H	1.63	0.62
1:A:428:G:H4'	1:A:429:U:O5'	1.98	0.62
1:A:1182:G:O2'	1:A:1183:A:OP2	2.12	0.62
21:S:49:ILE:HD12	21:S:49:ILE:N	2.14	0.62
8:F:33:TYR:CB	8:F:75:LEU:HD23	2.25	0.62
5:C:100:ALA:O	5:C:101:LEU:HB2	1.98	0.62
5:C:83:ARG:O	5:C:85:ARG:N	2.24	0.62
4:B:59:GLU:HG3	4:B:60:ASP:N	2.13	0.62
4:B:178:ARG:NH1	4:B:178:ARG:HG3	2.13	0.62
17:O:87:ILE:O	17:O:88:ARG:HB2	1.99	0.62
20:R:34:TYR:HA	20:R:69:THR:HG23	1.82	0.62
5:C:25:GLY:O	5:C:27:LYS:N	2.33	0.62
11:I:85:LEU:O	11:I:92:TYR:HD1	1.81	0.62
15:M:78:ILE:O	15:M:81:LEU:HD23	1.99	0.62
22:T:79:ARG:HD2	22:T:83:ARG:HH12	1.63	0.62
13:K:121:PRO:HG2	13:K:126:ARG:HG2	1.80	0.62
1:A:689:C:P	13:K:46:GLY:HA3	2.39	0.62
4:B:139:LYS:O	4:B:143:GLU:HG2	2.00	0.62
14:L:24:VAL:O	14:L:26:ALA:N	2.26	0.62
4:B:27:LYS:HD3	4:B:195:ASP:OD2	2.00	0.62
23:V:12:LYS:HB3	23:V:22:ARG:HD2	1.81	0.62
4:B:13:ALA:HB1	4:B:17:PHE:HE2	1.65	0.62
1:A:1347:G:N2	1:A:1373:G:H2'	2.13	0.62
4:B:102:LEU:HD21	4:B:162:ILE:CD1	2.28	0.62
1:A:1195:C:H2'	1:A:1197:G:H5'	1.81	0.62
1:A:556:C:C2'	1:A:557:G:H5'	2.29	0.62
20:R:25:THR:HG22	20:R:42:ARG:HH22	1.62	0.62
19:Q:59:ILE:HG22	19:Q:71:PHE:CD1	2.35	0.62
1:A:148:G:H2'	1:A:149:A:C8	2.35	0.62
1:A:1048:G:H5''	16:N:3:ARG:HG3	1.82	0.62
22:T:57:ARG:HE	22:T:102:GLY:HA3	1.59	0.62
1:A:1052:U:H2'	1:A:1055:A:OP1	2.00	0.62
5:C:191:THR:HG21	5:C:193:TYR:CZ	2.35	0.62
6:D:62:GLN:HE22	6:D:65:ARG:NH1	1.97	0.62
9:G:145:ALA:O	9:G:147:ALA:N	2.30	0.62
4:B:166:ASP:OD2	4:B:169:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:50:ALA:HA	21:S:58:VAL:O	2.00	0.62
4:B:80:ILE:HD12	4:B:208:ILE:HG12	1.82	0.62
1:A:1031:G:H2'	1:A:1032:G:C8	2.35	0.62
10:H:80:ILE:HG22	10:H:80:ILE:O	1.99	0.62
1:A:1315:U:OP2	21:S:6:LYS:NZ	2.33	0.62
14:L:24:VAL:HG12	14:L:24:VAL:O	2.00	0.62
14:L:34:ARG:O	14:L:61:THR:HG23	2.00	0.62
12:J:39:PRO:O	12:J:40:LEU:HB2	2.00	0.61
2:Y:34:G:H2'	2:Y:35:A:C8	2.35	0.61
1:A:112:G:N2	1:A:354:G:H5'	2.14	0.61
15:M:78:ILE:HA	15:M:81:LEU:HD21	1.82	0.61
21:S:51:VAL:O	21:S:58:VAL:HG22	2.00	0.61
7:E:5:ASP:CG	7:E:6:PHE:H	2.04	0.61
12:J:16:LEU:HD22	12:J:94:VAL:HG22	1.82	0.61
1:A:1369:C:H2'	1:A:1370:G:C8	2.34	0.61
5:C:112:SER:HB3	5:C:115:LEU:HD12	1.81	0.61
6:D:64:LEU:HD12	6:D:75:PHE:CZ	2.35	0.61
1:A:794:A:H2'	1:A:795:C:C6	2.34	0.61
5:C:126:ARG:O	5:C:127:ARG:HB2	1.99	0.61
4:B:59:GLU:HG3	4:B:60:ASP:H	1.65	0.61
14:L:75:HIS:CD2	14:L:77:LEU:H	2.18	0.61
18:P:74:LEU:HB3	18:P:79:VAL:HG21	1.82	0.61
1:A:353:A:H5'	1:A:353:A:C8	2.35	0.61
4:B:76:GLN:NE2	4:B:207:ALA:N	2.49	0.61
5:C:177:THR:O	5:C:177:THR:HG23	2.00	0.61
18:P:51:VAL:O	18:P:52:ASP:HB2	2.01	0.61
1:A:269:C:H2'	1:A:270:A:H8	1.62	0.61
4:B:101:MET:CE	4:B:108:ILE:HG21	2.30	0.61
18:P:20:VAL:HG11	18:P:32:TYR:HB2	1.81	0.61
1:A:1292:U:H5'	11:I:38:GLN:NE2	2.16	0.61
1:A:792:A:H4'	1:A:793:U:H5''	1.82	0.61
20:R:46:GLU:CD	20:R:46:GLU:H	2.04	0.61
4:B:76:GLN:HE21	4:B:207:ALA:H	1.47	0.61
12:J:49:VAL:O	12:J:60:ARG:HA	2.00	0.61
5:C:91:LEU:HD21	5:C:99:VAL:CG1	2.28	0.61
1:A:1193:G:O2'	1:A:1194:U:H5'	1.99	0.61
1:A:523:A:H61	14:L:92:ASP:HB2	1.65	0.61
1:A:148:G:H2'	1:A:149:A:H8	1.64	0.61
18:P:4:ILE:HG23	18:P:36:ILE:HD11	1.82	0.61
4:B:201:ILE:HG21	4:B:214:ILE:HG21	1.81	0.61
1:A:1259:C:H42	1:A:1276:G:H1	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:34:LEU:HD23	5:C:34:LEU:O	2.01	0.61
1:A:1286:A:H2'	1:A:1287:A:H4'	1.82	0.61
22:T:67:ALA:HB2	22:T:77:ALA:HB2	1.83	0.61
20:R:26:LEU:HD23	20:R:42:ARG:HD3	1.83	0.61
10:H:103:VAL:HG21	10:H:109:ILE:O	2.01	0.61
21:S:36:ARG:NH2	21:S:75:ALA:O	2.34	0.61
15:M:49:THR:HG22	15:M:51:ALA:N	2.15	0.61
1:A:64:G:O2'	1:A:65:U:OP2	2.19	0.61
6:D:13:ARG:HD2	6:D:38:TYR:O	2.01	0.61
7:E:26:PHE:N	7:E:26:PHE:CD1	2.69	0.61
12:J:45:ARG:HH11	12:J:45:ARG:CB	2.06	0.61
1:A:840:C:H5''	1:A:841:U:OP1	2.01	0.61
11:I:32:ASP:HB3	11:I:35:GLU:HB2	1.83	0.61
1:A:1427:U:H2'	1:A:1428:A:H8	1.65	0.61
1:A:190(L):U:O2	22:T:105:SER:HB2	2.00	0.61
15:M:36:LYS:HB2	15:M:59:TYR:HE2	1.66	0.61
1:A:989:C:O2'	1:A:990:C:H5'	2.00	0.61
1:A:77:G:O2'	1:A:78:G:H5'	2.01	0.61
1:A:1347:G:O2'	1:A:1348:U:P	2.59	0.61
14:L:126:LYS:H	14:L:126:LYS:HE3	1.65	0.61
1:A:1116:C:H2'	1:A:1117:G:C5'	2.30	0.61
1:A:1117:G:H8	1:A:1117:G:H5'	1.66	0.61
7:E:12:LEU:CD1	7:E:31:LEU:HB2	2.31	0.61
7:E:11:ILE:HB	7:E:31:LEU:HB3	1.83	0.61
1:A:979:C:H2'	1:A:980:C:H5'	1.83	0.61
1:A:1477:C:H2'	1:A:1478:C:C6	2.36	0.61
1:A:496:A:H4'	1:A:497:A:OP1	1.99	0.61
4:B:156:LYS:NZ	4:B:156:LYS:HA	2.15	0.61
16:N:36:PHE:O	16:N:36:PHE:CD1	2.54	0.61
4:B:76:GLN:HG3	4:B:206:ASP:OD1	2.01	0.60
9:G:23:VAL:O	9:G:27:ILE:HG13	2.00	0.60
19:Q:70:ARG:HG3	19:Q:70:ARG:HH11	1.66	0.60
16:N:9:LYS:HG3	16:N:21:TYR:O	2.01	0.60
7:E:43:LEU:HB2	7:E:136:MET:HE2	1.82	0.60
1:A:1250:A:H4'	11:I:68:GLY:CA	2.31	0.60
1:A:216:G:H2'	1:A:217:C:C6	2.36	0.60
1:A:1223:C:P	21:S:78:ARG:NH1	2.74	0.60
9:G:138:LYS:HE2	9:G:142:GLU:OE1	2.02	0.60
8:F:101:ALA:HA	20:R:28:GLU:HB3	1.83	0.60
1:A:918:A:H2'	1:A:919:A:C8	2.35	0.60
1:A:242:C:H2'	1:A:243:A:H5'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:89:ARG:HG2	14:L:97:ARG:CA	2.31	0.60
1:A:107:G:H2'	1:A:108:G:H5'	1.83	0.60
20:R:37:VAL:O	20:R:41:LYS:HG2	2.01	0.60
6:D:102:ASP:OD1	6:D:103:ASN:N	2.34	0.60
12:J:24:VAL:O	12:J:28:ARG:HG3	2.02	0.60
1:A:1370:G:O2'	1:A:1371:G:H5'	2.01	0.60
5:C:64:VAL:O	5:C:99:VAL:HG23	2.01	0.60
21:S:3:ARG:HH22	21:S:69:HIS:CE1	2.19	0.60
4:B:19:HIS:CD2	4:B:20:GLU:HG2	2.37	0.60
1:A:1278:U:H4'	1:A:1279:A:O5'	2.02	0.60
12:J:4:ILE:HA	12:J:100:THR:HA	1.84	0.60
22:T:54:LYS:HA	22:T:57:ARG:CD	2.31	0.60
11:I:97:LYS:CG	11:I:102:LEU:HD12	2.31	0.60
1:A:247:G:OP2	19:Q:100:LYS:HG3	2.01	0.60
4:B:143:GLU:O	4:B:147:LYS:HG3	2.02	0.60
18:P:34:GLU:OE2	18:P:55:ARG:HD3	2.02	0.60
9:G:135:VAL:O	9:G:139:GLU:HG3	2.02	0.60
18:P:51:VAL:HG12	18:P:52:ASP:N	2.17	0.60
1:A:977:A:H2'	1:A:978:A:H5''	1.84	0.60
1:A:314:C:O2'	1:A:315:A:H5'	2.00	0.60
4:B:135:GLN:HG2	4:B:139:LYS:NZ	2.16	0.60
20:R:86:VAL:O	20:R:87:ARG:CB	2.50	0.60
1:A:706:A:C1'	13:K:29:ILE:HD11	2.31	0.60
14:L:41:ARG:HG2	14:L:42:THR:O	2.02	0.60
15:M:84:ILE:CG2	21:S:65:ASN:HD22	2.14	0.60
8:F:97:PHE:HB2	20:R:32:ARG:HH21	1.66	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.37	0.60
1:A:420:U:H2'	1:A:422:C:C5	2.37	0.60
19:Q:66:SER:O	19:Q:70:ARG:NH1	2.34	0.60
7:E:12:LEU:HD13	7:E:31:LEU:HB2	1.83	0.60
20:R:53:ARG:HH11	20:R:59:SER:HA	1.66	0.60
11:I:48:GLU:N	11:I:49:PRO:HD2	2.16	0.60
5:C:94:LEU:HD22	5:C:95:THR:CG2	2.31	0.60
4:B:71:VAL:O	4:B:165:VAL:HG23	2.02	0.60
6:D:4:TYR:O	6:D:5:ILE:HB	2.00	0.60
1:A:743:U:H2'	1:A:744:C:C6	2.35	0.60
21:S:16:LEU:C	21:S:18:LYS:H	2.05	0.60
19:Q:97:SER:HB2	19:Q:102:GLY:O	2.00	0.60
1:A:76:C:O2'	1:A:77:G:H5'	2.01	0.60
12:J:49:VAL:HG13	16:N:41:ARG:HB2	1.84	0.60
1:A:542:G:H2'	1:A:543:C:H6	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:84:ILE:O	5:C:88:ARG:HD2	2.02	0.60
21:S:41:VAL:HG12	21:S:42:PRO:CD	2.32	0.60
1:A:1004:A:H5''	1:A:1025:U:O4	2.01	0.60
1:A:1064:G:H4'	1:A:1065:U:C5'	2.32	0.60
15:M:78:ILE:HA	15:M:81:LEU:CD2	2.31	0.60
9:G:71:PRO:HD3	9:G:103:TRP:HZ3	1.67	0.60
4:B:28:PHE:CZ	4:B:189:ASP:HA	2.37	0.60
12:J:8:LEU:HB2	12:J:70:ARG:HB2	1.83	0.60
15:M:22:ILE:CD1	15:M:25:ILE:HD12	2.32	0.60
17:O:75:PRO:O	17:O:79:ARG:HG3	2.02	0.60
5:C:145:GLY:O	5:C:146:ALA:HB3	2.02	0.60
4:B:187:LEU:HD23	4:B:201:ILE:O	2.02	0.59
1:A:1060:C:O2'	1:A:1061:G:H5'	2.01	0.59
1:A:542:G:OP1	6:D:10:ARG:NH2	2.35	0.59
1:A:1108:G:H5'	1:A:1191:A:H4'	1.82	0.59
1:A:748:C:HO2'	1:A:749:C:H6	1.43	0.59
12:J:89:ASP:C	12:J:90:LEU:HD12	2.23	0.59
1:A:673:G:H2'	1:A:674:G:C8	2.37	0.59
15:M:5:ALA:O	15:M:7:VAL:N	2.35	0.59
9:G:48:LYS:O	9:G:51:GLN:HB2	2.02	0.59
1:A:19:C:H2'	1:A:20:U:H6	1.68	0.59
7:E:57:LYS:HG2	7:E:61:TYR:CE2	2.37	0.59
13:K:74:ALA:C	13:K:76:GLY:H	2.06	0.59
1:A:484:G:H4'	1:A:485:G:O5'	2.02	0.59
12:J:38:ILE:HB	12:J:71:LEU:CB	2.24	0.59
1:A:1250:A:H5''	11:I:68:GLY:N	2.17	0.59
6:D:150:GLU:HG3	6:D:153:ARG:CZ	2.33	0.59
9:G:149:ARG:HB3	9:G:149:ARG:HH11	1.66	0.59
10:H:95:VAL:HB	10:H:99:GLU:HB2	1.83	0.59
1:A:219:C:H2'	1:A:220:G:O4'	2.02	0.59
1:A:285:G:O2'	1:A:286:G:H5'	2.01	0.59
8:F:80:ARG:NH1	8:F:88:VAL:HB	2.17	0.59
18:P:20:VAL:HG11	18:P:32:TYR:CG	2.38	0.59
4:B:181:PHE:HD2	10:H:70:GLN:HB3	1.66	0.59
13:K:98:LEU:HA	13:K:101:SER:HB3	1.84	0.59
1:A:1104:G:OP1	4:B:111:ARG:HD2	2.03	0.59
6:D:8:VAL:HG11	6:D:21:LEU:HB2	1.84	0.59
20:R:26:LEU:HD12	20:R:27:GLY:O	2.02	0.59
10:H:86:ILE:O	10:H:88:LYS:HG3	2.02	0.59
5:C:40:ARG:O	5:C:44:GLU:HB2	2.02	0.59
5:C:191:THR:HG22	5:C:193:TYR:N	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:51:GLN:HE21	9:G:58:PRO:HD3	1.68	0.59
6:D:23:GLY:HA3	6:D:112:VAL:CG1	2.32	0.59
1:A:254:G:OP1	19:Q:67:LYS:O	2.20	0.59
6:D:111:ALA:HA	6:D:161:ASN:HD22	1.68	0.59
1:A:1241:G:H2'	1:A:1242:C:H6	1.68	0.59
17:O:10:LYS:NZ	17:O:10:LYS:HA	2.18	0.59
8:F:2:ARG:HD2	8:F:69:GLU:CB	2.33	0.59
1:A:1053:G:C3'	1:A:1054:C:H5'	2.33	0.59
18:P:67:THR:HG22	18:P:68:ASP:N	2.18	0.59
4:B:73:THR:HG23	4:B:95:GLN:O	2.02	0.59
20:R:26:LEU:HD11	20:R:29:PHE:CE2	2.37	0.59
6:D:64:LEU:HD12	6:D:75:PHE:HZ	1.68	0.59
4:B:156:LYS:HA	4:B:156:LYS:HZ3	1.68	0.59
7:E:9:LYS:HB2	7:E:112:LEU:HD11	1.84	0.59
18:P:21:VAL:HG21	18:P:59:TRP:CD1	2.37	0.59
1:A:407:G:O2'	6:D:116:GLN:HG3	2.02	0.59
5:C:19:GLU:O	5:C:40:ARG:NH2	2.35	0.59
7:E:74:GLY:HA3	7:E:116:THR:HG22	1.85	0.59
1:A:1118:C:H1'	1:A:1179:A:C4	2.37	0.59
4:B:76:GLN:OE1	4:B:208:ILE:HG13	2.02	0.59
4:B:9:GLU:HB3	4:B:12:GLU:CD	2.22	0.59
12:J:20:ALA:O	12:J:24:VAL:HG23	2.03	0.59
7:E:89:ILE:HD13	7:E:90:VAL:H	1.67	0.59
7:E:87:SER:HB3	7:E:131:ILE:HD13	1.84	0.59
5:C:107:GLN:O	5:C:108:ASN:HB3	2.01	0.58
5:C:91:LEU:CD2	5:C:99:VAL:HG13	2.32	0.58
1:A:376:G:OP2	18:P:67:THR:HG21	2.02	0.58
19:Q:68:ARG:HH11	19:Q:68:ARG:CG	2.16	0.58
4:B:50:GLU:HB3	4:B:200:ILE:O	2.02	0.58
7:E:80:ILE:H	7:E:80:ILE:HD12	1.67	0.58
5:C:55:VAL:HG12	5:C:55:VAL:O	2.02	0.58
5:C:33:LEU:HD11	16:N:53:LEU:HD23	1.83	0.58
1:A:1454:G:H2'	1:A:1455:G:H8	1.68	0.58
1:A:620:C:N1	6:D:135:LEU:HD13	2.18	0.58
1:A:424:G:O2'	1:A:425:G:H5'	2.03	0.58
4:B:77:ALA:CB	4:B:211:ILE:HG21	2.32	0.58
4:B:87:ARG:HH12	4:B:233:SER:HA	1.68	0.58
1:A:501:C:H2'	1:A:502:G:C8	2.38	0.58
1:A:1497:G:H2'	1:A:1498:U:H5'	1.85	0.58
8:F:98:LEU:H	8:F:98:LEU:HD12	1.67	0.58
1:A:370:C:O2'	1:A:371:G:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:C:C1'	6:D:135:LEU:HD13	2.34	0.58
11:I:111:ARG:HD3	11:I:112:LYS:N	2.18	0.58
1:A:168:G:O2'	1:A:169:C:H5'	2.03	0.58
6:D:145:GLU:OE2	6:D:182:LYS:HD2	2.04	0.58
4:B:10:LEU:HD22	4:B:48:MET:HE1	1.84	0.58
1:A:255:G:H1'	19:Q:16:GLN:NE2	2.19	0.58
5:C:154:SER:O	5:C:165:THR:HA	2.03	0.58
4:B:112:VAL:C	4:B:114:ARG:H	2.06	0.58
4:B:140:HIS:HA	4:B:143:GLU:CG	2.33	0.58
6:D:150:GLU:HA	6:D:153:ARG:HG3	1.85	0.58
8:F:95:GLU:H	8:F:95:GLU:CD	2.06	0.58
4:B:19:HIS:NE2	4:B:206:ASP:HB3	2.19	0.58
1:A:1423:G:O2'	1:A:1424:C:H5'	2.03	0.58
1:A:1425:U:H2'	1:A:1426:C:H6	1.69	0.58
9:G:146:GLU:C	9:G:148:ASN:H	2.07	0.58
9:G:115:ARG:HB2	9:G:115:ARG:HH11	1.69	0.58
5:C:113:ALA:HB3	5:C:114:PRO:HD3	1.86	0.58
1:A:1061:G:C2'	1:A:1062:U:H5'	2.34	0.58
5:C:84:ILE:O	5:C:84:ILE:HG12	2.04	0.58
5:C:34:LEU:HD21	5:C:38:ARG:CZ	2.34	0.58
4:B:60:ASP:O	4:B:64:ARG:NH1	2.37	0.58
22:T:67:ALA:HA	22:T:73:HIS:H	1.68	0.58
14:L:27:LEU:C	14:L:29:GLY:N	2.57	0.58
15:M:37:THR:O	15:M:37:THR:HG22	2.03	0.58
22:T:94:ALA:O	22:T:95:ALA:HB3	2.02	0.58
5:C:54:ARG:HG2	5:C:55:VAL:H	1.67	0.58
17:O:29:VAL:HG11	17:O:67:LEU:HD21	1.85	0.58
4:B:111:ARG:HB3	4:B:149:LEU:HD11	1.85	0.58
1:A:883:C:O2'	1:A:884:U:H5'	2.04	0.58
10:H:64:LYS:HG2	10:H:79:VAL:HG21	1.86	0.58
22:T:36:LEU:HD12	22:T:62:LEU:HD12	1.84	0.58
12:J:3:LYS:N	12:J:75:ILE:HG12	2.18	0.58
5:C:179:ARG:HG3	5:C:179:ARG:HH11	1.68	0.58
1:A:940:C:H2'	1:A:941:G:C8	2.37	0.58
1:A:337:C:H2'	1:A:338:A:C8	2.38	0.58
13:K:126:ARG:O	13:K:127:LYS:HB2	2.03	0.58
11:I:117:HIS:C	11:I:118:LYS:HG3	2.24	0.58
4:B:91:PRO:HG3	4:B:154:LEU:HB2	1.86	0.58
13:K:21:ILE:HD13	13:K:94:ALA:HB3	1.86	0.58
6:D:24:GLU:HG2	6:D:25:ARG:N	2.19	0.58
19:Q:96:GLN:HB3	19:Q:103:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:84:GLN:O	12:J:88:LEU:HD12	2.04	0.58
4:B:82:ARG:O	4:B:86:GLU:HG3	2.04	0.58
1:A:1149:C:H2'	1:A:1150:U:C6	2.38	0.58
22:T:10:LEU:O	22:T:12:ALA:N	2.36	0.58
1:A:740:U:O2'	1:A:741:G:H5'	2.03	0.58
1:A:1320:C:N3	21:S:36:ARG:HG3	2.19	0.58
7:E:144:THR:H	7:E:147:ASP:HB2	1.68	0.58
1:A:444:C:H2'	1:A:445:G:H8	1.69	0.58
10:H:86:ILE:HD12	10:H:133:LEU:HD22	1.86	0.58
1:A:1454:G:O2'	1:A:1455:G:H5'	2.04	0.58
8:F:50:TYR:CE1	20:R:77:GLY:HA2	2.39	0.58
5:C:191:THR:CG2	5:C:192:THR:N	2.67	0.57
1:A:1352:C:H2'	1:A:1353:G:H8	1.68	0.57
9:G:52:GLU:C	9:G:53:LYS:HD2	2.24	0.57
1:A:824:C:H2'	1:A:825:G:C8	2.36	0.57
9:G:113:GLU:HG2	9:G:119:ARG:HG2	1.85	0.57
1:A:1216:G:H5''	16:N:5:ALA:HB2	1.86	0.57
16:N:37:PHE:CE2	16:N:53:LEU:HD13	2.39	0.57
1:A:1510:U:H2'	1:A:1511:G:C8	2.38	0.57
5:C:139:GLN:CA	5:C:139:GLN:HE21	2.17	0.57
1:A:243:A:H4'	1:A:244:U:C5'	2.24	0.57
8:F:4:TYR:CE2	8:F:72:VAL:HG21	2.39	0.57
4:B:100:GLY:C	4:B:108:ILE:HD12	2.25	0.57
5:C:159:GLY:HA2	5:C:193:TYR:CZ	2.39	0.57
1:A:1238:A:H5'	1:A:1336:C:N4	2.15	0.57
11:I:111:ARG:HD3	11:I:112:LYS:C	2.23	0.57
1:A:895:G:H2'	1:A:896:C:C6	2.39	0.57
19:Q:101:ARG:CZ	19:Q:101:ARG:HA	2.34	0.57
8:F:86:ARG:HH11	8:F:86:ARG:HG2	1.69	0.57
1:A:1152:A:H5''	12:J:13:HIS:CG	2.39	0.57
1:A:390:C:O3'	18:P:28:ARG:NH2	2.37	0.57
1:A:949:A:N7	15:M:106:ASN:ND2	2.52	0.57
1:A:765:G:H1	1:A:812:C:H2'	1.68	0.57
20:R:33:ASP:OD2	20:R:36:ASN:HB2	2.04	0.57
1:A:1342:C:O2'	1:A:1343:G:H5'	2.03	0.57
10:H:119:LEU:HD12	10:H:124:ALA:HA	1.85	0.57
1:A:976:G:H5'	1:A:1358:U:O2'	2.05	0.57
4:B:101:MET:HE3	4:B:108:ILE:HD13	1.86	0.57
1:A:1054:C:N3	2:Y:34:G:O4'	2.37	0.57
18:P:67:THR:HG22	18:P:69:THR:H	1.69	0.57
5:C:188:LEU:O	5:C:189:ALA:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:H5'	1:A:1258:G:H1'	1.86	0.57
1:A:1424:C:O2'	1:A:1425:U:H5'	2.04	0.57
16:N:29:ARG:HG2	16:N:29:ARG:HH11	1.69	0.57
1:A:407:G:H2'	1:A:408:A:H8	1.70	0.57
1:A:1258:G:O2'	1:A:1259:C:H5'	2.04	0.57
7:E:80:ILE:HD11	7:E:91:LEU:HB2	1.81	0.57
7:E:79:GLU:HG3	7:E:93:PRO:CD	2.28	0.57
16:N:25:VAL:HG12	16:N:38:GLY:O	2.03	0.57
14:L:42:THR:HA	14:L:53:ARG:O	2.04	0.57
19:Q:27:PHE:CE1	19:Q:36:ILE:HD11	2.38	0.57
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.39	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.57
21:S:19:VAL:HG13	21:S:20:LEU:N	2.20	0.57
1:A:954:G:H2'	1:A:955:U:H6	1.69	0.57
18:P:58:TYR:O	18:P:62:VAL:HG23	2.04	0.57
1:A:1338:G:H2'	1:A:1339:A:C8	2.40	0.57
19:Q:45:HIS:CD2	19:Q:47:PRO:HG3	2.39	0.57
1:A:1157:A:H4'	1:A:1158:C:O5'	2.04	0.57
14:L:60:LEU:HD21	14:L:85:ILE:HD12	1.85	0.57
1:A:560:U:H5'	1:A:566:G:N2	2.20	0.57
4:B:30:ARG:HG3	4:B:31:TYR:CD2	2.40	0.57
10:H:68:ARG:HH11	10:H:68:ARG:HG2	1.69	0.57
12:J:6:ILE:HG22	12:J:98:ILE:HG23	1.87	0.57
21:S:20:LEU:HA	21:S:23:ASN:ND2	2.19	0.57
1:A:1128:C:H42	1:A:1143:G:H1	1.53	0.57
1:A:1053:G:C4'	1:A:1054:C:H5'	2.34	0.57
1:A:1053:G:HO2'	1:A:1199:U:H5	1.53	0.57
5:C:136:GLN:O	5:C:139:GLN:HB2	2.05	0.57
6:D:191:ARG:O	6:D:191:ARG:HD2	2.05	0.57
1:A:1227:A:O3'	15:M:115:LYS:HE3	2.05	0.57
8:F:19:LEU:HD23	8:F:19:LEU:C	2.24	0.57
1:A:1060:C:C5	5:C:2:GLY:HA3	2.40	0.57
1:A:950:U:OP2	15:M:102:ARG:HG2	2.05	0.57
1:A:939:G:H5''	9:G:102:ARG:HH22	1.70	0.57
1:A:1117:G:H21	1:A:1180:A:H1'	1.69	0.57
19:Q:59:ILE:HG23	19:Q:71:PHE:HB3	1.87	0.57
9:G:114:ARG:HH11	9:G:114:ARG:HG2	1.70	0.57
1:A:1056:U:H5'	5:C:163:ALA:HB2	1.85	0.57
9:G:15:ASP:OD1	9:G:17:VAL:N	2.38	0.57
21:S:7:LYS:HG2	21:S:7:LYS:O	2.04	0.57
5:C:70:VAL:HG12	5:C:71:ALA:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:38:LEU:HD12	9:G:38:LEU:O	2.05	0.56
1:A:364:A:H62	14:L:28:LYS:NZ	2.02	0.56
1:A:865:A:H5'	1:A:1078:U:O4	2.05	0.56
7:E:30:ALA:O	7:E:45:PHE:HA	2.05	0.56
9:G:85:TYR:HD1	9:G:154:TYR:HE1	1.53	0.56
11:I:10:ARG:O	11:I:12:GLU:N	2.38	0.56
20:R:88:LYS:HG2	20:R:88:LYS:OXT	2.05	0.56
1:A:1477:C:H2'	1:A:1478:C:H6	1.70	0.56
8:F:48:LEU:HD13	8:F:52:ILE:HG13	1.87	0.56
12:J:51:ARG:HG3	12:J:59:SER:HB2	1.87	0.56
14:L:47:LYS:CG	14:L:48:PRO:HD3	2.35	0.56
4:B:230:VAL:HG12	4:B:231:GLU:N	2.20	0.56
2:Y:30:C:O2'	2:Y:31:C:H5'	2.04	0.56
14:L:89:ARG:HH22	14:L:97:ARG:HH21	1.52	0.56
1:A:1015:A:H2'	1:A:1016:A:C8	2.40	0.56
1:A:748:C:O2'	1:A:749:C:C6	2.56	0.56
1:A:882:C:O2'	1:A:883:C:H5'	2.04	0.56
14:L:8:ASN:O	14:L:12:ARG:HG3	2.05	0.56
1:A:1468:A:H2'	1:A:1469:G:O4'	2.06	0.56
21:S:20:LEU:HD12	21:S:21:GLU:N	2.20	0.56
8:F:97:PHE:HB2	20:R:32:ARG:NH2	2.20	0.56
1:A:748:C:O2'	1:A:749:C:H6	1.87	0.56
1:A:1121:U:H2'	1:A:1122:U:H6	1.71	0.56
1:A:127:G:HO2'	19:Q:2:PRO:N	2.03	0.56
1:A:176:C:H2'	1:A:177:C:H6	1.71	0.56
12:J:38:ILE:O	12:J:70:ARG:HA	2.06	0.56
6:D:58:LEU:O	6:D:62:GLN:HG2	2.05	0.56
4:B:64:ARG:HG2	4:B:64:ARG:O	2.05	0.56
1:A:112:G:H21	1:A:354:G:C5'	2.17	0.56
6:D:111:ALA:HB2	6:D:120:LEU:HD12	1.86	0.56
1:A:1163:C:H2'	1:A:1164:G:H8	1.70	0.56
1:A:1176:A:H2'	1:A:1177:G:C8	2.41	0.56
11:I:127:LYS:HZ3	11:I:127:LYS:H	1.51	0.56
6:D:131:ARG:H	6:D:131:ARG:HD2	1.71	0.56
1:A:1305:G:H5''	23:V:4:GLY:C	2.26	0.56
1:A:1125:U:H3	12:J:5:ARG:HE	1.54	0.56
1:A:1054:C:H2'	1:A:1055:A:H5''	1.88	0.56
4:B:140:HIS:HA	4:B:143:GLU:HG2	1.88	0.56
6:D:63:LYS:HD2	6:D:198:VAL:HG22	1.87	0.56
15:M:10:PRO:CB	15:M:18:ALA:HB1	2.20	0.56
21:S:42:PRO:HA	21:S:45:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:G:P	21:S:77:THR:HG21	2.46	0.56
5:C:131:ARG:O	5:C:135:LYS:HG3	2.06	0.56
1:A:748:C:H6	1:A:748:C:OP2	1.89	0.56
22:T:59:ALA:O	22:T:63:ILE:HG13	2.05	0.56
1:A:1007:C:H2'	1:A:1008:C:H6	1.71	0.56
7:E:82:VAL:HG11	7:E:137:GLU:HB3	1.87	0.56
7:E:24:ARG:HH11	7:E:24:ARG:HG2	1.70	0.56
5:C:85:ARG:HA	5:C:88:ARG:HB2	1.88	0.56
1:A:1005:A:C2'	1:A:1006:C:H5'	2.34	0.56
11:I:44:VAL:HG12	11:I:51:ARG:NH2	2.21	0.56
1:A:1312:G:O2'	1:A:1313:U:H5'	2.05	0.56
1:A:1311:G:N7	21:S:2:PRO:HA	2.21	0.56
1:A:1227:A:OP2	15:M:111:LYS:HE3	2.05	0.56
1:A:1187:G:OP1	11:I:113:LYS:HE2	2.05	0.56
6:D:121:VAL:O	6:D:134:ASP:HA	2.06	0.56
1:A:1256:A:O3'	1:A:1257:U:H4'	2.06	0.56
1:A:1305:G:OP2	1:A:1305:G:C8	2.59	0.56
4:B:162:ILE:CG2	4:B:164:VAL:HG23	2.36	0.56
11:I:17:VAL:HG11	11:I:81:ILE:HA	1.88	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.56
1:A:1234:C:O2'	1:A:1235:U:H5'	2.06	0.56
19:Q:24:GLU:CD	19:Q:37:LYS:HD3	2.26	0.56
8:F:22:GLU:O	8:F:26:ILE:HG13	2.05	0.56
1:A:112:G:H5'	1:A:389:A:H4'	1.88	0.56
1:A:1128:C:H1'	1:A:1146:A:H61	1.70	0.55
5:C:26:LYS:N	5:C:26:LYS:HD3	2.17	0.55
1:A:328:C:H4'	1:A:329:A:H5'	1.88	0.55
1:A:861:G:O2'	1:A:862:C:H5'	2.06	0.55
13:K:116:HIS:O	13:K:117:ASN:HB2	2.04	0.55
6:D:32:ALA:C	6:D:34:GLU:N	2.58	0.55
1:A:88:A:H2'	1:A:89:C:O4'	2.06	0.55
1:A:195:A:H4'	22:T:68:LYS:HE2	1.88	0.55
1:A:1441:G:H4'	1:A:1442:G:C5	2.40	0.55
4:B:97:TRP:HH2	4:B:176:GLU:CD	2.09	0.55
5:C:76:VAL:HG11	5:C:103:VAL:CG2	2.36	0.55
16:N:57:ARG:HG2	16:N:58:LYS:N	2.20	0.55
13:K:93:GLN:HE21	13:K:96:ARG:NH2	2.05	0.55
4:B:25:ASN:C	4:B:25:ASN:HD22	2.10	0.55
1:A:135:C:O2	18:P:1:MET:HB2	2.07	0.55
12:J:75:ILE:O	12:J:76:ASN:HB2	2.05	0.55
1:A:629:G:O2'	1:A:630:G:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:51:VAL:HG12	10:H:52:ASP:H	1.71	0.55
1:A:178:C:O2'	1:A:179:A:H5'	2.06	0.55
18:P:51:VAL:O	18:P:52:ASP:CB	2.55	0.55
1:A:1090:U:O2'	1:A:1091:U:H5'	2.06	0.55
1:A:450:G:N7	1:A:481:G:C6	2.74	0.55
1:A:1461:G:O2'	1:A:1462:G:H5'	2.06	0.55
20:R:47:THR:HG23	20:R:83:GLU:H	1.70	0.55
16:N:25:VAL:O	16:N:25:VAL:HG22	2.06	0.55
1:A:1064:G:H4'	1:A:1065:U:H5'	1.87	0.55
1:A:1412:C:H2'	1:A:1413:A:C8	2.41	0.55
18:P:81:ARG:HB2	18:P:81:ARG:NH1	2.20	0.55
1:A:1139:G:H4'	1:A:1140:C:H5'	1.87	0.55
4:B:18:GLY:HA2	4:B:41:ILE:HA	1.88	0.55
1:A:1392:G:O2'	1:A:1393:U:H5'	2.07	0.55
11:I:93:ARG:HD3	11:I:97:LYS:NZ	2.16	0.55
11:I:9:ARG:HG2	11:I:13:ALA:O	2.06	0.55
5:C:52:LEU:HD23	5:C:52:LEU:N	2.21	0.55
4:B:83:MET:HE2	4:B:234:PRO:HG2	1.87	0.55
10:H:86:ILE:HG22	10:H:87:SER:N	2.21	0.55
5:C:134:ILE:HG22	5:C:168:ALA:HB3	1.88	0.55
7:E:28:PHE:O	7:E:47:LYS:HA	2.06	0.55
21:S:44:MET:HA	21:S:47:HIS:HD2	1.71	0.55
4:B:55:PHE:HA	4:B:58:ILE:HD12	1.88	0.55
19:Q:65:ILE:N	19:Q:65:ILE:HD12	2.21	0.55
5:C:23:TYR:OH	12:J:9:ARG:HD3	2.06	0.55
1:A:406:G:H2'	1:A:407:G:H8	1.72	0.55
4:B:69:LEU:HD12	4:B:155:LEU:HD11	1.87	0.55
4:B:47:THR:HA	4:B:202:PRO:HG2	1.88	0.55
21:S:64:GLU:O	21:S:67:VAL:HG23	2.06	0.55
11:I:108:VAL:HG12	11:I:109:VAL:N	2.22	0.55
1:A:1216:G:O2'	1:A:1217:C:H5'	2.07	0.55
5:C:139:GLN:NE2	5:C:139:GLN:HA	2.22	0.55
1:A:1091:U:O2	1:A:1093:A:C8	2.60	0.55
1:A:993:G:H4'	1:A:994:A:OP2	2.06	0.55
1:A:832:C:O2'	1:A:833:U:H5'	2.06	0.55
1:A:1145:C:O2'	1:A:1146:A:H8	1.90	0.55
4:B:136:VAL:HA	4:B:139:LYS:CG	2.36	0.55
8:F:14:LEU:HA	8:F:18:GLN:HE21	1.69	0.55
1:A:1315:U:H2'	1:A:1316:G:O4'	2.07	0.55
1:A:414:A:OP2	1:A:428:G:N2	2.33	0.55
19:Q:45:HIS:NE2	19:Q:47:PRO:HG3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:30:LYS:C	6:D:32:ALA:H	2.09	0.55
1:A:192:U:C1'	22:T:103:GLY:HA2	2.37	0.55
8:F:87:ARG:NH1	8:F:87:ARG:HG3	2.10	0.55
1:A:701:C:O2'	1:A:702:A:OP2	2.21	0.55
18:P:10:GLY:HA3	18:P:14:ASN:O	2.06	0.55
4:B:12:GLU:C	4:B:14:GLY:N	2.60	0.55
4:B:80:ILE:CD1	4:B:208:ILE:HG23	2.35	0.55
4:B:142:LEU:O	4:B:144:ARG:N	2.40	0.55
5:C:70:VAL:O	5:C:106:VAL:HG23	2.06	0.55
1:A:640:A:O2'	1:A:641:U:H5'	2.07	0.55
12:J:46:ARG:HH11	12:J:64:GLU:HB3	1.71	0.55
1:A:248:C:O2'	1:A:249:U:H5'	2.06	0.55
1:A:858:G:O2'	1:A:859:A:H5'	2.07	0.55
1:A:961:U:C2'	1:A:962:C:H5'	2.37	0.55
9:G:90:GLU:H	9:G:155:ARG:HH12	1.54	0.54
6:D:151:LYS:N	6:D:151:LYS:HD2	2.14	0.54
11:I:93:ARG:HA	11:I:96:LEU:HB3	1.89	0.54
4:B:59:GLU:HB3	4:B:221:LEU:CD1	2.35	0.54
4:B:127:ILE:HB	4:B:128:GLU:OE2	2.06	0.54
15:M:36:LYS:HD2	15:M:59:TYR:CE2	2.42	0.54
6:D:122:ARG:HH21	6:D:134:ASP:CG	2.09	0.54
1:A:1109:C:OP2	5:C:176:HIS:CD2	2.60	0.54
15:M:22:ILE:HD12	15:M:25:ILE:HD12	1.88	0.54
1:A:1072:G:H2'	1:A:1073:U:C6	2.42	0.54
4:B:98:LEU:N	4:B:98:LEU:HD23	2.22	0.54
1:A:838:G:H2'	1:A:839:U:C5'	2.30	0.54
10:H:119:LEU:HB3	10:H:123:GLU:HB2	1.89	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.08	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.54
8:F:91:VAL:HG13	20:R:72:ARG:NH2	2.22	0.54
4:B:17:PHE:O	4:B:18:GLY:C	2.45	0.54
21:S:30:LEU:HD13	21:S:31:ILE:N	2.22	0.54
1:A:268:C:O2'	1:A:269:C:H5'	2.07	0.54
4:B:87:ARG:HH12	4:B:233:SER:CA	2.21	0.54
9:G:145:ALA:O	9:G:146:GLU:HB2	2.06	0.54
5:C:19:GLU:HB3	5:C:40:ARG:NH2	2.22	0.54
1:A:860:A:H2'	1:A:861:G:O4'	2.07	0.54
11:I:19:LEU:HB3	11:I:59:PHE:CD2	2.42	0.54
11:I:116:LYS:HE2	11:I:122:ALA:HB2	1.90	0.54
5:C:171:GLY:O	5:C:173:VAL:HG23	2.07	0.54
4:B:87:ARG:HH12	4:B:233:SER:CB	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:37:THR:CG2	15:M:55:ARG:HD2	2.38	0.54
9:G:140:ASP:HA	9:G:143:ARG:HD2	1.87	0.54
1:A:1420:C:H2'	1:A:1421:G:H8	1.73	0.54
5:C:177:THR:CG2	5:C:180:ALA:HB2	2.38	0.54
1:A:1128:C:H2'	1:A:1129:C:H5''	1.89	0.54
1:A:540:G:H2'	1:A:541:G:O4'	2.08	0.54
1:A:149:A:H2'	1:A:150:C:H6	1.70	0.54
4:B:25:ASN:HD22	4:B:27:LYS:H	1.53	0.54
19:Q:60:ILE:HD13	19:Q:61:GLU:N	2.22	0.54
18:P:81:ARG:HB2	18:P:81:ARG:HH11	1.73	0.54
14:L:59:ARG:NE	14:L:65:GLU:HG3	2.22	0.54
4:B:52:GLU:O	4:B:56:ARG:HG3	2.08	0.54
1:A:583:A:H2'	1:A:584:G:O4'	2.08	0.54
5:C:110:ASN:O	5:C:141:VAL:HG22	2.08	0.54
4:B:10:LEU:HD22	4:B:48:MET:HE2	1.88	0.54
4:B:80:ILE:O	4:B:80:ILE:HG22	2.06	0.54
5:C:15:THR:HG21	5:C:179:ARG:O	2.07	0.54
1:A:1125:U:H5''	1:A:1126:U:H5	1.73	0.54
6:D:57:ARG:NH1	6:D:205:GLU:OE2	2.40	0.54
12:J:46:ARG:HG2	12:J:46:ARG:HH11	1.71	0.54
1:A:485:G:O2'	1:A:486:U:P	2.65	0.54
15:M:107:ALA:O	15:M:111:LYS:HG3	2.08	0.54
1:A:789:U:H5'	1:A:1540:U:O2	2.07	0.54
13:K:13:GLN:HA	13:K:75:TYR:O	2.07	0.54
1:A:1305:G:N2	1:A:1331:G:C2'	2.71	0.54
15:M:6:GLY:O	15:M:7:VAL:HG22	2.08	0.54
1:A:344:A:H5''	1:A:345:C:H5	1.71	0.54
8:F:94:GLN:HE21	20:R:32:ARG:HH11	1.54	0.54
4:B:23:ARG:HH11	4:B:24:TRP:HA	1.72	0.54
16:N:3:ARG:NH2	16:N:6:LEU:HD11	2.23	0.54
6:D:78:LEU:HD22	6:D:96:LEU:HB3	1.89	0.54
22:T:101:GLY:C	22:T:103:GLY:H	2.11	0.54
1:A:1054:C:N4	2:Y:34:G:C8	2.76	0.54
15:M:5:ALA:O	15:M:6:GLY:C	2.46	0.54
20:R:53:ARG:NH1	20:R:59:SER:HA	2.22	0.54
18:P:38:TYR:CE2	18:P:50:LYS:HE2	2.43	0.54
17:O:6:GLU:H	17:O:6:GLU:CD	2.09	0.54
6:D:192:GLU:OE1	6:D:192:GLU:HA	2.08	0.54
19:Q:67:LYS:HG2	19:Q:68:ARG:N	2.23	0.54
1:A:659:U:O2'	1:A:660:G:H5'	2.08	0.54
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:108:ASN:HD21	5:C:110:ASN:HB2	1.73	0.54
1:A:1057:G:H2'	1:A:1058:G:O4'	2.08	0.54
1:A:1038:C:H2'	1:A:1039:C:C6	2.39	0.54
15:M:59:TYR:O	15:M:63:THR:HG22	2.08	0.54
11:I:23:ASN:HD21	11:I:25:LYS:HD2	1.73	0.54
1:A:1307:U:H2'	1:A:1308:U:C6	2.43	0.54
1:A:105:G:H2'	1:A:106:C:C6	2.42	0.54
22:T:56:MET:HE2	22:T:88:VAL:HB	1.89	0.54
4:B:187:LEU:HA	4:B:201:ILE:HB	1.89	0.53
8:F:2:ARG:HH11	8:F:69:GLU:CB	2.20	0.53
8:F:63:TYR:N	8:F:63:TYR:HD2	2.06	0.53
4:B:115:LEU:O	4:B:119:GLU:HG2	2.08	0.53
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.09	0.53
4:B:137:ARG:HH11	4:B:137:ARG:HB3	1.73	0.53
18:P:28:ARG:HG3	18:P:29:ASP:OD2	2.08	0.53
1:A:985:C:H2'	1:A:986:A:H8	1.71	0.53
7:E:116:THR:HG23	7:E:117:ASP:OD2	2.07	0.53
19:Q:4:LYS:HE3	19:Q:6:LEU:HD21	1.89	0.53
5:C:36:ASP:O	5:C:39:ILE:HB	2.07	0.53
1:A:352:C:H4'	1:A:354:G:OP1	2.08	0.53
6:D:135:LEU:HB2	6:D:138:TYR:HB2	1.91	0.53
1:A:1305:G:N2	1:A:1331:G:O2'	2.41	0.53
22:T:11:SER:HA	22:T:13:LEU:HD12	1.90	0.53
4:B:121:LEU:O	4:B:127:ILE:HG12	2.07	0.53
16:N:12:ARG:O	16:N:14:PRO:HD3	2.09	0.53
14:L:49:ASN:ND2	14:L:92:ASP:OD2	2.42	0.53
1:A:405:U:H3'	1:A:406:G:H5'	1.90	0.53
14:L:85:ILE:HG22	14:L:86:ARG:N	2.24	0.53
6:D:2:GLY:O	6:D:3:ARG:HD3	2.07	0.53
15:M:80:ARG:C	15:M:82:MET:H	2.10	0.53
13:K:54:ARG:NH1	13:K:54:ARG:HG3	2.24	0.53
21:S:30:LEU:O	21:S:31:ILE:HD13	2.08	0.53
8:F:22:GLU:OE1	8:F:25:ILE:HD12	2.08	0.53
1:A:1057:G:O2'	1:A:1058:G:H5'	2.07	0.53
4:B:136:VAL:HA	4:B:139:LYS:HG2	1.89	0.53
16:N:14:PRO:O	16:N:15:LYS:CB	2.55	0.53
14:L:26:ALA:O	14:L:27:LEU:O	2.26	0.53
6:D:98:GLU:HG2	6:D:189:PRO:HG3	1.91	0.53
1:A:1481:U:O2'	1:A:1482:G:H5'	2.07	0.53
1:A:1326:C:C5	23:V:6:ARG:NH2	2.76	0.53
1:A:1108:G:H4'	1:A:1191:A:O4'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:20:VAL:HG13	18:P:34:GLU:O	2.08	0.53
1:A:1281:U:H6	1:A:1281:U:H3'	1.74	0.53
6:D:165:MET:SD	6:D:168:ARG:HD3	2.48	0.53
4:B:10:LEU:N	4:B:10:LEU:HD23	2.23	0.53
1:A:1207:G:H2'	1:A:1208:C:H6	1.73	0.53
1:A:1222:G:O2'	1:A:1223:C:H5'	2.07	0.53
1:A:1004:A:H5''	1:A:1025:U:C4	2.44	0.53
8:F:44:GLY:HA3	8:F:59:TYR:CE1	2.44	0.53
13:K:57:THR:HG22	13:K:60:ALA:CB	2.39	0.53
20:R:59:SER:O	20:R:60:GLY:C	2.47	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.44	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.44	0.53
4:B:17:PHE:HA	4:B:42:ILE:HB	1.90	0.53
1:A:1399:C:C2	1:A:1502:A:N6	2.77	0.53
1:A:1054:C:C2'	1:A:1055:A:H5''	2.38	0.53
6:D:62:GLN:HE22	6:D:65:ARG:HH12	1.54	0.53
5:C:23:TYR:CE1	5:C:24:ALA:O	2.62	0.53
1:A:131:C:H2'	1:A:132:C:H6	1.74	0.53
1:A:162:A:H2'	1:A:163:C:O4'	2.09	0.53
1:A:1405:G:O4'	1:A:1519:A:H4'	2.09	0.53
19:Q:79:SER:O	19:Q:80:GLY:O	2.26	0.53
5:C:186:PHE:O	5:C:187:ALA:HB2	2.08	0.53
6:D:141:ARG:HG2	6:D:141:ARG:HH11	1.73	0.53
18:P:43:LYS:HA	18:P:48:TRP:HB3	1.90	0.53
1:A:1060:C:H5''	12:J:51:ARG:HB3	1.90	0.53
1:A:332:G:O2'	1:A:333:G:H5'	2.08	0.53
8:F:2:ARG:HD2	8:F:69:GLU:CG	2.39	0.53
15:M:85:GLY:O	15:M:86:CYS:O	2.27	0.53
1:A:404:U:O2'	1:A:405:U:H5'	2.09	0.53
1:A:955:U:O2'	1:A:956:U:H5'	2.09	0.53
12:J:6:ILE:HD11	12:J:72:VAL:HG11	1.90	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.56	0.53
4:B:142:LEU:HD22	4:B:146:GLN:CD	2.29	0.53
6:D:100:ARG:HH12	6:D:137:SER:HB3	1.72	0.53
11:I:49:PRO:O	11:I:52:ALA:HB3	2.09	0.53
1:A:1497:G:O2'	1:A:1498:U:H5'	2.09	0.53
1:A:401:C:H1'	1:A:622:A:H1'	1.90	0.53
1:A:974:A:OP2	16:N:41:ARG:NH1	2.42	0.53
1:A:1085:U:H3'	1:A:1086:U:C5	2.44	0.53
17:O:17:ARG:HG3	17:O:17:ARG:NH1	2.21	0.53
9:G:144:MET:C	9:G:145:ALA:O	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:C:H1'	14:L:15:ARG:HB3	1.90	0.53
13:K:16:SER:HA	13:K:79:SER:O	2.09	0.53
1:A:287:U:O2'	1:A:288:A:H5'	2.10	0.53
6:D:140:VAL:HG11	6:D:146:ILE:HD11	1.90	0.52
14:L:119:LYS:O	14:L:120:TYR:HB2	2.10	0.52
5:C:150:LYS:HG3	5:C:169:ALA:HB2	1.90	0.52
17:O:10:LYS:HA	17:O:10:LYS:HZ3	1.74	0.52
1:A:456:C:H2'	1:A:457:C:H6	1.73	0.52
14:L:39:VAL:HG12	14:L:40:VAL:N	2.23	0.52
1:A:1124:G:C5'	12:J:35:SER:O	2.55	0.52
15:M:17:VAL:O	15:M:20:THR:HB	2.09	0.52
7:E:93:PRO:HG2	10:H:105:ARG:CZ	2.39	0.52
22:T:43:LEU:HD11	22:T:55:ILE:HD12	1.91	0.52
4:B:101:MET:N	4:B:108:ILE:HD12	2.24	0.52
2:Y:29:A:H2'	2:Y:30:C:C5	2.44	0.52
1:A:1286:A:C8	1:A:1287:A:H4'	2.44	0.52
9:G:20:ASP:HB3	9:G:23:VAL:HG23	1.92	0.52
1:A:1004:A:H5''	1:A:1025:U:C5	2.45	0.52
20:R:26:LEU:C	20:R:26:LEU:HD12	2.29	0.52
11:I:53:VAL:HG21	11:I:85:LEU:HD21	1.90	0.52
1:A:364:A:H61	14:L:28:LYS:HE2	1.74	0.52
9:G:108:ALA:O	9:G:119:ARG:HD2	2.10	0.52
6:D:30:LYS:O	6:D:32:ALA:N	2.43	0.52
5:C:43:LEU:HD22	5:C:68:VAL:HG21	1.91	0.52
14:L:54:LYS:HD2	14:L:54:LYS:N	2.24	0.52
4:B:76:GLN:HE21	4:B:207:ALA:N	2.07	0.52
1:A:1250:A:C5'	11:I:68:GLY:H	2.22	0.52
1:A:1054:C:O2'	1:A:1055:A:H5''	2.09	0.52
1:A:922:G:H2'	1:A:923:A:C8	2.43	0.52
7:E:18:ARG:HH21	7:E:25:ARG:HB3	1.74	0.52
1:A:528:C:H5'	1:A:535:A:C6	2.43	0.52
9:G:124:LEU:O	9:G:127:ALA:HB3	2.09	0.52
1:A:957:U:H3	1:A:960:U:H5''	1.75	0.52
8:F:63:TYR:CD2	8:F:63:TYR:N	2.75	0.52
22:T:54:LYS:HA	22:T:57:ARG:HD2	1.92	0.52
4:B:132:LYS:HD3	4:B:135:GLN:OE1	2.09	0.52
1:A:1351:U:H4'	9:G:33:ASP:OD2	2.10	0.52
1:A:532:A:H2'	1:A:533:A:C5'	2.40	0.52
1:A:545:C:H5''	6:D:72:GLU:HG3	1.90	0.52
7:E:107:ARG:HG2	7:E:108:ALA:N	2.24	0.52
8:F:43:LEU:N	8:F:43:LEU:HD22	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:73:THR:O	4:B:75:LYS:N	2.43	0.52
1:A:1054:C:C3'	1:A:1054:C:O2	2.57	0.52
7:E:144:THR:HG23	7:E:146:ALA:H	1.75	0.52
11:I:19:LEU:HB3	11:I:59:PHE:CE2	2.45	0.52
1:A:1080:A:O3'	7:E:16:THR:OG1	2.27	0.52
4:B:200:ILE:HG22	4:B:202:PRO:HD3	1.92	0.52
12:J:16:LEU:CD2	12:J:94:VAL:HG22	2.39	0.52
21:S:28:LYS:HD3	21:S:31:ILE:CD1	2.40	0.52
4:B:100:GLY:HA3	4:B:104:ASN:HB3	1.92	0.52
4:B:138:LEU:HA	4:B:141:GLU:HB2	1.92	0.52
7:E:76:ILE:HD11	7:E:115:VAL:CG2	2.40	0.52
1:A:457:C:H2'	1:A:458:C:C6	2.45	0.52
1:A:124:G:C6	1:A:125:U:C4	2.97	0.52
7:E:60:TYR:HE1	7:E:64:ARG:NH2	2.07	0.52
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.10	0.52
4:B:76:GLN:HE22	4:B:208:ILE:N	2.08	0.52
12:J:19:SER:HB2	12:J:91:PRO:HG3	1.91	0.52
1:A:1300:G:O2'	1:A:1301:U:H6	1.93	0.52
15:M:22:ILE:O	15:M:23:TYR:O	2.28	0.52
1:A:1422:G:O2'	1:A:1423:G:H5'	2.09	0.52
1:A:392:G:H2'	1:A:393:A:H8	1.75	0.52
4:B:54:THR:HG23	4:B:199:TYR:HB3	1.92	0.52
1:A:586:C:O2'	1:A:587:G:H5'	2.10	0.52
1:A:1206:G:H2'	1:A:1207:G:C8	2.45	0.52
17:O:87:ILE:O	17:O:88:ARG:CB	2.58	0.52
13:K:54:ARG:HH11	13:K:54:ARG:HG3	1.75	0.52
1:A:457:C:H2'	1:A:458:C:H6	1.74	0.52
4:B:57:PHE:CE2	4:B:185:ILE:HD11	2.45	0.52
16:N:33:VAL:HA	16:N:40:CYS:HA	1.92	0.52
8:F:24:GLU:HG3	8:F:25:ILE:N	2.25	0.52
5:C:91:LEU:HD11	5:C:99:VAL:HG13	1.92	0.52
11:I:118:LYS:O	11:I:119:ALA:HB3	2.10	0.52
1:A:1394:A:C5	1:A:1501:C:H4'	2.44	0.52
7:E:36:ASP:OD1	7:E:38:GLN:N	2.40	0.52
18:P:2:VAL:O	18:P:64:ALA:HA	2.10	0.52
1:A:1160:G:O2'	1:A:1161:C:H5'	2.10	0.52
1:A:1470:G:O2'	1:A:1471:G:H5'	2.09	0.52
1:A:1373:G:O6	11:I:11:LYS:HE2	2.10	0.52
1:A:1300:G:HO2'	1:A:1301:U:H6	1.57	0.52
1:A:270:A:H2'	1:A:271:C:C6	2.45	0.52
9:G:146:GLU:HA	9:G:149:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:35:ARG:C	16:N:37:PHE:H	2.13	0.52
18:P:11:SER:OG	18:P:14:ASN:HB3	2.09	0.52
1:A:828:A:H2'	1:A:829:G:O4'	2.09	0.52
23:V:6:ARG:CD	23:V:15:ARG:HH12	2.19	0.51
7:E:18:ARG:HE	7:E:25:ARG:HB2	1.74	0.51
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.51
1:A:1030(C):G:H2'	1:A:1030(D):A:H8	1.76	0.51
14:L:85:ILE:CG2	14:L:98:TYR:HB3	2.40	0.51
14:L:59:ARG:HH21	14:L:65:GLU:HB3	1.75	0.51
9:G:122:HIS:HD2	9:G:125:MET:CE	2.23	0.51
1:A:1030:C:O2'	1:A:1030(A):G:H5'	2.10	0.51
1:A:434:U:H2'	1:A:435:C:C6	2.45	0.51
1:A:636:U:H2'	1:A:637:G:H8	1.74	0.51
21:S:9:VAL:HG12	21:S:10:PHE:N	2.25	0.51
12:J:4:ILE:HG13	12:J:74:ILE:O	2.11	0.51
5:C:181:ASN:C	5:C:182:ILE:HD12	2.30	0.51
16:N:25:VAL:O	16:N:25:VAL:HG13	2.10	0.51
21:S:45:VAL:HA	21:S:62:ILE:HG22	1.92	0.51
1:A:730:G:N2	1:A:765:G:H5''	2.25	0.51
1:A:498:U:O2'	1:A:499:A:H5'	2.10	0.51
4:B:227:GLY:O	4:B:229:VAL:N	2.39	0.51
10:H:83:ILE:O	10:H:83:ILE:HG23	2.10	0.51
17:O:36:ILE:HG12	17:O:59:MET:HE3	1.92	0.51
5:C:47:LEU:N	5:C:47:LEU:HD12	2.25	0.51
4:B:47:THR:HG23	4:B:202:PRO:O	2.10	0.51
12:J:8:LEU:CD2	12:J:96:ILE:HG12	2.39	0.51
1:A:664:G:H2'	1:A:666:G:OP1	2.10	0.51
19:Q:98:LEU:O	19:Q:98:LEU:HD12	2.09	0.51
1:A:948:C:O2'	1:A:949:A:H5'	2.11	0.51
14:L:126:LYS:CE	14:L:126:LYS:H	2.23	0.51
4:B:178:ARG:HH21	4:B:196:LEU:HA	1.75	0.51
14:L:50:SER:O	14:L:51:ALA:HB2	2.09	0.51
1:A:782:A:H2'	1:A:783:C:O4'	2.11	0.51
7:E:120:THR:HG23	7:E:121:LYS:N	2.25	0.51
1:A:52:G:O2'	1:A:53:A:H5'	2.11	0.51
1:A:192:U:H1'	22:T:103:GLY:HA2	1.93	0.51
9:G:51:GLN:NE2	9:G:56:GLN:O	2.44	0.51
4:B:124:SER:CB	4:B:125:PRO:HD2	2.37	0.51
1:A:945:G:C2	1:A:946:A:C8	2.97	0.51
1:A:537:G:OP1	14:L:113:ARG:NH2	2.43	0.51
10:H:85:ARG:CD	10:H:87:SER:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:121:PRO:HG2	13:K:126:ARG:CG	2.40	0.51
16:N:22:THR:O	16:N:23:ARG:HB2	2.08	0.51
5:C:20:SER:O	16:N:54:PRO:HB3	2.11	0.51
13:K:46:GLY:O	13:K:48:ILE:O	2.29	0.51
4:B:78:GLN:O	4:B:94:ASN:OD1	2.29	0.51
5:C:14:ILE:HD13	5:C:14:ILE:N	2.13	0.51
6:D:127:THR:CG2	6:D:147:ALA:HB3	2.36	0.51
21:S:40:ILE:HD13	21:S:62:ILE:HD11	1.91	0.51
20:R:25:THR:HG22	20:R:42:ARG:NH2	2.25	0.51
1:A:393:A:C2'	1:A:394:G:H5'	2.41	0.51
1:A:190(L):U:C2	22:T:105:SER:HB2	2.46	0.51
15:M:14:ARG:HH12	15:M:16:ASP:CG	2.13	0.51
22:T:50:GLU:HG3	22:T:100:ILE:HG13	1.92	0.51
5:C:195:VAL:O	5:C:196:LEU:HD23	2.09	0.51
6:D:8:VAL:HG13	6:D:21:LEU:CD1	2.33	0.51
5:C:70:VAL:HG21	5:C:76:VAL:HG21	1.93	0.51
15:M:62:ASN:O	15:M:63:THR:CB	2.58	0.51
1:A:1132:C:H2'	1:A:1133:G:C8	2.46	0.51
1:A:404:U:H2'	1:A:405:U:C6	2.46	0.51
17:O:54:ARG:O	17:O:58:MET:HG3	2.11	0.51
12:J:34:VAL:HG12	12:J:35:SER:N	2.25	0.51
1:A:1206:G:H2'	1:A:1207:G:H8	1.76	0.51
6:D:103:ASN:O	6:D:106:TYR:HB3	2.11	0.51
4:B:57:PHE:CD2	4:B:185:ILE:HD11	2.46	0.51
1:A:51:A:H4'	1:A:52:G:C5'	2.41	0.51
9:G:28:ASN:OD1	9:G:36:LYS:NZ	2.44	0.51
1:A:973:G:H3'	1:A:974:A:H5''	1.93	0.51
19:Q:97:SER:N	19:Q:103:GLY:HA2	2.23	0.51
1:A:161:A:H2'	1:A:162:A:C8	2.46	0.51
11:I:48:GLU:HG3	11:I:101:PHE:CZ	2.46	0.51
21:S:52:TYR:HA	21:S:56:GLN:O	2.11	0.51
18:P:4:ILE:CG2	18:P:36:ILE:HD11	2.40	0.51
16:N:23:ARG:NH1	16:N:30:ALA:HB2	2.26	0.51
8:F:7:ASN:HB2	8:F:89:MET:HB3	1.92	0.51
12:J:87:THR:O	12:J:87:THR:HG22	2.11	0.51
5:C:114:PRO:O	5:C:118:GLN:HB2	2.10	0.51
4:B:189:ASP:O	4:B:191:ASP:N	2.43	0.51
12:J:4:ILE:HA	12:J:100:THR:CA	2.41	0.51
12:J:4:ILE:O	12:J:73:ASP:HA	2.11	0.51
10:H:4:ASP:OD2	10:H:7:ALA:HB2	2.10	0.51
11:I:32:ASP:O	11:I:35:GLU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:G:H2'	1:A:503:C:C6	2.46	0.51
1:A:991:U:C4	1:A:1212:U:H1'	2.46	0.51
13:K:126:ARG:O	13:K:127:LYS:CB	2.59	0.51
21:S:11:VAL:HG13	21:S:38:SER:HB2	1.92	0.51
9:G:16:LEU:H	9:G:16:LEU:HD22	1.75	0.51
4:B:14:GLY:C	4:B:15:VAL:HG22	2.31	0.51
4:B:42:ILE:HD11	4:B:189:ASP:HB2	1.92	0.51
21:S:30:LEU:HD13	21:S:31:ILE:O	2.11	0.51
1:A:1299:A:C8	1:A:1301:U:H1'	2.45	0.51
1:A:922:G:H5'	7:E:20:GLN:NE2	2.25	0.51
16:N:9:LYS:HD3	16:N:9:LYS:C	2.31	0.51
1:A:1165:C:O2'	1:A:1166:G:H5'	2.10	0.51
2:Y:38:PSU:H2'	2:Y:39:G:O4'	2.11	0.51
1:A:1110:A:O5'	1:A:1110:A:H8	1.94	0.51
4:B:42:ILE:HD12	4:B:203:GLY:HA2	1.94	0.50
1:A:877:C:H1'	10:H:3:THR:HG23	1.90	0.50
11:I:77:ILE:O	11:I:79:LEU:N	2.43	0.50
1:A:1152:A:H2'	1:A:1153:C:H6	1.74	0.50
1:A:730:G:H21	1:A:765:G:H5''	1.76	0.50
1:A:532:A:H2'	1:A:533:A:H5''	1.93	0.50
21:S:81:ARG:O	21:S:81:ARG:HD3	2.11	0.50
19:Q:81:ARG:O	19:Q:81:ARG:HG3	2.11	0.50
22:T:94:ALA:O	22:T:95:ALA:CB	2.59	0.50
18:P:19:ILE:N	18:P:19:ILE:HD12	2.26	0.50
9:G:156:TRP:C	9:G:156:TRP:CD1	2.84	0.50
1:A:575:G:H4'	1:A:575:G:OP1	2.11	0.50
22:T:100:ILE:C	22:T:102:GLY:N	2.63	0.50
8:F:87:ARG:HH11	8:F:87:ARG:CG	2.15	0.50
13:K:84:VAL:CG2	13:K:110:ASP:HA	2.37	0.50
1:A:112:G:H4'	1:A:389:A:C5'	2.41	0.50
1:A:1270:C:O2'	1:A:1271:G:H5'	2.12	0.50
13:K:93:GLN:NE2	13:K:96:ARG:HH21	2.09	0.50
19:Q:80:GLY:O	19:Q:81:ARG:CB	2.60	0.50
1:A:106:C:O2	1:A:379:C:H4'	2.11	0.50
1:A:258:G:O2'	1:A:259:G:H5'	2.12	0.50
23:V:24:ARG:O	23:V:25:LYS:CB	2.59	0.50
19:Q:12:SER:HB3	19:Q:20:THR:HB	1.93	0.50
4:B:204:ASN:ND2	4:B:206:ASP:H	2.09	0.50
4:B:98:LEU:O	4:B:101:MET:HG2	2.12	0.50
1:A:1195:C:C3'	1:A:1196:U:H5''	2.35	0.50
13:K:110:ASP:HB2	20:R:88:LYS:CD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:115:LYS:O	14:L:117:ARG:N	2.40	0.50
19:Q:2:PRO:O	19:Q:3:LYS:C	2.50	0.50
12:J:82:ILE:O	12:J:86:MET:HB2	2.11	0.50
10:H:30:ARG:O	10:H:33:GLU:HB3	2.12	0.50
4:B:16:HIS:O	4:B:17:PHE:O	2.30	0.50
21:S:16:LEU:O	21:S:18:LYS:N	2.44	0.50
15:M:26:GLY:O	15:M:28:ALA:N	2.44	0.50
1:A:217:C:H2'	1:A:218:C:H6	1.77	0.50
4:B:134:GLU:O	4:B:134:GLU:HG2	2.12	0.50
1:A:438:G:C4'	1:A:439:A:OP1	2.57	0.50
1:A:691:G:O2'	1:A:797:C:H4'	2.11	0.50
1:A:547:A:H4'	1:A:548:G:O5'	2.11	0.50
1:A:554:C:H2'	1:A:555:C:C6	2.47	0.50
1:A:397:A:H5'	1:A:398:C:OP1	2.10	0.50
1:A:1250:A:H5''	11:I:68:GLY:H	1.75	0.50
5:C:15:THR:HB	5:C:181:ASN:HB2	1.94	0.50
1:A:939:G:H5''	9:G:102:ARG:CZ	2.40	0.50
5:C:134:ILE:HG23	5:C:151:VAL:HB	1.93	0.50
1:A:485:G:C2'	1:A:486:U:OP2	2.59	0.50
1:A:335:C:H2'	1:A:336:C:C6	2.47	0.50
1:A:189:G:H2'	1:A:190:C:C6	2.47	0.50
22:T:44:ALA:C	22:T:46:GLU:H	2.15	0.50
1:A:1298:C:H4'	1:A:1299:A:O4'	2.11	0.50
5:C:5:ILE:N	5:C:5:ILE:HD12	2.26	0.50
22:T:67:ALA:O	22:T:73:HIS:ND1	2.44	0.50
11:I:48:GLU:HG3	11:I:101:PHE:HZ	1.75	0.50
1:A:1201:A:O2'	1:A:1202:G:OP2	2.28	0.50
5:C:42:LEU:HD12	5:C:94:LEU:HD12	1.92	0.50
19:Q:68:ARG:NH1	19:Q:68:ARG:CG	2.73	0.50
1:A:458:C:H2'	1:A:459:G:H8	1.76	0.50
19:Q:33:GLY:O	19:Q:34:LYS:C	2.49	0.50
4:B:16:HIS:HA	4:B:204:ASN:CB	2.39	0.50
21:S:77:THR:HG22	21:S:78:ARG:N	2.27	0.50
9:G:42:ILE:HG22	9:G:120:ILE:HD12	1.94	0.50
6:D:142:PRO:CB	6:D:187:ARG:HH21	2.24	0.50
6:D:187:ARG:HG3	6:D:188:LEU:N	2.27	0.50
1:A:1491:G:C5	24:A:1545:PAR:H21	2.46	0.50
9:G:16:LEU:N	9:G:16:LEU:HD22	2.26	0.50
1:A:657:G:H4'	17:O:28:GLN:HG2	1.93	0.50
1:A:1256:A:H61	1:A:1278:U:H1'	1.76	0.50
1:A:1223:C:OP1	1:A:1224:G:H3'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:G:OP1	1:A:367:U:H2'	2.11	0.50
10:H:60:ARG:HH11	10:H:60:ARG:HG3	1.76	0.50
13:K:17:GLY:HA3	13:K:77:MET:HE1	1.94	0.50
23:V:12:LYS:HG2	23:V:22:ARG:HB3	1.92	0.50
14:L:60:LEU:N	14:L:64:TYR:O	2.37	0.50
1:A:731:G:H5'	1:A:766:A:H4'	1.93	0.50
22:T:26:ASN:OD1	22:T:71:THR:HA	2.12	0.50
12:J:6:ILE:HA	12:J:97:GLU:O	2.12	0.50
1:A:1347:G:H2'	1:A:1373:G:H1	1.77	0.50
18:P:67:THR:CG2	18:P:68:ASP:N	2.74	0.50
15:M:88:ARG:HH11	21:S:3:ARG:HH21	1.58	0.50
1:A:1499:A:C1'	1:A:1520:G:H5'	2.41	0.50
11:I:17:VAL:HG21	11:I:81:ILE:N	2.27	0.50
9:G:113:GLU:H	9:G:113:GLU:CD	2.16	0.50
4:B:23:ARG:NH1	4:B:24:TRP:HA	2.27	0.50
1:A:1090:U:H2'	1:A:1091:U:H6	1.77	0.50
18:P:45:THR:HB	18:P:46:PRO:HD2	1.94	0.50
1:A:431:A:O2'	1:A:432:A:H5'	2.12	0.50
6:D:83:SER:HA	6:D:89:THR:OG1	2.12	0.50
20:R:40:LEU:HB3	20:R:79:LEU:HD11	1.94	0.50
1:A:109:A:H2'	1:A:326:G:N2	2.26	0.50
4:B:189:ASP:HB3	4:B:203:GLY:O	2.12	0.49
5:C:14:ILE:H	5:C:14:ILE:CD1	2.12	0.49
5:C:86:VAL:O	5:C:89:GLU:HB3	2.12	0.49
9:G:51:GLN:C	9:G:53:LYS:H	2.15	0.49
5:C:24:ALA:CB	5:C:32:LEU:HD12	2.38	0.49
1:A:436:C:H2'	1:A:437:U:C6	2.47	0.49
1:A:1405:G:O2'	1:A:1406:U:H5'	2.12	0.49
14:L:61:THR:C	14:L:63:GLY:H	2.15	0.49
12:J:47:PHE:HD2	16:N:34:TYR:CD2	2.30	0.49
16:N:24:CYS:HB3	16:N:28:GLY:H	1.77	0.49
15:M:44:ARG:HB3	15:M:46:LYS:HG2	1.94	0.49
16:N:44:LEU:O	16:N:44:LEU:HD12	2.11	0.49
7:E:150:ARG:HH11	7:E:150:ARG:HG3	1.75	0.49
16:N:45:ARG:NH1	16:N:45:ARG:HG3	2.26	0.49
22:T:54:LYS:HA	22:T:57:ARG:HD3	1.94	0.49
11:I:7:THR:HG22	11:I:8:GLY:N	2.26	0.49
5:C:22:TRP:CG	5:C:59:ARG:HD2	2.47	0.49
17:O:70:LEU:HD13	17:O:78:TYR:HA	1.93	0.49
5:C:139:GLN:O	5:C:140:ARG:C	2.50	0.49
23:V:24:ARG:O	23:V:25:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:57:GLU:O	9:G:60:LYS:HB2	2.11	0.49
7:E:143:ARG:NH1	10:H:77:GLU:OE2	2.39	0.49
1:A:1368:G:OP1	12:J:62:HIS:HE1	1.94	0.49
1:A:1056:U:O2'	1:A:1057:G:H5'	2.12	0.49
4:B:110:GLN:O	4:B:114:ARG:HB2	2.12	0.49
1:A:1196:U:OP1	1:A:1197:G:H5'	2.12	0.49
4:B:119:GLU:HG3	4:B:153:ARG:HH22	1.77	0.49
4:B:87:ARG:NH2	4:B:233:SER:HB2	2.27	0.49
1:A:533:A:O2'	1:A:534:U:OP1	2.30	0.49
1:A:952:U:O4	15:M:104:ARG:HD3	2.12	0.49
1:A:413:G:N2	1:A:428:G:O2'	2.42	0.49
9:G:71:PRO:HD3	9:G:103:TRP:CZ3	2.45	0.49
15:M:14:ARG:NH1	15:M:16:ASP:OD1	2.45	0.49
1:A:570:G:H2'	1:A:571:U:C6	2.47	0.49
4:B:97:TRP:HZ2	4:B:102:LEU:HD13	1.76	0.49
6:D:8:VAL:C	6:D:10:ARG:N	2.65	0.49
15:M:40:ASN:HB3	15:M:43:THR:HG23	1.94	0.49
1:A:939:G:H2'	1:A:940:C:H6	1.78	0.49
1:A:922:G:H4'	7:E:20:GLN:HA	1.95	0.49
9:G:146:GLU:C	9:G:148:ASN:N	2.66	0.49
7:E:13:ILE:HG13	7:E:13:ILE:O	2.11	0.49
1:A:197:A:N1	1:A:220:G:O2'	2.41	0.49
13:K:19:ALA:HB2	13:K:80:VAL:HG21	1.94	0.49
10:H:45:ILE:HG13	10:H:47:GLY:H	1.77	0.49
8:F:35:ALA:O	8:F:36:ARG:CB	2.59	0.49
1:A:1053:G:N7	1:A:1200:C:H5'	2.27	0.49
4:B:118:LEU:HD11	4:B:141:GLU:HB3	1.94	0.49
5:C:23:TYR:HE2	12:J:9:ARG:HG3	1.78	0.49
14:L:55:VAL:HG12	14:L:56:ALA:N	2.24	0.49
5:C:6:HIS:CD2	5:C:8:ILE:H	2.24	0.49
4:B:54:THR:O	4:B:58:ILE:HG13	2.11	0.49
1:A:961:U:H2'	1:A:962:C:H5'	1.93	0.49
11:I:126:SER:O	11:I:128:ARG:N	2.45	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.48	0.49
1:A:653:A:C8	10:H:56:LYS:HG2	2.47	0.49
1:A:99:C:H2'	1:A:101:A:O4'	2.13	0.49
1:A:200:G:H2'	1:A:201:C:O4'	2.11	0.49
12:J:3:LYS:HG2	12:J:75:ILE:HG23	1.95	0.49
1:A:1251:A:H2'	1:A:1252:A:H8	1.73	0.49
7:E:76:ILE:HD13	7:E:118:ILE:HD12	1.95	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:45:VAL:HA	15:M:48:LEU:HG	1.94	0.49
1:A:668:G:O2'	17:O:46:HIS:CD2	2.66	0.49
1:A:1278:U:C5'	1:A:1279:A:H5'	2.43	0.49
12:J:34:VAL:HG22	12:J:74:ILE:CG2	2.35	0.49
21:S:30:LEU:C	21:S:30:LEU:HD13	2.32	0.49
12:J:49:VAL:O	12:J:60:ARG:CA	2.61	0.49
5:C:182:ILE:N	5:C:182:ILE:HD12	2.27	0.49
4:B:97:TRP:CZ2	4:B:101:MET:HB2	2.48	0.49
4:B:114:ARG:O	4:B:117:GLU:HB3	2.12	0.49
11:I:51:ARG:HB2	11:I:51:ARG:NH1	2.27	0.49
14:L:53:ARG:HG2	14:L:69:TYR:CE1	2.41	0.49
1:A:1314:C:H3'	21:S:6:LYS:HZ3	1.75	0.49
7:E:101:ILE:HD12	7:E:119:LEU:HD23	1.95	0.49
22:T:101:GLY:O	22:T:103:GLY:N	2.45	0.49
1:A:971:G:OP1	1:A:972:C:H5"	2.13	0.49
1:A:1085:U:H3'	1:A:1086:U:H5	1.78	0.49
15:M:84:ILE:HG22	21:S:65:ASN:ND2	2.24	0.49
1:A:1228:C:H4'	15:M:116:THR:HA	1.95	0.49
9:G:87:VAL:HG11	9:G:154:TYR:O	2.13	0.49
11:I:20:ARG:O	11:I:60:ASP:N	2.45	0.49
6:D:119:GLN:CG	6:D:123:HIS:CD2	2.95	0.49
4:B:74:LYS:HZ2	4:B:206:ASP:HA	1.77	0.49
12:J:3:LYS:C	12:J:4:ILE:HG13	2.32	0.49
1:A:1347:G:C8	11:I:107:ARG:NH1	2.81	0.49
1:A:1073:U:H2'	1:A:1074:G:C8	2.48	0.49
1:A:1111:A:H61	5:C:177:THR:HA	1.78	0.49
9:G:115:ARG:HB3	9:G:118:VAL:HG23	1.94	0.49
5:C:139:GLN:HE21	5:C:139:GLN:HA	1.77	0.49
1:A:1245:A:H2'	1:A:1246:C:C6	2.48	0.49
1:A:427:U:OP1	6:D:13:ARG:NH2	2.45	0.49
2:Y:40:G:H2'	2:Y:41:U:C6	2.48	0.49
13:K:57:THR:HG23	13:K:60:ALA:H	1.76	0.49
1:A:1480:G:O2'	1:A:1481:U:H5'	2.12	0.49
1:A:637:G:O2'	1:A:638:G:H5'	2.13	0.49
13:K:27:ASN:HA	13:K:56:GLY:HA2	1.95	0.49
6:D:118:ARG:HG3	6:D:136:PRO:HB3	1.95	0.49
7:E:145:LYS:O	7:E:149:GLU:HB2	2.12	0.49
7:E:15:ARG:O	7:E:16:THR:O	2.31	0.48
4:B:13:ALA:C	4:B:15:VAL:N	2.66	0.48
22:T:12:ALA:N	22:T:13:LEU:HD12	2.20	0.48
4:B:102:LEU:HD12	4:B:102:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:G:H5'	1:A:1191:A:C4'	2.43	0.48
4:B:124:SER:HB2	4:B:125:PRO:CD	2.39	0.48
1:A:613:C:O2'	1:A:614:A:H5'	2.13	0.48
12:J:42:THR:HG23	12:J:67:THR:C	2.34	0.48
10:H:51:VAL:HG21	10:H:60:ARG:HG2	1.95	0.48
17:O:66:LEU:O	17:O:69:TYR:HB3	2.13	0.48
15:M:65:LYS:O	15:M:70:LEU:HG	2.14	0.48
13:K:48:ILE:CG2	13:K:49:GLY:N	2.58	0.48
12:J:35:SER:HB2	12:J:72:VAL:O	2.12	0.48
1:A:349:A:C3'	1:A:350:G:H5''	2.43	0.48
4:B:97:TRP:CE2	4:B:101:MET:HG3	2.48	0.48
21:S:63:THR:HG22	21:S:64:GLU:N	2.28	0.48
1:A:131:C:H2'	1:A:132:C:C6	2.48	0.48
1:A:1499:A:O2'	1:A:1500:A:H5'	2.12	0.48
22:T:96:GLY:O	22:T:97:ALA:CB	2.61	0.48
1:A:980:C:H2'	1:A:981:U:O4'	2.12	0.48
8:F:48:LEU:HD13	8:F:52:ILE:CG1	2.43	0.48
1:A:797:C:OP1	13:K:124:LYS:HD3	2.12	0.48
1:A:596:C:O2'	1:A:597:G:H5'	2.12	0.48
1:A:735:C:O2'	1:A:736:C:H5'	2.12	0.48
7:E:15:ARG:O	7:E:27:ARG:O	2.31	0.48
1:A:1278:U:H4'	1:A:1279:A:O4'	2.12	0.48
1:A:350:G:H5'	1:A:350:G:H8	1.78	0.48
4:B:141:GLU:O	4:B:145:LEU:HG	2.14	0.48
9:G:42:ILE:CG2	9:G:120:ILE:HD12	2.42	0.48
1:A:628:G:H2'	1:A:629:G:H8	1.78	0.48
4:B:69:LEU:HD23	4:B:70:PHE:N	2.27	0.48
10:H:10:LEU:HD22	10:H:83:ILE:HD11	1.96	0.48
13:K:44:SER:H	13:K:47:VAL:HB	1.77	0.48
1:A:519:C:H2'	1:A:520:A:C8	2.49	0.48
1:A:60:A:H4'	1:A:61:G:O5'	2.13	0.48
12:J:6:ILE:CG2	12:J:98:ILE:HG23	2.43	0.48
12:J:71:LEU:O	12:J:72:VAL:HB	2.12	0.48
1:A:974:A:OP1	1:A:974:A:H8	1.95	0.48
12:J:84:GLN:C	12:J:88:LEU:HD12	2.34	0.48
7:E:76:ILE:HD11	7:E:115:VAL:HG21	1.94	0.48
1:A:1005:A:H2'	1:A:1006:C:C5'	2.42	0.48
5:C:58:GLU:H	5:C:65:ALA:HB3	1.78	0.48
5:C:10:PHE:O	5:C:178:LEU:HD11	2.13	0.48
18:P:19:ILE:HG22	18:P:36:ILE:CG1	2.43	0.48
11:I:118:LYS:O	11:I:120:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:29:TYR:CZ	16:N:54:PRO:HG2	2.49	0.48
17:O:61:GLY:O	17:O:64:ARG:HG2	2.13	0.48
7:E:33:VAL:HG11	7:E:109:ILE:HA	1.95	0.48
1:A:925:G:C6	1:A:927:G:N7	2.81	0.48
10:H:3:THR:HG23	10:H:4:ASP:N	2.29	0.48
1:A:1001:A:H2'	1:A:1002:G:C8	2.48	0.48
1:A:407:G:H2'	1:A:408:A:C8	2.47	0.48
11:I:19:LEU:HD23	11:I:61:ALA:HB2	1.95	0.48
7:E:41:VAL:HG13	7:E:113:ALA:HA	1.94	0.48
1:A:115:G:H1'	1:A:116:A:N7	2.29	0.48
4:B:13:ALA:C	4:B:15:VAL:H	2.15	0.48
1:A:1123:A:O2'	1:A:1124:G:H5'	2.13	0.48
1:A:1277:C:O2'	1:A:1279:A:H1'	2.14	0.48
5:C:119:ARG:O	5:C:122:GLU:N	2.46	0.48
1:A:364:A:N6	14:L:28:LYS:NZ	2.61	0.48
1:A:22:G:H4'	1:A:885:G:C8	2.49	0.48
5:C:29:TYR:OH	16:N:54:PRO:HG2	2.13	0.48
10:H:45:ILE:C	10:H:47:GLY:H	2.17	0.48
6:D:119:GLN:HG3	6:D:123:HIS:CD2	2.48	0.48
1:A:1360:A:O2'	1:A:1361:G:H5'	2.14	0.48
1:A:119:A:H4'	1:A:120:A:O5'	2.14	0.48
4:B:238:LEU:C	4:B:240:GLN:H	2.16	0.48
4:B:17:PHE:HD2	4:B:44:LEU:HD11	1.79	0.48
12:J:94:VAL:HG12	12:J:95:GLU:N	2.27	0.48
15:M:40:ASN:HD22	15:M:41:PRO:N	2.10	0.48
6:D:59:ARG:NH2	6:D:62:GLN:HG3	2.29	0.48
13:K:109:VAL:HG22	20:R:86:VAL:HA	1.95	0.48
17:O:26:GLU:HA	17:O:81:LEU:HD11	1.96	0.48
1:A:35:G:H2'	1:A:36:C:H6	1.76	0.48
1:A:1333:A:H2'	1:A:1334:G:O4'	2.14	0.48
1:A:1247:U:O2'	1:A:1248:A:H5'	2.14	0.48
1:A:157:G:O2'	1:A:158:G:H5'	2.13	0.48
1:A:521:G:OP1	14:L:73:GLU:O	2.31	0.48
6:D:80:GLU:O	6:D:84:LYS:HG3	2.13	0.48
1:A:452:A:HO2'	1:A:453:A:H8	1.59	0.48
1:A:674:G:H2'	1:A:675:A:H8	1.78	0.48
5:C:87:LEU:C	5:C:89:GLU:N	2.66	0.48
4:B:136:VAL:HG12	4:B:140:HIS:NE2	2.28	0.48
14:L:126:LYS:HZ1	14:L:127:GLU:N	2.11	0.48
1:A:112:G:C2'	1:A:113:G:H5'	2.43	0.48
21:S:4:SER:O	21:S:5:LEU:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:143:ARG:O	9:G:145:ALA:O	2.31	0.48
5:C:151:VAL:HG12	5:C:152:ILE:N	2.27	0.48
5:C:157:ILE:HG21	5:C:164:ARG:NH2	2.28	0.48
11:I:4:TYR:CZ	11:I:88:TYR:HD1	2.32	0.48
16:N:35:ARG:O	16:N:37:PHE:N	2.47	0.48
1:A:992:U:H4'	1:A:993:G:O5'	2.14	0.48
15:M:80:ARG:C	15:M:82:MET:N	2.66	0.48
15:M:11:ARG:HA	15:M:45:VAL:HB	1.96	0.48
4:B:76:GLN:OE1	4:B:76:GLN:C	2.51	0.48
12:J:16:LEU:O	12:J:19:SER:N	2.47	0.48
1:A:1064:G:C4'	1:A:1065:U:H5'	2.43	0.48
1:A:1202:G:H2'	1:A:1203:C:O4'	2.14	0.48
1:A:628:G:H2'	1:A:629:G:C8	2.49	0.48
14:L:25:PRO:C	14:L:27:LEU:N	2.66	0.48
12:J:42:THR:HG23	12:J:68:HIS:HA	1.94	0.48
4:B:25:ASN:ND2	4:B:27:LYS:H	2.12	0.48
10:H:103:VAL:HG21	10:H:109:ILE:C	2.34	0.48
7:E:57:LYS:HG2	7:E:61:TYR:HE2	1.77	0.48
6:D:94:LEU:HD12	6:D:191:ARG:HD3	1.96	0.48
1:A:653:A:OP1	10:H:56:LYS:NZ	2.40	0.48
1:A:983:A:H2	1:A:984:C:C6	2.31	0.48
1:A:1371:G:OP1	11:I:11:LYS:O	2.31	0.48
1:A:1074:G:O3'	4:B:103:THR:HG22	2.14	0.48
5:C:179:ARG:HG3	5:C:179:ARG:NH1	2.29	0.48
1:A:1178:G:P	11:I:97:LYS:HZ2	2.36	0.48
5:C:155:GLY:O	5:C:156:ARG:CB	2.62	0.48
5:C:72:LYS:HE2	5:C:75:VAL:CG2	2.44	0.48
2:Y:30:C:H2'	2:Y:31:C:H6	1.79	0.48
10:H:63:LEU:H	10:H:63:LEU:HD22	1.78	0.48
7:E:51:VAL:CB	7:E:52:PRO:HD3	2.41	0.48
18:P:20:VAL:HG12	18:P:21:VAL:N	2.29	0.48
1:A:1314:C:H3'	21:S:6:LYS:HZ1	1.77	0.48
5:C:157:ILE:CG2	5:C:164:ARG:HH21	2.26	0.48
20:R:38:GLU:HA	20:R:38:GLU:OE2	2.14	0.48
1:A:176:C:H2'	1:A:177:C:C6	2.48	0.48
1:A:738:C:OP1	8:F:92:LYS:HE2	2.13	0.48
6:D:76:ARG:HG2	6:D:76:ARG:HH11	1.79	0.48
1:A:1044:A:H2'	1:A:1045:C:C5'	2.43	0.48
11:I:10:ARG:HH22	11:I:107:ARG:NH2	2.11	0.47
1:A:1392:G:O2'	1:A:1502:A:H5''	2.13	0.47
1:A:1298:C:C4	9:G:114:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:C:H42	2:Y:34:G:C1'	2.27	0.47
4:B:144:ARG:HG3	4:B:145:LEU:N	2.29	0.47
14:L:114:LYS:HE2	14:L:125:PRO:HG3	1.96	0.47
18:P:18:ARG:HD3	18:P:35:LYS:CD	2.44	0.47
1:A:941:G:O2'	1:A:942:G:H5'	2.14	0.47
1:A:1281:U:H3'	1:A:1281:U:C6	2.48	0.47
9:G:72:ARG:HH12	9:G:138:LYS:HZ1	1.60	0.47
10:H:112:LEU:CD2	10:H:112:LEU:N	2.76	0.47
5:C:95:THR:C	5:C:97:LYS:H	2.18	0.47
5:C:130:VAL:HG21	5:C:157:ILE:HG23	1.96	0.47
1:A:1216:G:H5''	16:N:5:ALA:CB	2.44	0.47
7:E:74:GLY:CA	7:E:116:THR:HG22	2.44	0.47
19:Q:3:LYS:HD3	19:Q:61:GLU:O	2.13	0.47
5:C:155:GLY:O	5:C:196:LEU:HD22	2.14	0.47
13:K:84:VAL:HG11	13:K:95:ILE:HD11	1.96	0.47
9:G:72:ARG:HH12	9:G:138:LYS:HZ3	1.61	0.47
1:A:1520:G:O2'	1:A:1521:G:H5'	2.14	0.47
5:C:95:THR:O	5:C:97:LYS:N	2.43	0.47
19:Q:67:LYS:O	19:Q:69:LYS:N	2.46	0.47
1:A:353:A:C5'	1:A:353:A:H8	2.27	0.47
10:H:126:LYS:C	10:H:128:GLY:H	2.17	0.47
1:A:322:C:O2'	1:A:323:U:H5'	2.14	0.47
1:A:567:G:H2'	1:A:568:G:O4'	2.14	0.47
4:B:73:THR:O	4:B:74:LYS:C	2.52	0.47
11:I:10:ARG:HG2	11:I:11:LYS:N	2.29	0.47
4:B:102:LEU:CD1	4:B:102:LEU:N	2.76	0.47
6:D:8:VAL:CG2	6:D:115:ARG:NH1	2.72	0.47
5:C:75:VAL:O	5:C:83:ARG:HD3	2.14	0.47
9:G:43:PHE:O	9:G:46:ALA:HB3	2.14	0.47
18:P:67:THR:HG22	18:P:69:THR:N	2.29	0.47
8:F:14:LEU:HB3	8:F:18:GLN:HB2	1.96	0.47
7:E:120:THR:CG2	7:E:121:LYS:N	2.77	0.47
1:A:147:G:O2'	1:A:148:G:H5'	2.15	0.47
1:A:235:C:H5'	19:Q:70:ARG:HD3	1.96	0.47
5:C:130:VAL:O	5:C:134:ILE:HG13	2.13	0.47
9:G:31:MET:SD	9:G:34:GLY:HA2	2.55	0.47
1:A:975:A:O2'	16:N:32:SER:HA	2.14	0.47
8:F:62:TRP:C	8:F:63:TYR:HD2	2.17	0.47
1:A:1056:U:C5'	5:C:163:ALA:HB2	2.45	0.47
6:D:126:ILE:HG22	6:D:127:THR:N	2.29	0.47
13:K:108:ILE:O	13:K:109:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:A:H2'	1:A:384:G:H5'	1.96	0.47
1:A:533:A:O2'	1:A:534:U:P	2.72	0.47
1:A:56:U:H2'	1:A:57:G:C8	2.49	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.50	0.47
18:P:26:ARG:HD3	18:P:31:LYS:N	2.28	0.47
4:B:15:VAL:HB	4:B:210:SER:HB2	1.97	0.47
4:B:77:ALA:HB1	4:B:211:ILE:HG21	1.95	0.47
1:A:1277:C:HO2'	1:A:1279:A:C1'	2.27	0.47
21:S:31:ILE:O	21:S:32:LYS:HB3	2.14	0.47
1:A:1075:C:H5'	4:B:103:THR:HG21	1.95	0.47
11:I:93:ARG:NH1	11:I:97:LYS:NZ	2.62	0.47
1:A:1004:A:N7	1:A:1037:C:N3	2.61	0.47
18:P:3:LYS:HD2	18:P:24:ALA:HB2	1.95	0.47
1:A:411:A:N6	1:A:413:G:N2	2.63	0.47
5:C:131:ARG:HG3	5:C:135:LYS:HE3	1.96	0.47
20:R:34:TYR:O	20:R:73:ALA:HB2	2.14	0.47
1:A:1176:A:H2'	1:A:1177:G:H8	1.79	0.47
7:E:82:VAL:HG21	7:E:138:ALA:HA	1.96	0.47
6:D:98:GLU:HG2	6:D:194:LEU:HD11	1.95	0.47
11:I:10:ARG:O	11:I:11:LYS:C	2.52	0.47
1:A:1302:U:OP2	15:M:17:VAL:HG13	2.15	0.47
5:C:195:VAL:C	5:C:196:LEU:HD23	2.35	0.47
19:Q:98:LEU:HA	19:Q:102:GLY:HA2	1.96	0.47
1:A:781:A:H2'	1:A:782:A:C5'	2.44	0.47
7:E:102:ALA:HB1	7:E:120:THR:HG21	1.97	0.47
18:P:43:LYS:HB3	18:P:48:TRP:CD1	2.50	0.47
10:H:35:ILE:O	10:H:39:LEU:HD22	2.14	0.47
1:A:427:U:OP2	6:D:36:ARG:NH2	2.47	0.47
6:D:36:ARG:N	6:D:37:PRO:CD	2.60	0.47
5:C:113:ALA:HA	5:C:202:ILE:HD11	1.97	0.47
11:I:10:ARG:HG2	11:I:10:ARG:HH11	1.78	0.47
12:J:60:ARG:N	12:J:60:ARG:HD2	2.29	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.47
8:F:67:MET:HE1	8:F:72:VAL:HA	1.96	0.47
5:C:15:THR:O	5:C:16:ARG:CB	2.62	0.47
4:B:231:GLU:CB	4:B:232:PRO:CD	2.89	0.47
12:J:81:THR:C	12:J:83:GLU:H	2.18	0.47
1:A:920:U:H2'	1:A:921:U:C6	2.49	0.47
13:K:34:ASP:HB2	13:K:35:PRO:HD2	1.95	0.47
5:C:132:ARG:O	5:C:135:LYS:N	2.48	0.47
15:M:31:LYS:O	15:M:35:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:C:N4	16:N:18:VAL:HG12	2.30	0.47
1:A:1501:C:OP2	1:A:1504:G:H2'	2.15	0.47
6:D:35:ARG:O	6:D:36:ARG:HB2	2.14	0.47
1:A:1073:U:H2'	1:A:1074:G:H8	1.80	0.47
1:A:1206:G:C6	1:A:1207:G:C6	3.03	0.47
5:C:72:LYS:HE2	5:C:75:VAL:HG21	1.97	0.47
1:A:1194:U:O2'	1:A:1195:C:H5'	2.15	0.47
12:J:9:ARG:HB3	12:J:9:ARG:NH1	2.29	0.47
1:A:1343:G:OP1	11:I:125:TYR:HE2	1.98	0.47
1:A:921:U:H2'	1:A:922:G:O4'	2.15	0.47
9:G:146:GLU:HA	9:G:149:ARG:HD3	1.97	0.47
10:H:51:VAL:HG21	10:H:60:ARG:CG	2.44	0.47
4:B:24:TRP:N	4:B:24:TRP:CD1	2.83	0.47
1:A:1439:C:H2'	1:A:1440:C:C6	2.50	0.47
4:B:204:ASN:HD22	4:B:206:ASP:H	1.61	0.47
4:B:75:LYS:HA	4:B:78:GLN:HB2	1.97	0.47
5:C:180:ALA:HB1	5:C:203:PHE:CE1	2.49	0.47
1:A:204:U:H6	1:A:204:U:O5'	1.97	0.47
5:C:35:GLU:O	5:C:36:ASP:C	2.53	0.47
4:B:59:GLU:O	4:B:63:MET:HG2	2.14	0.47
18:P:5:ARG:HH21	18:P:28:ARG:HA	1.80	0.47
6:D:173:TRP:HB2	6:D:187:ARG:O	2.15	0.47
1:A:1226:C:C4	15:M:104:ARG:HG3	2.50	0.47
1:A:1232:U:P	11:I:124:GLN:HE21	2.38	0.47
1:A:1347:G:O2'	1:A:1348:U:OP2	2.33	0.47
6:D:70:ILE:HG23	6:D:74:GLN:HB2	1.97	0.47
1:A:1066:C:O2'	1:A:1067:A:H5'	2.14	0.47
18:P:21:VAL:HG21	18:P:59:TRP:CG	2.50	0.47
4:B:194:PRO:O	4:B:196:LEU:N	2.48	0.47
11:I:48:GLU:N	11:I:49:PRO:CD	2.78	0.47
7:E:43:LEU:HD11	7:E:132:ALA:HB1	1.96	0.47
1:A:1244:C:O2'	1:A:1245:A:H5'	2.15	0.47
17:O:63:ARG:O	17:O:66:LEU:N	2.47	0.47
1:A:607:A:O2'	1:A:608:A:H5'	2.15	0.47
6:D:19:LEU:HD22	6:D:67:ILE:CG1	2.45	0.47
1:A:1042:G:O2'	1:A:1043:C:H5'	2.15	0.47
1:A:1372:U:O2'	1:A:1373:G:H5'	2.15	0.46
15:M:23:TYR:CB	15:M:67:GLU:HA	2.46	0.46
8:F:2:ARG:CD	8:F:69:GLU:HG2	2.45	0.46
1:A:1111:A:N6	5:C:177:THR:HA	2.30	0.46
22:T:100:ILE:O	22:T:101:GLY:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:93:ARG:CD	11:I:97:LYS:HZ1	2.17	0.46
6:D:61:LYS:NZ	6:D:62:GLN:NE2	2.63	0.46
1:A:327:A:O3'	1:A:328:C:H4'	2.15	0.46
1:A:922:G:H5'	7:E:19:MET:O	2.15	0.46
13:K:33:THR:HB	13:K:38:ASN:C	2.35	0.46
1:A:1017:G:H2'	1:A:1018:C:C6	2.50	0.46
1:A:408:A:O2'	1:A:409:G:H5'	2.15	0.46
13:K:57:THR:HG22	13:K:60:ALA:HB2	1.97	0.46
1:A:485:G:O2'	1:A:486:U:OP2	2.33	0.46
13:K:26:ASN:O	13:K:27:ASN:HB2	2.15	0.46
1:A:603:U:H2'	1:A:604:G:H8	1.80	0.46
21:S:30:LEU:C	21:S:31:ILE:HD13	2.36	0.46
21:S:41:VAL:CG1	21:S:42:PRO:CD	2.92	0.46
1:A:376:G:O3'	18:P:5:ARG:HD2	2.16	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.73	0.46
18:P:9:PHE:CD2	18:P:18:ARG:HG3	2.51	0.46
14:L:51:ALA:O	14:L:52:LEU:HD23	2.15	0.46
15:M:59:TYR:CD1	15:M:59:TYR:C	2.88	0.46
5:C:167:TRP:O	5:C:168:ALA:HB3	2.15	0.46
13:K:74:ALA:C	13:K:76:GLY:N	2.69	0.46
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.46
4:B:227:GLY:C	4:B:229:VAL:H	2.18	0.46
18:P:82:GLN:O	18:P:83:GLU:C	2.53	0.46
1:A:1060:C:O2	1:A:1198:G:C2	2.68	0.46
1:A:1060:C:H5	5:C:2:GLY:HA3	1.78	0.46
12:J:48:THR:HG23	12:J:62:HIS:CD2	2.50	0.46
5:C:174:PRO:HB2	5:C:177:THR:CG2	2.41	0.46
1:A:1125:U:H3	12:J:5:ARG:NE	2.14	0.46
9:G:23:VAL:HG13	9:G:43:PHE:CE2	2.51	0.46
14:L:75:HIS:HD2	14:L:77:LEU:N	2.11	0.46
7:E:18:ARG:NE	7:E:25:ARG:HB2	2.30	0.46
9:G:141:VAL:O	9:G:144:MET:N	2.48	0.46
5:C:145:GLY:O	5:C:146:ALA:CB	2.64	0.46
12:J:38:ILE:HD12	12:J:71:LEU:CD1	2.46	0.46
10:H:104:ARG:O	10:H:105:ARG:C	2.54	0.46
1:A:1206:G:H1'	5:C:193:TYR:O	2.16	0.46
5:C:5:ILE:H	5:C:5:ILE:HD12	1.80	0.46
1:A:1190:G:P	5:C:5:ILE:HG13	2.56	0.46
9:G:50:ILE:O	9:G:50:ILE:HG22	2.16	0.46
9:G:51:GLN:C	9:G:53:LYS:N	2.68	0.46
1:A:113:G:C1'	1:A:354:G:H5'	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:U:OP2	24:A:1545:PAR:N24	2.43	0.46
9:G:78:ARG:HD2	9:G:156:TRP:CE3	2.50	0.46
14:L:93:LEU:O	14:L:96:VAL:HG23	2.15	0.46
20:R:18:ARG:HA	20:R:18:ARG:NE	2.30	0.46
15:M:20:THR:C	15:M:22:ILE:H	2.18	0.46
22:T:13:LEU:N	22:T:13:LEU:HD12	2.13	0.46
7:E:89:ILE:HD13	7:E:90:VAL:N	2.30	0.46
1:A:628:G:O2'	1:A:629:G:H5'	2.15	0.46
5:C:134:ILE:CG2	5:C:168:ALA:HB3	2.46	0.46
5:C:170:GLN:O	5:C:171:GLY:O	2.33	0.46
14:L:59:ARG:NH2	14:L:65:GLU:HB3	2.31	0.46
1:A:1229:A:H2'	1:A:1230:C:C6	2.51	0.46
1:A:359:U:O2'	1:A:360:A:H5'	2.16	0.46
1:A:28:G:O2'	1:A:296:U:OP1	2.33	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.97	0.46
8:F:1:MET:CE	8:F:1:MET:H3	2.27	0.46
1:A:760:G:H2'	1:A:761:G:H5'	1.98	0.46
1:A:1441:G:H4'	1:A:1442:G:C4	2.51	0.46
1:A:333:G:H4'	22:T:16:HIS:NE2	2.30	0.46
4:B:116:GLU:HA	4:B:119:GLU:CG	2.45	0.46
1:A:1320:C:C2	21:S:72:GLY:HA3	2.51	0.46
4:B:212:GLN:NE2	4:B:216:SER:HB2	2.31	0.46
4:B:84:GLU:HB3	4:B:219:VAL:CG2	2.37	0.46
10:H:63:LEU:HD22	10:H:63:LEU:N	2.30	0.46
15:M:36:LYS:CB	15:M:59:TYR:HE2	2.29	0.46
19:Q:69:LYS:C	19:Q:70:ARG:HG3	2.35	0.46
12:J:42:THR:HG21	12:J:66:ARG:HB2	1.98	0.46
1:A:179:A:H2'	1:A:180:U:C6	2.51	0.46
1:A:1478:C:O2'	1:A:1479:C:H5'	2.15	0.46
1:A:636:U:H2'	1:A:637:G:C8	2.50	0.46
22:T:26:ASN:HA	22:T:71:THR:HG23	1.97	0.46
22:T:26:ASN:OD1	22:T:71:THR:HG23	2.16	0.46
1:A:967:C:O3'	11:I:128:ARG:NH2	2.49	0.46
19:Q:48:GLU:O	19:Q:49:GLU:C	2.53	0.46
6:D:163:GLU:HA	6:D:163:GLU:OE2	2.15	0.46
1:A:1296:C:H4'	1:A:1302:U:C5	2.51	0.46
8:F:2:ARG:HD2	8:F:69:GLU:HG2	1.96	0.46
1:A:674:G:H2'	1:A:675:A:C8	2.51	0.46
1:A:203:U:H4'	1:A:204:U:OP1	2.16	0.46
12:J:9:ARG:CB	12:J:9:ARG:NH1	2.78	0.46
22:T:74:LYS:HB3	22:T:75:ASN:H	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:119:LYS:O	14:L:120:TYR:CB	2.63	0.46
10:H:9:MET:SD	10:H:32:LYS:HB3	2.55	0.46
11:I:104:ARG:O	11:I:105:ASP:C	2.54	0.46
4:B:32:ILE:HD13	4:B:40:HIS:CD2	2.51	0.46
8:F:30:LEU:HB3	8:F:35:ALA:HB3	1.98	0.46
5:C:147:LYS:HE3	5:C:203:PHE:CE2	2.51	0.46
1:A:1053:G:O2'	1:A:1199:U:H5	1.99	0.46
19:Q:97:SER:C	19:Q:99:SER:H	2.14	0.46
6:D:62:GLN:HA	6:D:62:GLN:NE2	2.31	0.46
1:A:528:C:N4	14:L:49:ASN:HD21	2.14	0.46
11:I:89:ASN:O	11:I:92:TYR:HB2	2.16	0.46
19:Q:70:ARG:HH11	19:Q:70:ARG:CG	2.29	0.46
22:T:95:ALA:O	22:T:96:GLY:C	2.54	0.46
6:D:109:GLY:C	6:D:111:ALA:N	2.69	0.46
1:A:6:G:H4'	1:A:298:A:H4'	1.98	0.46
18:P:7:ALA:O	18:P:17:TYR:HA	2.15	0.46
15:M:108:ARG:HD3	15:M:114:ARG:NH1	2.31	0.46
5:C:156:ARG:NH2	5:C:161:GLU:HA	2.31	0.46
1:A:848:C:H2'	1:A:849:C:C6	2.50	0.46
5:C:88:ARG:HG3	5:C:101:LEU:CD1	2.45	0.46
1:A:1353:G:O2'	1:A:1354:C:H5'	2.15	0.46
20:R:87:ARG:HB3	20:R:88:LYS:H	1.49	0.46
1:A:1381:U:C2'	1:A:1382:C:H5'	2.46	0.46
1:A:413:G:H2'	1:A:428:G:H22	1.79	0.46
9:G:145:ALA:O	9:G:146:GLU:CB	2.63	0.46
17:O:70:LEU:C	17:O:72:ARG:H	2.19	0.46
1:A:1441:G:H1'	1:A:1460:A:H61	1.81	0.46
11:I:8:GLY:CA	11:I:79:LEU:HB3	2.46	0.46
6:D:100:ARG:HH12	6:D:137:SER:CB	2.29	0.46
21:S:40:ILE:CD1	21:S:62:ILE:HD11	2.46	0.46
16:N:11:LYS:O	16:N:13:THR:N	2.48	0.46
14:L:75:HIS:HA	14:L:102:ARG:HH22	1.80	0.46
1:A:1495:U:H2'	1:A:1496:C:H6	1.80	0.46
1:A:1183:A:O2'	1:A:1184:G:P	2.74	0.46
11:I:111:ARG:HD3	11:I:112:LYS:O	2.16	0.46
1:A:1230:C:O2'	1:A:1231:G:H5'	2.16	0.46
9:G:79:ARG:HH12	9:G:82:GLY:HA2	1.80	0.46
6:D:24:GLU:CG	6:D:25:ARG:N	2.79	0.45
6:D:26:CYS:HA	6:D:31:CYS:HB2	1.98	0.45
1:A:1256:A:H5'	1:A:1258:G:O4'	2.16	0.45
1:A:244:U:O4	1:A:906:G:H1'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:3:THR:HG23	10:H:4:ASP:H	1.81	0.45
22:T:16:HIS:O	22:T:17:ARG:C	2.53	0.45
1:A:1053:G:C4	1:A:1199:U:C5	3.04	0.45
14:L:47:LYS:HG2	14:L:48:PRO:HD3	1.98	0.45
5:C:83:ARG:HA	5:C:86:VAL:CG2	2.44	0.45
5:C:50:ALA:HB1	5:C:70:VAL:CG1	2.37	0.45
9:G:32:ARG:O	9:G:33:ASP:HB2	2.16	0.45
1:A:813:U:OP1	1:A:904:C:H5'	2.17	0.45
14:L:114:LYS:HE3	14:L:114:LYS:CA	2.44	0.45
11:I:48:GLU:HA	11:I:51:ARG:NH1	2.31	0.45
1:A:1225:A:H2'	1:A:1225:A:N3	2.31	0.45
5:C:129:ALA:CB	5:C:132:ARG:HH12	2.28	0.45
10:H:41:ARG:NH1	10:H:123:GLU:OE2	2.49	0.45
10:H:45:ILE:C	10:H:47:GLY:N	2.70	0.45
1:A:102:G:N3	1:A:151:A:H2	2.14	0.45
1:A:1451:A:O2'	1:A:1452:C:OP1	2.31	0.45
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.16	0.45
13:K:12:ARG:O	13:K:13:GLN:C	2.54	0.45
4:B:76:GLN:NE2	4:B:207:ALA:H	2.10	0.45
4:B:77:ALA:O	4:B:81:VAL:HG23	2.17	0.45
5:C:88:ARG:HG3	5:C:101:LEU:HD13	1.99	0.45
13:K:106:LYS:HA	13:K:106:LYS:CE	2.44	0.45
11:I:50:LEU:C	11:I:52:ALA:H	2.19	0.45
1:A:780:A:C2	1:A:801:U:C5	3.04	0.45
15:M:59:TYR:HD1	15:M:59:TYR:C	2.19	0.45
20:R:53:ARG:NH1	20:R:60:GLY:N	2.64	0.45
1:A:1439:C:OP2	22:T:38:LYS:NZ	2.49	0.45
6:D:208:SER:O	6:D:209:ARG:C	2.55	0.45
1:A:1542:U:H2'	1:A:1543:C:O4'	2.16	0.45
19:Q:86:GLU:O	19:Q:87:LYS:C	2.51	0.45
11:I:5:TYR:CG	11:I:6:GLY:N	2.84	0.45
6:D:33:MET:HE3	6:D:37:PRO:HB3	1.98	0.45
4:B:44:LEU:HA	4:B:47:THR:OG1	2.16	0.45
1:A:1178:G:P	11:I:97:LYS:NZ	2.90	0.45
6:D:62:GLN:NE2	6:D:65:ARG:NH1	2.64	0.45
1:A:556:C:H2'	1:A:557:G:H5'	1.99	0.45
1:A:683:G:H21	13:K:38:ASN:ND2	2.14	0.45
5:C:62:ASP:HA	5:C:97:LYS:HB3	1.99	0.45
8:F:98:LEU:N	8:F:98:LEU:HD12	2.32	0.45
22:T:45:GLN:HB2	22:T:91:LEU:HD13	1.98	0.45
1:A:1349:A:H2'	1:A:1350:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.52	0.45
1:A:46:G:O2'	1:A:365:U:H1'	2.16	0.45
16:N:4:LYS:O	16:N:7:ILE:HG12	2.17	0.45
11:I:58:ARG:HG3	11:I:58:ARG:HH11	1.80	0.45
4:B:17:PHE:HD1	4:B:18:GLY:N	2.14	0.45
5:C:82:GLU:O	5:C:85:ARG:HB3	2.17	0.45
4:B:153:ARG:HG2	4:B:153:ARG:HH11	1.82	0.45
5:C:115:LEU:O	5:C:119:ARG:N	2.47	0.45
11:I:48:GLU:CD	11:I:51:ARG:HH12	2.19	0.45
14:L:83:VAL:CG1	14:L:100:ILE:HG23	2.44	0.45
1:A:501:C:OP1	14:L:117:ARG:NH2	2.50	0.45
10:H:48:TYR:HB2	10:H:60:ARG:O	2.17	0.45
8:F:98:LEU:HD23	20:R:28:GLU:OE1	2.17	0.45
11:I:20:ARG:HH12	11:I:62:TYR:HB3	1.81	0.45
1:A:1044:A:C2'	1:A:1045:C:H5'	2.47	0.45
1:A:564:C:C2	19:Q:31:LEU:HD11	2.52	0.45
1:A:340:U:H2'	1:A:341:C:C6	2.51	0.45
1:A:1206:G:C6	1:A:1207:G:C5	3.05	0.45
11:I:77:ILE:HG22	11:I:78:LYS:N	2.32	0.45
1:A:1056:U:H5'	5:C:163:ALA:HB3	1.96	0.45
1:A:1138:G:N3	1:A:1138:G:H3'	2.32	0.45
7:E:18:ARG:NH2	7:E:25:ARG:HB3	2.30	0.45
15:M:59:TYR:CD1	15:M:63:THR:HG21	2.52	0.45
15:M:115:LYS:N	15:M:115:LYS:HD3	2.31	0.45
1:A:1044:A:H2'	1:A:1045:C:H5'	1.99	0.45
14:L:33:ARG:HG2	14:L:62:SER:HB3	1.99	0.45
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.45
20:R:54:ARG:H	20:R:54:ARG:HG3	1.56	0.45
8:F:22:GLU:OE1	8:F:22:GLU:HA	2.17	0.45
1:A:1129:C:O2'	1:A:1131:G:C8	2.66	0.45
5:C:87:LEU:C	5:C:89:GLU:H	2.18	0.45
5:C:35:GLU:CG	5:C:59:ARG:HH22	2.21	0.45
1:A:133:U:P	22:T:74:LYS:HE3	2.56	0.45
15:M:105:THR:HB	15:M:106:ASN:H	1.64	0.45
1:A:1292:U:P	9:G:41:ARG:NH2	2.88	0.45
4:B:86:GLU:C	4:B:88:ALA:N	2.69	0.45
5:C:135:LYS:HE2	7:E:50:GLU:OE1	2.17	0.45
4:B:24:TRP:CG	4:B:25:ASN:N	2.80	0.45
10:H:68:ARG:NH1	10:H:68:ARG:HG2	2.30	0.45
1:A:716:A:N3	13:K:117:ASN:O	2.50	0.45
1:A:458:C:H2'	1:A:459:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:G:H2'	1:A:259:G:H8	1.81	0.45
1:A:1283:G:O2'	1:A:1284:C:H5'	2.17	0.45
1:A:491:G:O2'	1:A:492:G:H5'	2.16	0.45
9:G:75:VAL:CG1	9:G:86:GLN:HB3	2.47	0.45
21:S:22:LEU:CD2	21:S:28:LYS:HD2	2.45	0.45
14:L:46:LYS:HG3	14:L:47:LYS:N	2.32	0.45
5:C:83:ARG:C	5:C:85:ARG:N	2.67	0.45
19:Q:97:SER:H	19:Q:103:GLY:CA	2.25	0.45
1:A:1320:C:H2'	1:A:1321:C:O4'	2.17	0.45
1:A:129(A):G:O2'	1:A:130:A:OP2	2.35	0.45
1:A:1289:A:H2'	1:A:1290:G:H5'	1.99	0.45
18:P:18:ARG:HD3	18:P:35:LYS:HD2	1.99	0.45
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.45
4:B:23:ARG:HD3	4:B:23:ARG:C	2.37	0.45
1:A:484:G:O2'	1:A:485:G:OP2	2.30	0.45
11:I:25:LYS:O	11:I:60:ASP:OD1	2.35	0.45
23:V:14:TRP:C	23:V:16:GLY:H	2.19	0.45
6:D:162:LEU:HD12	6:D:181:MET:CE	2.47	0.45
9:G:66:VAL:HG12	9:G:70:LYS:HE3	1.98	0.45
4:B:206:ASP:CG	4:B:207:ALA:H	2.20	0.45
1:A:1278:U:H5''	1:A:1279:A:H5'	1.99	0.45
12:J:6:ILE:HD11	12:J:72:VAL:CG1	2.47	0.45
11:I:9:ARG:HG2	11:I:14:VAL:HA	1.99	0.45
1:A:664:G:OP1	20:R:64:ARG:HD2	2.17	0.45
5:C:38:ARG:HG3	5:C:38:ARG:HH11	1.82	0.45
7:E:76:ILE:HG23	7:E:142:LEU:HD22	1.98	0.45
7:E:78:HIS:CD2	10:H:107:LEU:HD12	2.52	0.45
8:F:14:LEU:CA	8:F:18:GLN:HE21	2.29	0.45
1:A:1313:U:O4	21:S:4:SER:HB2	2.16	0.45
1:A:1496:C:H2'	1:A:1497:G:O4'	2.17	0.45
1:A:718:G:H5'	1:A:719:C:OP2	2.17	0.45
1:A:482:A:H2'	1:A:483:C:O4'	2.16	0.45
1:A:963:G:HO2'	12:J:54:PHE:HZ	1.63	0.45
1:A:554:C:H2'	1:A:555:C:H6	1.81	0.45
6:D:35:ARG:O	6:D:36:ARG:CB	2.64	0.45
12:J:90:LEU:H	12:J:91:PRO:HD2	1.82	0.45
1:A:1143:G:H2'	1:A:1144:G:C8	2.52	0.45
11:I:8:GLY:HA3	11:I:79:LEU:HB3	1.98	0.45
1:A:542:G:O2'	1:A:543:C:H5'	2.17	0.45
6:D:58:LEU:O	6:D:58:LEU:HD22	2.16	0.45
1:A:262:A:C6	1:A:263:A:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:50:LEU:C	11:I:52:ALA:N	2.70	0.45
9:G:111:ARG:NH2	9:G:126:ASP:OD2	2.49	0.45
21:S:49:ILE:HD12	21:S:49:ILE:H	1.81	0.45
8:F:86:ARG:NH1	8:F:86:ARG:HG2	2.31	0.45
1:A:379:C:O2'	1:A:380:G:H5'	2.17	0.45
18:P:42:ARG:O	18:P:43:LYS:C	2.56	0.45
1:A:279:A:H5'	1:A:281:G:H5'	1.99	0.45
5:C:56:ASP:OD1	5:C:56:ASP:N	2.49	0.45
1:A:1372:U:OP2	11:I:11:LYS:HD3	2.17	0.45
12:J:60:ARG:O	12:J:61:GLU:CB	2.65	0.45
1:A:1072:G:O6	1:A:1102:A:N6	2.50	0.45
8:F:10:LEU:HD12	8:F:59:TYR:O	2.16	0.45
1:A:1014:A:H2'	1:A:1015:A:C8	2.52	0.45
1:A:428:G:O2'	1:A:429:U:P	2.75	0.45
1:A:982:U:H5''	16:N:6:LEU:CD1	2.47	0.45
16:N:3:ARG:NH2	16:N:6:LEU:CD1	2.80	0.45
22:T:68:LYS:HA	22:T:68:LYS:HD2	1.69	0.45
18:P:43:LYS:HA	18:P:48:TRP:CB	2.47	0.45
1:A:101:A:O2'	1:A:102:G:H5'	2.18	0.45
1:A:116:A:H2'	1:A:117:G:O4'	2.17	0.45
1:A:299:G:H2'	1:A:300:A:C8	2.52	0.45
1:A:686:U:HO2'	1:A:687:A:H8	1.64	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.17	0.45
1:A:1367:C:C2	1:A:1368:G:C8	3.05	0.44
1:A:1250:A:C5'	11:I:68:GLY:N	2.79	0.44
5:C:11:ARG:O	5:C:14:ILE:O	2.34	0.44
4:B:142:LEU:O	4:B:143:GLU:C	2.55	0.44
5:C:34:LEU:HD21	5:C:38:ARG:NH1	2.32	0.44
18:P:8:ARG:HB2	18:P:28:ARG:NH1	2.32	0.44
1:A:394:G:H2'	1:A:395:C:H6	1.82	0.44
12:J:47:PHE:CZ	16:N:37:PHE:HE1	2.35	0.44
6:D:117:ALA:O	6:D:121:VAL:HG23	2.17	0.44
1:A:828:A:H5''	1:A:859:A:C2	2.53	0.44
7:E:60:TYR:CE1	7:E:64:ARG:NH2	2.84	0.44
16:N:24:CYS:HB2	16:N:40:CYS:HB3	1.98	0.44
15:M:16:ASP:OD1	15:M:16:ASP:N	2.50	0.44
5:C:60:ALA:O	5:C:61:ALA:HB3	2.17	0.44
1:A:252:U:H2'	1:A:253:U:C6	2.51	0.44
6:D:128:VAL:HG12	6:D:129:ASN:ND2	2.32	0.44
1:A:255:G:O6	1:A:266:G:O6	2.35	0.44
1:A:1053:G:O3'	1:A:1054:C:H4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:G:H5'	1:A:726:C:H1'	1.99	0.44
1:A:130:A:H1'	1:A:263:A:O2'	2.16	0.44
17:O:21:ASP:OD2	17:O:24:SER:HB3	2.17	0.44
9:G:15:ASP:O	9:G:19:GLY:HA2	2.17	0.44
7:E:51:VAL:O	7:E:54:ALA:HB3	2.17	0.44
1:A:1168:A:C6	1:A:1169:A:C6	3.05	0.44
1:A:382:A:C2	1:A:383:A:C4	3.05	0.44
15:M:37:THR:O	15:M:55:ARG:NH1	2.47	0.44
9:G:65:ALA:HB1	9:G:127:ALA:HB3	1.99	0.44
1:A:1176:A:O2'	1:A:1177:G:H5'	2.16	0.44
1:A:335:C:H2'	1:A:336:C:H6	1.81	0.44
1:A:1508:G:O2'	1:A:1509:C:H5'	2.17	0.44
4:B:9:GLU:C	4:B:10:LEU:HD23	2.38	0.44
1:A:974:A:P	16:N:41:ARG:HH12	2.39	0.44
11:I:77:ILE:O	11:I:78:LYS:C	2.56	0.44
4:B:230:VAL:CG1	4:B:231:GLU:N	2.80	0.44
8:F:97:PHE:CB	20:R:32:ARG:HH21	2.30	0.44
9:G:41:ARG:O	9:G:42:ILE:C	2.56	0.44
11:I:127:LYS:HA	11:I:127:LYS:HZ2	1.82	0.44
14:L:59:ARG:HA	14:L:59:ARG:HE	1.82	0.44
12:J:86:MET:C	12:J:86:MET:HE3	2.38	0.44
22:T:90:GLN:O	22:T:93:GLU:HG2	2.17	0.44
1:A:265:G:H2'	1:A:267:C:H5	1.83	0.44
1:A:976:G:OP1	16:N:32:SER:N	2.43	0.44
22:T:12:ALA:C	22:T:14:LYS:N	2.69	0.44
6:D:7:PRO:O	6:D:10:ARG:HD2	2.18	0.44
1:A:673:G:H5''	8:F:87:ARG:NH1	2.33	0.44
1:A:216:G:H2'	1:A:217:C:H6	1.81	0.44
5:C:5:ILE:H	5:C:5:ILE:CD1	2.31	0.44
1:A:1223:C:OP1	21:S:78:ARG:NH1	2.51	0.44
1:A:1223:C:H3'	1:A:1224:G:H5''	1.99	0.44
6:D:146:ILE:N	6:D:146:ILE:CD1	2.79	0.44
5:C:134:ILE:HG22	5:C:168:ALA:CB	2.48	0.44
5:C:126:ARG:O	5:C:127:ARG:CB	2.62	0.44
5:C:188:LEU:HB3	5:C:189:ALA:H	1.57	0.44
1:A:833:U:H2'	1:A:834:C:C6	2.52	0.44
7:E:60:TYR:O	7:E:64:ARG:HG2	2.17	0.44
10:H:126:LYS:C	10:H:128:GLY:N	2.71	0.44
1:A:46:G:H2'	1:A:366:C:H41	1.82	0.44
12:J:65:LEU:O	12:J:65:LEU:HG	2.18	0.44
1:A:1329:A:P	15:M:28:ALA:HB3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:13:LEU:H	22:T:13:LEU:CD1	2.06	0.44
20:R:47:THR:O	20:R:49:LYS:N	2.50	0.44
4:B:213:LEU:HD23	4:B:213:LEU:C	2.37	0.44
5:C:3:ASN:O	5:C:4:LYS:HB2	2.17	0.44
7:E:51:VAL:HB	7:E:52:PRO:CD	2.42	0.44
14:L:125:PRO:C	14:L:127:GLU:H	2.21	0.44
8:F:12:PRO:HD3	8:F:58:GLY:HA2	2.00	0.44
1:A:528:C:N4	14:L:49:ASN:ND2	2.66	0.44
1:A:783:C:O2'	1:A:784:C:H5'	2.17	0.44
1:A:1316:G:N2	1:A:1318:A:H3'	2.31	0.44
13:K:34:ASP:C	13:K:34:ASP:OD1	2.56	0.44
1:A:191:G:N3	22:T:105:SER:HB3	2.32	0.44
14:L:117:ARG:O	14:L:119:LYS:O	2.36	0.44
15:M:36:LYS:HB2	15:M:59:TYR:CE2	2.48	0.44
1:A:979:C:H42	16:N:18:VAL:HG12	1.83	0.44
1:A:895:G:H2'	1:A:896:C:H6	1.80	0.44
1:A:1163:C:H2'	1:A:1164:G:C8	2.52	0.44
1:A:718:G:H1'	13:K:116:HIS:HA	1.99	0.44
1:A:962:C:H2'	1:A:963:G:O4'	2.18	0.44
6:D:175:SER:OG	6:D:184:LYS:HB2	2.17	0.44
13:K:14:VAL:HG12	13:K:14:VAL:O	2.18	0.44
1:A:1123:A:H2	12:J:39:PRO:HG3	1.83	0.44
12:J:6:ILE:O	12:J:6:ILE:HG13	2.17	0.44
7:E:80:ILE:N	7:E:80:ILE:HD12	2.33	0.44
8:F:4:TYR:OH	8:F:69:GLU:HA	2.17	0.44
1:A:1191:A:H2'	1:A:1192:C:C6	2.53	0.44
9:G:15:ASP:OD1	9:G:18:TYR:N	2.45	0.44
12:J:9:ARG:HH11	12:J:9:ARG:HB2	1.82	0.44
14:L:126:LYS:C	14:L:126:LYS:NZ	2.71	0.44
15:M:58:GLU:OE2	15:M:58:GLU:HA	2.18	0.44
7:E:78:HIS:HD2	10:H:107:LEU:HD12	1.82	0.44
7:E:19:MET:O	7:E:20:GLN:NE2	2.51	0.44
15:M:77:ASN:O	15:M:81:LEU:HD22	2.18	0.44
5:C:52:LEU:N	5:C:52:LEU:CD2	2.80	0.44
7:E:101:ILE:O	7:E:120:THR:HB	2.17	0.44
1:A:406:G:H2'	1:A:407:G:C8	2.50	0.44
20:R:53:ARG:HG3	20:R:63:GLN:HG2	1.99	0.44
14:L:60:LEU:HD22	14:L:66:VAL:HG22	2.00	0.44
1:A:22:G:H2'	1:A:23:C:C6	2.53	0.44
1:A:153:C:O2'	1:A:154:C:H5'	2.18	0.44
1:A:1251:A:H1'	1:A:1369:C:O2'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:H2'	1:A:1373:G:N1	2.32	0.44
14:L:46:LYS:CG	14:L:47:LYS:N	2.79	0.44
1:A:217:C:O2'	1:A:218:C:H5'	2.17	0.44
16:N:11:LYS:HG2	16:N:11:LYS:O	2.16	0.44
15:M:36:LYS:HD2	15:M:59:TYR:OH	2.17	0.44
16:N:16:PHE:C	16:N:18:VAL:N	2.70	0.44
1:A:1451:A:H4'	1:A:1452:C:OP2	2.18	0.44
1:A:1027:C:H2'	1:A:1028:C:C6	2.52	0.44
4:B:16:HIS:HB3	4:B:17:PHE:H	1.56	0.44
1:A:1257:U:O2'	1:A:1258:G:C8	2.71	0.44
1:A:877:C:O2'	1:A:878:G:H5'	2.18	0.44
5:C:11:ARG:O	5:C:13:GLY:N	2.51	0.44
1:A:1314:C:OP2	21:S:6:LYS:HD3	2.17	0.44
1:A:157:G:C2	1:A:158:G:C8	3.06	0.44
11:I:65:VAL:HG21	11:I:73:GLN:HB3	2.00	0.44
20:R:43:PHE:C	20:R:51:LEU:HD12	2.38	0.44
4:B:177:ALA:O	4:B:180:LEU:N	2.51	0.44
11:I:27:THR:HG22	11:I:28:VAL:N	2.33	0.44
15:M:71:ARG:HG2	15:M:71:ARG:HH11	1.82	0.44
1:A:1460:A:H2'	1:A:1461:G:O4'	2.17	0.44
15:M:25:ILE:HG22	15:M:26:GLY:N	2.33	0.44
22:T:100:ILE:O	22:T:102:GLY:N	2.50	0.44
1:A:1055:A:N7	1:A:1206:G:N1	2.66	0.44
11:I:8:GLY:O	11:I:9:ARG:HG3	2.18	0.44
4:B:60:ASP:OD1	4:B:64:ARG:NH2	2.50	0.44
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.52	0.44
1:A:812:C:OP1	1:A:903:G:H1'	2.18	0.44
8:F:10:LEU:HD11	8:F:59:TYR:HD2	1.82	0.44
1:A:938:A:C6	1:A:939:G:C5	3.06	0.44
1:A:1405:G:H1'	1:A:1519:A:O4'	2.18	0.44
1:A:1133:G:O2'	1:A:1134:G:H5'	2.18	0.44
16:N:35:ARG:C	16:N:37:PHE:N	2.71	0.44
15:M:80:ARG:O	15:M:82:MET:N	2.51	0.44
1:A:1232:U:OP1	11:I:124:GLN:NE2	2.48	0.44
15:M:108:ARG:NH2	15:M:114:ARG:HA	2.32	0.44
8:F:34:GLY:O	8:F:68:PRO:HD3	2.18	0.44
13:K:99:GLN:HA	13:K:105:VAL:CG2	2.48	0.44
1:A:1060:C:C5	5:C:2:GLY:CA	3.01	0.43
22:T:13:LEU:O	22:T:16:HIS:HB3	2.18	0.43
1:A:129(A):G:O2'	1:A:190(E):U:C6	2.71	0.43
1:A:706:A:H1'	13:K:29:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:A:C2	1:A:627:G:C2	3.06	0.43
9:G:141:VAL:O	9:G:144:MET:HB2	2.18	0.43
1:A:961:U:O2'	1:A:962:C:H5'	2.17	0.43
22:T:56:MET:CE	22:T:88:VAL:HG11	2.48	0.43
1:A:458:C:C2	1:A:459:G:C8	3.06	0.43
4:B:78:GLN:HG2	4:B:78:GLN:O	2.18	0.43
4:B:79:ASP:HB3	4:B:238:LEU:HD13	1.99	0.43
12:J:14:LYS:C	12:J:16:LEU:H	2.20	0.43
1:A:242:C:C2'	1:A:243:A:H5'	2.48	0.43
1:A:1053:G:C3'	1:A:1054:C:C5'	2.95	0.43
19:Q:97:SER:C	19:Q:99:SER:N	2.72	0.43
1:A:190(L):U:O2'	1:A:191:G:H5'	2.18	0.43
19:Q:59:ILE:CG2	19:Q:71:PHE:CD1	3.00	0.43
1:A:981:U:H5'	16:N:21:TYR:CE1	2.53	0.43
1:A:865:A:C2	1:A:918:A:H4'	2.52	0.43
13:K:43:SER:OG	13:K:67:ASP:HB3	2.18	0.43
1:A:867:G:O2'	1:A:868:C:H5'	2.17	0.43
12:J:89:ASP:O	12:J:90:LEU:HD12	2.18	0.43
8:F:35:ALA:HA	8:F:67:MET:HB3	1.99	0.43
8:F:2:ARG:NH1	8:F:69:GLU:CB	2.81	0.43
1:A:579:G:C5'	1:A:728:A:H1'	2.34	0.43
11:I:16:ARG:CG	11:I:64:THR:HB	2.37	0.43
11:I:86:VAL:HG11	11:I:93:ARG:HE	1.84	0.43
1:A:1287:A:H2'	1:A:1288:A:C8	2.53	0.43
1:A:1288:A:H1'	1:A:1352:C:O2'	2.18	0.43
9:G:15:ASP:O	9:G:19:GLY:N	2.48	0.43
9:G:46:ALA:O	9:G:50:ILE:HG13	2.18	0.43
6:D:152:SER:O	6:D:155:LEU:HD12	2.18	0.43
1:A:1202:G:O2'	1:A:1203:C:H5'	2.18	0.43
1:A:364:A:N6	14:L:28:LYS:HE2	2.32	0.43
19:Q:59:ILE:HA	19:Q:59:ILE:HD13	1.77	0.43
7:E:137:GLU:O	7:E:141:GLN:HG3	2.18	0.43
1:A:668:G:O2'	17:O:46:HIS:HD2	2.00	0.43
13:K:26:ASN:O	13:K:27:ASN:CB	2.67	0.43
19:Q:7:THR:O	19:Q:23:VAL:HG13	2.19	0.43
15:M:117:VAL:CG1	15:M:118:ALA:N	2.81	0.43
4:B:18:GLY:HA2	4:B:40:HIS:O	2.18	0.43
4:B:74:LYS:NZ	4:B:206:ASP:HA	2.32	0.43
8:F:26:ILE:O	8:F:30:LEU:HG	2.19	0.43
19:Q:98:LEU:O	19:Q:98:LEU:CD1	2.67	0.43
1:A:1095:U:P	1:A:1108:G:H1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:126:LYS:CE	14:L:126:LYS:N	2.82	0.43
16:N:11:LYS:O	16:N:12:ARG:C	2.57	0.43
12:J:47:PHE:CD1	12:J:47:PHE:N	2.86	0.43
1:A:1411:C:O2'	1:A:1412:C:H5'	2.18	0.43
1:A:686:U:C2	1:A:687:A:N7	2.86	0.43
19:Q:13:ASP:O	19:Q:15:MET:N	2.52	0.43
4:B:131:PRO:C	4:B:133:LYS:N	2.72	0.43
14:L:44:THR:HA	14:L:45:PRO:HD3	1.91	0.43
19:Q:76:LEU:CD2	19:Q:76:LEU:C	2.87	0.43
15:M:90:LEU:O	15:M:93:ARG:N	2.51	0.43
4:B:16:HIS:CA	4:B:204:ASN:HB2	2.46	0.43
12:J:8:LEU:HD22	12:J:94:VAL:HG11	1.99	0.43
12:J:53:PRO:HA	16:N:41:ARG:NH2	2.27	0.43
5:C:191:THR:HG21	5:C:193:TYR:CD1	2.54	0.43
1:A:510:A:O2'	1:A:542:G:H1'	2.18	0.43
5:C:148:GLY:HA3	5:C:172:ARG:O	2.19	0.43
20:R:87:ARG:HG2	20:R:87:ARG:NH1	2.32	0.43
17:O:17:ARG:NH1	17:O:77:ARG:NH1	2.67	0.43
14:L:71:PRO:O	14:L:102:ARG:CD	2.64	0.43
6:D:173:TRP:O	6:D:186:LEU:HB2	2.18	0.43
19:Q:81:ARG:HE	19:Q:81:ARG:HB2	1.53	0.43
1:A:1132:C:H2'	1:A:1133:G:H8	1.84	0.43
7:E:87:SER:HB3	7:E:131:ILE:CD1	2.49	0.43
7:E:36:ASP:OD2	7:E:40:ARG:HB2	2.19	0.43
6:D:162:LEU:HD12	6:D:181:MET:HE1	2.00	0.43
4:B:14:GLY:O	4:B:15:VAL:HG22	2.18	0.43
1:A:1207:G:H2'	1:A:1208:C:C6	2.53	0.43
11:I:7:THR:O	11:I:80:GLY:HA3	2.18	0.43
6:D:8:VAL:CG1	6:D:21:LEU:HB2	2.48	0.43
4:B:142:LEU:O	4:B:145:LEU:N	2.52	0.43
4:B:144:ARG:HG3	4:B:145:LEU:H	1.83	0.43
21:S:37:ARG:HA	21:S:37:ARG:HD3	1.81	0.43
4:B:124:SER:CB	4:B:125:PRO:CD	2.97	0.43
1:A:1003(A):G:C2'	1:A:1004:A:H4'	2.43	0.43
14:L:126:LYS:N	14:L:126:LYS:HE3	2.32	0.43
5:C:119:ARG:HG2	5:C:119:ARG:HH11	1.83	0.43
1:A:1116:C:O2'	1:A:1117:G:H5''	2.18	0.43
8:F:11:ASN:HA	8:F:12:PRO:HD2	1.87	0.43
1:A:1015:A:H2'	1:A:1016:A:H8	1.83	0.43
5:C:139:GLN:NE2	5:C:139:GLN:CA	2.78	0.43
1:A:709:G:O2'	1:A:710:G:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:U:H6	1:A:81:U:H5'	1.83	0.43
1:A:1330:U:C2'	1:A:1331:G:H5'	2.49	0.43
5:C:180:ALA:O	5:C:181:ASN:CB	2.56	0.43
4:B:212:GLN:O	4:B:213:LEU:C	2.56	0.43
1:A:1003(A):G:C6	1:A:1004:A:N3	2.87	0.43
1:A:765:G:N2	1:A:812:C:O2'	2.52	0.43
1:A:26:A:N6	1:A:558:G:H1'	2.33	0.43
14:L:89:ARG:HG2	14:L:97:ARG:CB	2.48	0.43
10:H:51:VAL:CG1	10:H:52:ASP:N	2.79	0.43
1:A:283:C:O2'	1:A:284:G:H5'	2.19	0.43
4:B:90:MET:HA	4:B:91:PRO:HD3	1.74	0.43
10:H:97:VAL:HG13	10:H:98:LYS:N	2.34	0.43
8:F:23:LYS:NZ	8:F:42:GLU:OE2	2.48	0.43
13:K:128:ALA:O	13:K:129:SER:HB3	2.17	0.43
1:A:1294:G:O2'	1:A:1295:G:H5'	2.19	0.43
15:M:21:TYR:HD1	15:M:21:TYR:H	1.67	0.43
1:A:1346:A:O4'	1:A:1348:U:C6	2.72	0.43
1:A:1305:G:H2'	1:A:1331:G:N2	2.33	0.43
22:T:39:LYS:O	22:T:43:LEU:HG	2.19	0.43
12:J:9:ARG:HH11	12:J:9:ARG:CB	2.31	0.43
1:A:1036:G:H2'	1:A:1037:C:C6	2.54	0.43
16:N:12:ARG:HB3	16:N:13:THR:H	1.58	0.43
5:C:6:HIS:CD2	5:C:8:ILE:HB	2.53	0.43
1:A:1270:C:O2'	1:A:1314:C:H5'	2.19	0.43
13:K:33:THR:HA	13:K:39:PRO:HA	2.00	0.43
19:Q:68:ARG:O	19:Q:68:ARG:HG3	2.19	0.43
1:A:1439:C:H2'	1:A:1440:C:H6	1.84	0.43
1:A:1229:A:C2	1:A:1230:C:C4	3.06	0.43
9:G:79:ARG:HG3	9:G:84:ASN:HB3	1.99	0.43
1:A:632:A:C2'	1:A:633:G:H5'	2.48	0.43
8:F:82:ARG:HB2	8:F:85:VAL:CG2	2.48	0.43
15:M:96:LEU:HB3	15:M:97:PRO:HD2	2.01	0.43
1:A:1370:G:C2	1:A:1371:G:N7	2.87	0.43
11:I:107:ARG:HB3	11:I:107:ARG:HH11	1.83	0.43
16:N:45:ARG:CG	16:N:45:ARG:HH11	2.27	0.43
23:V:2:GLY:C	23:V:4:GLY:N	2.72	0.43
1:A:1074:G:O3'	4:B:103:THR:CG2	2.66	0.43
8:F:87:ARG:NH1	8:F:87:ARG:CG	2.77	0.43
4:B:107:THR:HA	4:B:110:GLN:OE1	2.19	0.43
9:G:54:THR:HG22	9:G:56:GLN:N	2.24	0.43
11:I:45:ALA:O	11:I:47:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:150:GLU:C	6:D:152:SER:H	2.22	0.43
1:A:64:G:HO2'	1:A:65:U:P	2.40	0.43
6:D:64:LEU:HB2	6:D:198:VAL:HG11	2.01	0.43
16:N:16:PHE:C	16:N:18:VAL:H	2.21	0.43
14:L:60:LEU:HD11	14:L:85:ILE:HD12	2.01	0.43
16:N:44:LEU:O	16:N:48:ALA:CB	2.67	0.43
1:A:321:A:O2'	1:A:322:C:H5'	2.18	0.43
4:B:159:PRO:HB2	4:B:161:ALA:O	2.19	0.43
1:A:642:A:C8	10:H:115:SER:HA	2.54	0.43
5:C:107:GLN:O	5:C:108:ASN:CB	2.67	0.43
13:K:12:ARG:O	13:K:13:GLN:O	2.37	0.43
4:B:80:ILE:CD1	4:B:208:ILE:HG12	2.48	0.43
11:I:10:ARG:C	11:I:12:GLU:N	2.68	0.43
4:B:97:TRP:C	4:B:98:LEU:HD23	2.40	0.43
10:H:125:ARG:HE	10:H:125:ARG:HB2	1.60	0.43
1:A:1137:C:H4'	1:A:1138:G:N1	2.33	0.43
4:B:212:GLN:HG3	4:B:239:VAL:CG2	2.49	0.43
1:A:217:C:H2'	1:A:218:C:C6	2.54	0.43
1:A:1351:U:O2'	1:A:1352:C:H5'	2.19	0.43
11:I:33:PHE:C	11:I:35:GLU:H	2.23	0.43
1:A:801:U:H2'	1:A:802:A:C8	2.54	0.43
1:A:640:A:C2'	1:A:641:U:H5'	2.48	0.43
1:A:614:A:H2'	1:A:615:C:C6	2.54	0.43
19:Q:26:GLN:O	19:Q:27:PHE:HB3	2.19	0.43
4:B:23:ARG:O	4:B:24:TRP:O	2.37	0.43
1:A:499:A:H4'	1:A:500:G:OP1	2.18	0.43
1:A:291:C:O2'	1:A:292:G:H5'	2.19	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.54	0.43
5:C:9:GLY:N	16:N:49:HIS:O	2.52	0.43
1:A:692:U:H1'	1:A:695:A:N7	2.34	0.43
4:B:15:VAL:HB	4:B:16:HIS:H	1.47	0.42
4:B:17:PHE:CD1	4:B:17:PHE:C	2.92	0.42
8:F:30:LEU:HB3	8:F:35:ALA:CB	2.48	0.42
1:A:1145:C:HO2'	1:A:1146:A:P	2.41	0.42
5:C:99:VAL:CG2	5:C:100:ALA:N	2.82	0.42
19:Q:97:SER:O	19:Q:102:GLY:N	2.51	0.42
4:B:114:ARG:HH11	4:B:118:LEU:HG	1.84	0.42
9:G:51:GLN:NE2	9:G:58:PRO:HD3	2.33	0.42
7:E:77:PRO:O	7:E:78:HIS:HB3	2.19	0.42
1:A:497:A:O2'	1:A:498:U:OP1	2.28	0.42
13:K:70:LYS:O	13:K:73:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:U:O2'	1:A:832:C:H5'	2.19	0.42
8:F:92:LYS:HE3	8:F:92:LYS:HB2	1.77	0.42
16:N:33:VAL:HG13	16:N:33:VAL:O	2.19	0.42
1:A:519:C:H2'	1:A:520:A:O4'	2.18	0.42
9:G:70:LYS:HG2	9:G:96:GLN:O	2.19	0.42
15:M:117:VAL:HG12	15:M:118:ALA:N	2.33	0.42
8:F:3:ARG:HG2	8:F:93:SER:OG	2.18	0.42
7:E:16:THR:HG22	7:E:27:ARG:O	2.18	0.42
5:C:108:ASN:ND2	5:C:110:ASN:HB2	2.32	0.42
1:A:1301:U:O2'	1:A:1302:U:P	2.77	0.42
1:A:542:G:H2'	1:A:543:C:C6	2.50	0.42
17:O:77:ARG:O	17:O:81:LEU:N	2.43	0.42
14:L:89:ARG:NH2	14:L:97:ARG:HE	2.18	0.42
11:I:31:GLN:HG2	11:I:35:GLU:HG2	2.00	0.42
14:L:110:VAL:O	14:L:113:ARG:HB2	2.19	0.42
1:A:444:C:H2'	1:A:445:G:C8	2.51	0.42
4:B:23:ARG:HH11	4:B:24:TRP:CA	2.33	0.42
1:A:865:A:H2	1:A:918:A:H4'	1.84	0.42
1:A:881:G:P	14:L:12:ARG:HH22	2.42	0.42
1:A:983:A:HO2'	1:A:1049:U:HO2'	1.66	0.42
10:H:31:PHE:O	10:H:35:ILE:HG13	2.19	0.42
9:G:81:GLY:C	9:G:83:ALA:H	2.22	0.42
1:A:851:G:H2'	1:A:852:G:H8	1.83	0.42
6:D:31:CYS:SG	6:D:31:CYS:O	2.77	0.42
12:J:45:ARG:HB2	12:J:65:LEU:HB3	2.02	0.42
1:A:1368:G:HO2'	1:A:1369:C:H5'	1.83	0.42
1:A:369:C:O2'	1:A:370:C:H5'	2.19	0.42
21:S:42:PRO:HD3	21:S:67:VAL:CG1	2.49	0.42
1:A:730:G:N3	1:A:765:G:H4'	2.34	0.42
14:L:89:ARG:HA	14:L:97:ARG:HA	2.00	0.42
7:E:76:ILE:HG23	7:E:77:PRO:CD	2.42	0.42
17:O:67:LEU:HD11	17:O:87:ILE:HD13	2.00	0.42
1:A:1339:A:H2'	1:A:1340:A:O4'	2.19	0.42
1:A:1227:A:H2'	1:A:1228:C:O5'	2.19	0.42
8:F:91:VAL:HG13	20:R:72:ARG:HH22	1.83	0.42
1:A:425:G:O2'	1:A:426:G:H5'	2.19	0.42
13:K:40:ILE:HG23	13:K:75:TYR:CD2	2.55	0.42
1:A:1145:C:O2'	1:A:1146:A:C8	2.72	0.42
4:B:101:MET:HE2	4:B:108:ILE:HG21	1.98	0.42
4:B:164:VAL:O	4:B:186:ALA:HA	2.19	0.42
15:M:34:LEU:CD1	15:M:41:PRO:HA	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:26:LEU:HD22	20:R:39:VAL:HG23	2.01	0.42
1:A:528:C:H5'	1:A:535:A:N6	2.34	0.42
1:A:1118:C:H1'	1:A:1179:A:N9	2.34	0.42
9:G:121:ALA:O	9:G:125:MET:HG3	2.19	0.42
10:H:36:LEU:HA	10:H:39:LEU:HD23	2.01	0.42
1:A:1465:C:O2'	1:A:1466:C:H5'	2.19	0.42
4:B:78:GLN:O	4:B:94:ASN:ND2	2.52	0.42
10:H:104:ARG:NH2	10:H:138:TRP:CZ3	2.88	0.42
1:A:247:G:OP2	19:Q:99:SER:HB2	2.20	0.42
1:A:264:U:H4'	19:Q:63:ARG:HD3	2.02	0.42
1:A:1004:A:N7	1:A:1036:G:O6	2.53	0.42
11:I:51:ARG:HG3	11:I:56:LEU:HD12	2.00	0.42
6:D:150:GLU:C	6:D:152:SER:N	2.73	0.42
1:A:437:U:C5'	6:D:155:LEU:HD22	2.47	0.42
1:A:794:A:C5	1:A:795:C:C4	3.07	0.42
7:E:12:LEU:HD22	7:E:13:ILE:N	2.34	0.42
11:I:117:HIS:O	11:I:118:LYS:HG3	2.20	0.42
1:A:635:G:O2'	1:A:636:U:H5'	2.19	0.42
1:A:1229:A:H2'	1:A:1230:C:H6	1.84	0.42
23:V:3:LYS:HB3	23:V:14:TRP:CG	2.54	0.42
1:A:1429:C:H2'	1:A:1430:C:C6	2.55	0.42
5:C:175:LEU:HD21	5:C:201:TYR:CD2	2.54	0.42
1:A:669:U:H2'	1:A:670:G:C8	2.55	0.42
1:A:1407:C:O2'	1:A:1408:A:H5'	2.20	0.42
21:S:20:LEU:HA	21:S:23:ASN:HD22	1.83	0.42
1:A:1459:C:O2'	1:A:1460:A:H5'	2.19	0.42
1:A:1251:A:H5'	11:I:12:GLU:OE1	2.20	0.42
17:O:34:LEU:O	17:O:38:ARG:HG2	2.20	0.42
22:T:57:ARG:HH11	22:T:57:ARG:CB	2.32	0.42
1:A:1130:A:OP2	1:A:1131:G:OP2	2.37	0.42
1:A:1117:G:N2	1:A:1180:A:H1'	2.34	0.42
15:M:84:ILE:O	15:M:85:GLY:C	2.58	0.42
13:K:18:ARG:NH1	13:K:35:PRO:O	2.52	0.42
5:C:132:ARG:O	5:C:133:ALA:C	2.58	0.42
19:Q:60:ILE:HD13	19:Q:61:GLU:H	1.85	0.42
1:A:992:U:O2'	1:A:993:G:P	2.78	0.42
1:A:1109:C:P	5:C:176:HIS:CD2	3.12	0.42
9:G:16:LEU:CD2	9:G:16:LEU:H	2.33	0.42
13:K:82:VAL:HG23	13:K:105:VAL:HG13	2.01	0.42
1:A:1514:C:O2'	1:A:1515:C:H5'	2.19	0.42
1:A:1487:G:O2'	1:A:1488:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:13:ARG:HD3	6:D:36:ARG:O	2.18	0.42
4:B:206:ASP:O	4:B:207:ALA:HB3	2.20	0.42
4:B:79:ASP:C	4:B:81:VAL:H	2.23	0.42
15:M:66:LEU:O	15:M:67:GLU:O	2.37	0.42
7:E:93:PRO:HG2	10:H:105:ARG:NH2	2.34	0.42
1:A:1102:A:H2'	1:A:1103:C:C6	2.55	0.42
1:A:270:A:H2'	1:A:271:C:H6	1.84	0.42
1:A:1207:G:HO2'	1:A:1208:C:H5'	1.84	0.42
1:A:542:G:H5'	6:D:41:GLY:HA3	2.01	0.42
5:C:101:LEU:CD2	5:C:101:LEU:O	2.67	0.42
15:M:6:GLY:O	15:M:7:VAL:CG2	2.67	0.42
1:A:558:G:H2'	1:A:559:A:H2	1.84	0.42
4:B:178:ARG:NH1	10:H:71:GLY:O	2.53	0.42
1:A:394:G:H2'	1:A:395:C:C6	2.54	0.42
10:H:119:LEU:CD1	10:H:124:ALA:HA	2.49	0.42
1:A:1089:G:O2'	1:A:1090:U:H5'	2.19	0.42
1:A:1091:U:C2	1:A:1093:A:OP2	2.72	0.42
4:B:177:ALA:CB	4:B:184:VAL:HG22	2.50	0.42
1:A:815:A:H4'	1:A:817:C:C5	2.55	0.42
1:A:644:G:C5	1:A:645:C:C5	3.08	0.42
23:V:2:GLY:O	23:V:4:GLY:N	2.53	0.42
1:A:579:G:H5'	1:A:728:A:C1'	2.33	0.42
22:T:101:GLY:C	22:T:103:GLY:N	2.71	0.42
15:M:2:ALA:O	15:M:4:ILE:HG13	2.20	0.42
1:A:1069:C:O2'	1:A:1192:C:H1'	2.19	0.42
14:L:89:ARG:NH2	14:L:97:ARG:NH2	2.65	0.42
1:A:533:A:O2'	1:A:535:A:OP2	2.21	0.42
13:K:20:TYR:O	13:K:30:VAL:HA	2.19	0.42
1:A:1226:C:H4'	21:S:80:TYR:CZ	2.55	0.42
7:E:43:LEU:O	7:E:62:ALA:HA	2.19	0.42
6:D:61:LYS:HD3	6:D:206:PHE:CD2	2.54	0.42
5:C:35:GLU:CG	5:C:59:ARG:NH2	2.77	0.42
14:L:42:THR:OG1	14:L:52:LEU:HB3	2.20	0.42
1:A:951:G:O2'	1:A:952:U:H5'	2.20	0.42
1:A:807:A:H2'	1:A:808:C:H6	1.82	0.42
8:F:60:PHE:CZ	20:R:78:LEU:HD21	2.55	0.42
14:L:98:TYR:N	14:L:98:TYR:CD1	2.87	0.42
1:A:1187:G:P	11:I:113:LYS:HE2	2.60	0.42
6:D:30:LYS:C	6:D:32:ALA:N	2.72	0.42
9:G:75:VAL:HG11	9:G:86:GLN:HB3	2.01	0.42
1:A:154:C:O2'	1:A:155:C:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:21:TYR:N	15:M:21:TYR:CD1	2.88	0.42
1:A:185:A:N3	22:T:81:LYS:NZ	2.55	0.42
1:A:190(B):C:H2'	1:A:190(C):C:O4'	2.20	0.42
6:D:17:VAL:CG1	6:D:18:LYS:N	2.83	0.42
1:A:310:G:H2'	1:A:311:C:H6	1.84	0.42
1:A:1061:G:C6	1:A:1062:U:N3	2.88	0.42
1:A:1347:G:C5	11:I:107:ARG:NH1	2.70	0.42
1:A:1060:C:N4	5:C:2:GLY:N	2.67	0.42
1:A:1392:G:H21	1:A:1502:A:H8	1.68	0.42
4:B:101:MET:HE3	4:B:108:ILE:HG21	2.01	0.42
11:I:97:LYS:C	11:I:99:LEU:N	2.73	0.42
4:B:64:ARG:HH11	4:B:64:ARG:CB	2.33	0.42
1:A:1014:A:H2	1:A:1219:U:H1'	1.80	0.42
13:K:69:ALA:CB	13:K:101:SER:HB2	2.50	0.42
1:A:169:C:O2'	1:A:170:U:H5'	2.19	0.42
1:A:718:G:H4'	13:K:117:ASN:HD21	1.84	0.42
1:A:1165:C:C2'	1:A:1166:G:H5'	2.50	0.42
1:A:603:U:H2'	1:A:604:G:C8	2.55	0.42
8:F:1:MET:CE	8:F:1:MET:N	2.82	0.42
1:A:489:C:H2'	1:A:490:G:H8	1.85	0.42
1:A:814:A:N7	1:A:816:A:C4	2.87	0.42
1:A:1079:G:O3'	7:E:14:ARG:NH2	2.53	0.42
1:A:474:G:H2'	1:A:475:G:H8	1.85	0.42
14:L:78:GLN:O	14:L:80:HIS:N	2.52	0.42
1:A:933:G:OP2	9:G:3:ARG:HB3	2.20	0.42
7:E:26:PHE:HD1	7:E:26:PHE:H	1.62	0.41
9:G:89:MET:HB2	9:G:155:ARG:NH1	2.34	0.41
1:A:1256:A:H61	1:A:1278:U:C1'	2.33	0.41
1:A:1364:U:O2'	1:A:1365:G:H5'	2.20	0.41
11:I:107:ARG:CB	11:I:107:ARG:HH11	2.32	0.41
9:G:49:ILE:C	9:G:51:GLN:H	2.23	0.41
1:A:1281:U:C6	1:A:1281:U:C3'	3.02	0.41
20:R:32:ARG:HE	20:R:32:ARG:HB2	1.61	0.41
1:A:1018:C:O2'	1:A:1019:C:H5'	2.20	0.41
12:J:44:VAL:HA	12:J:66:ARG:HA	2.02	0.41
1:A:791:G:C6	1:A:792:A:N7	2.87	0.41
1:A:1161:C:H2'	1:A:1162:C:C6	2.55	0.41
1:A:1030:C:H2'	1:A:1030(A):G:O4'	2.19	0.41
1:A:417:C:O2'	1:A:418:C:H5'	2.20	0.41
1:A:1365:G:O2'	1:A:1366:C:H5'	2.19	0.41
15:M:23:TYR:HB3	15:M:67:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:47:THR:C	20:R:49:LYS:H	2.24	0.41
11:I:95:LYS:C	11:I:98:PRO:HD2	2.40	0.41
5:C:191:THR:HG22	5:C:192:THR:N	2.35	0.41
1:A:1223:C:P	1:A:1224:G:H3'	2.60	0.41
5:C:112:SER:CB	5:C:115:LEU:HD12	2.48	0.41
1:A:1355:G:O2'	1:A:1356:G:H5'	2.20	0.41
19:Q:70:ARG:CG	19:Q:70:ARG:NH1	2.83	0.41
21:S:80:TYR:O	21:S:81:ARG:C	2.59	0.41
6:D:64:LEU:HD13	6:D:64:LEU:C	2.41	0.41
14:L:60:LEU:HB2	14:L:64:TYR:O	2.20	0.41
1:A:433:C:H2'	1:A:434:U:C6	2.55	0.41
1:A:490:G:O2'	1:A:491:G:H5'	2.20	0.41
1:A:632:A:H2'	1:A:633:G:H5'	2.01	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.85	0.41
1:A:58:C:O2'	1:A:59:A:H5'	2.20	0.41
15:M:91:ARG:HH22	15:M:103:THR:HG21	1.85	0.41
9:G:90:GLU:H	9:G:155:ARG:NH1	2.17	0.41
12:J:6:ILE:HG13	12:J:72:VAL:HB	2.02	0.41
1:A:926:G:H3'	1:A:1505:G:H21	1.85	0.41
15:M:20:THR:C	15:M:22:ILE:N	2.74	0.41
1:A:1072:G:C5	1:A:1073:U:C4	3.08	0.41
22:T:43:LEU:CD1	22:T:55:ILE:HD12	2.51	0.41
1:A:1125:U:H3	12:J:5:ARG:CZ	2.33	0.41
6:D:7:PRO:CB	6:D:10:ARG:HD2	2.49	0.41
4:B:7:VAL:O	4:B:7:VAL:HG23	2.20	0.41
1:A:132:C:O3'	22:T:74:LYS:CE	2.62	0.41
8:F:10:LEU:HD12	8:F:10:LEU:H	1.85	0.41
5:C:65:ALA:O	5:C:66:VAL:HB	2.19	0.41
9:G:30:ILE:HD13	9:G:120:ILE:HD13	2.01	0.41
5:C:97:LYS:O	5:C:98:ASN:C	2.59	0.41
22:T:89:ARG:NH2	22:T:106:ALA:HA	2.35	0.41
1:A:363:A:O2'	1:A:364:A:H5'	2.19	0.41
20:R:37:VAL:HG22	20:R:78:LEU:HB3	2.02	0.41
13:K:69:ALA:O	13:K:70:LYS:C	2.57	0.41
7:E:107:ARG:O	7:E:108:ALA:C	2.58	0.41
6:D:76:ARG:HD2	6:D:76:ARG:HA	1.87	0.41
1:A:645:C:H2'	1:A:646:U:C6	2.55	0.41
4:B:95:GLN:OE1	4:B:95:GLN:HA	2.21	0.41
12:J:39:PRO:O	12:J:69:ASN:O	2.38	0.41
21:S:19:VAL:CG1	21:S:20:LEU:N	2.83	0.41
12:J:48:THR:OG1	12:J:62:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:20:THR:O	15:M:22:ILE:N	2.52	0.41
8:F:30:LEU:HD11	8:F:63:TYR:CD1	2.56	0.41
1:A:838:G:N2	1:A:849:C:C2	2.89	0.41
5:C:64:VAL:CB	5:C:99:VAL:HB	2.38	0.41
1:A:1320:C:H5	21:S:37:ARG:CZ	2.33	0.41
2:Y:31:C:H1'	2:Y:40:G:N2	2.35	0.41
1:A:250:A:O5'	1:A:250:A:H8	2.02	0.41
12:J:80:LYS:HA	12:J:83:GLU:HB2	2.02	0.41
1:A:302:G:N3	1:A:556:C:H4'	2.35	0.41
1:A:1312:G:N7	21:S:3:ARG:O	2.54	0.41
1:A:533:A:C5	1:A:536:C:C4	3.08	0.41
15:M:81:LEU:HA	15:M:84:ILE:HD11	2.02	0.41
9:G:111:ARG:HB3	9:G:113:GLU:OE2	2.19	0.41
9:G:140:ASP:OD1	9:G:143:ARG:NH1	2.54	0.41
8:F:101:ALA:HB2	20:R:28:GLU:HB2	2.02	0.41
1:A:19:C:H2'	1:A:20:U:C6	2.50	0.41
7:E:152:ARG:HA	10:H:64:LYS:HZ3	1.85	0.41
1:A:1091:U:O2	1:A:1093:A:H8	2.01	0.41
8:F:91:VAL:CG1	8:F:92:LYS:N	2.82	0.41
1:A:1419:G:H2'	1:A:1420:C:C6	2.55	0.41
1:A:124:G:C5	1:A:125:U:C4	3.08	0.41
1:A:50:A:N6	1:A:361:G:H4'	2.35	0.41
6:D:24:GLU:C	6:D:26:CYS:H	2.23	0.41
12:J:8:LEU:HD12	12:J:20:ALA:HB2	2.03	0.41
16:N:45:ARG:CG	16:N:45:ARG:NH1	2.83	0.41
4:B:231:GLU:CD	4:B:231:GLU:H	2.22	0.41
1:A:344:A:H5''	1:A:345:C:C5	2.55	0.41
7:E:18:ARG:HG2	7:E:19:MET:N	2.36	0.41
1:A:1355:G:H2'	1:A:1356:G:C8	2.55	0.41
6:D:149:ALA:O	6:D:150:GLU:C	2.59	0.41
9:G:65:ALA:HB1	9:G:127:ALA:CB	2.50	0.41
5:C:187:ALA:HB3	5:C:198:VAL:HB	2.03	0.41
1:A:1182:G:HO2'	1:A:1183:A:P	2.37	0.41
1:A:1216:G:OP1	16:N:3:ARG:HG2	2.20	0.41
16:N:3:ARG:O	16:N:5:ALA:N	2.54	0.41
5:C:123:GLN:HB3	5:C:128:PHE:HB2	2.02	0.41
1:A:373:A:C2	1:A:482:A:C6	3.07	0.41
18:P:26:ARG:HD2	18:P:31:LYS:O	2.20	0.41
6:D:17:VAL:HG12	6:D:18:LYS:N	2.35	0.41
4:B:122:PHE:O	4:B:123:ALA:HB2	2.20	0.41
1:A:1249:C:H4'	11:I:36:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:84:ALA:HA	11:I:87:GLN:HB3	2.02	0.41
1:A:998:G:O2'	1:A:999:C:H5'	2.21	0.41
8:F:37:VAL:HA	8:F:65:VAL:HG12	2.02	0.41
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.41
1:A:123:C:OP1	1:A:312:C:H5'	2.21	0.41
6:D:31:CYS:C	6:D:33:MET:H	2.24	0.41
1:A:17:U:H4'	1:A:1080:A:O4'	2.21	0.41
1:A:723:U:O2	1:A:723:U:H2'	2.19	0.41
1:A:582:U:H2'	1:A:583:A:C8	2.56	0.41
5:C:141:VAL:HG11	5:C:202:ILE:HG23	2.01	0.41
8:F:75:LEU:HD13	8:F:75:LEU:C	2.41	0.41
5:C:147:LYS:HE3	5:C:203:PHE:CZ	2.56	0.41
4:B:114:ARG:NH1	4:B:118:LEU:HD21	2.36	0.41
4:B:239:VAL:O	4:B:239:VAL:CG1	2.65	0.41
20:R:36:ASN:CG	20:R:39:VAL:HG12	2.41	0.41
7:E:76:ILE:HD12	7:E:76:ILE:N	2.34	0.41
1:A:1381:U:HO2'	1:A:1382:C:H5'	1.85	0.41
1:A:284:G:O2'	1:A:285:G:H5'	2.21	0.41
7:E:99:GLY:O	7:E:117:ASP:HA	2.21	0.41
4:B:69:LEU:HD12	4:B:155:LEU:CD1	2.51	0.41
1:A:961:U:H2'	1:A:962:C:C5'	2.51	0.41
6:D:19:LEU:HD22	6:D:67:ILE:HG13	2.02	0.41
1:A:1327:C:O2'	1:A:1328:C:H5'	2.21	0.41
7:E:126:ARG:NH1	7:E:126:ARG:HG3	2.36	0.41
21:S:18:LYS:O	21:S:22:LEU:HG	2.21	0.41
8:F:62:TRP:CD1	20:R:35:ARG:CZ	3.04	0.41
1:A:1054:C:O2'	1:A:1055:A:C5'	2.69	0.41
5:C:85:ARG:HD2	5:C:85:ARG:O	2.21	0.41
4:B:59:GLU:CG	4:B:60:ASP:N	2.83	0.41
17:O:70:LEU:C	17:O:72:ARG:N	2.73	0.41
22:T:56:MET:HE2	22:T:88:VAL:CB	2.48	0.41
6:D:98:GLU:CG	6:D:189:PRO:HG3	2.51	0.41
17:O:36:ILE:CG1	17:O:59:MET:HE3	2.50	0.41
10:H:29:SER:O	10:H:30:ARG:C	2.59	0.41
1:A:1278:U:H5'	1:A:1279:A:O4'	2.21	0.41
21:S:14:HIS:O	21:S:18:LYS:HB2	2.21	0.41
21:S:16:LEU:C	21:S:18:LYS:N	2.72	0.41
12:J:49:VAL:O	12:J:60:ARG:C	2.59	0.41
8:F:67:MET:HE1	8:F:75:LEU:HB2	2.02	0.41
5:C:83:ARG:HE	5:C:87:LEU:CD1	2.33	0.41
19:Q:102:GLY:O	19:Q:103:GLY:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:151:GLY:C	4:B:153:ARG:H	2.24	0.41
6:D:62:GLN:NE2	6:D:65:ARG:HH12	2.18	0.41
15:M:4:ILE:HG23	15:M:57:ARG:HA	2.02	0.41
1:A:557:G:H2'	1:A:558:G:C8	2.56	0.41
1:A:479:C:H2'	1:A:480:U:O4'	2.21	0.41
1:A:1405:G:H1'	1:A:1519:A:C4'	2.50	0.41
10:H:51:VAL:HG21	10:H:60:ARG:NH1	2.35	0.41
4:B:155:LEU:HD23	4:B:155:LEU:HA	1.86	0.41
1:A:1121:U:O2'	1:A:1122:U:H5'	2.20	0.41
1:A:718:G:C5'	1:A:719:C:OP2	2.69	0.41
1:A:1029:C:H2'	1:A:1030:C:C6	2.54	0.41
1:A:1349:A:H2'	1:A:1350:A:C8	2.55	0.41
4:B:80:ILE:HD11	4:B:208:ILE:CG2	2.43	0.41
4:B:17:PHE:O	4:B:18:GLY:O	2.39	0.41
12:J:39:PRO:HA	12:J:70:ARG:HH11	1.84	0.41
1:A:1441:G:H1'	1:A:1460:A:N6	2.36	0.41
1:A:1126:U:C2	1:A:1127:G:C8	3.08	0.41
11:I:97:LYS:N	11:I:98:PRO:CD	2.83	0.41
4:B:118:LEU:HB3	4:B:142:LEU:HG	2.03	0.41
1:A:1153:C:C2	1:A:1154:G:C8	3.09	0.41
19:Q:63:ARG:HG2	19:Q:64:PRO:HD2	2.03	0.41
2:Y:30:C:O5'	2:Y:30:C:H6	2.03	0.41
15:M:105:THR:O	15:M:106:ASN:C	2.59	0.41
12:J:81:THR:C	12:J:83:GLU:N	2.73	0.41
18:P:20:VAL:HG12	18:P:21:VAL:O	2.20	0.41
1:A:682:G:O2'	1:A:683:G:H5'	2.21	0.41
4:B:82:ARG:HG3	4:B:83:MET:N	2.36	0.41
10:H:51:VAL:CG1	10:H:52:ASP:H	2.33	0.41
10:H:51:VAL:CG2	10:H:60:ARG:HG2	2.51	0.41
1:A:404:U:H2'	1:A:405:U:H6	1.86	0.41
7:E:5:ASP:CG	7:E:6:PHE:N	2.72	0.41
14:L:88:GLY:H	14:L:98:TYR:HA	1.85	0.41
15:M:82:MET:CE	15:M:92:HIS:HB3	2.50	0.41
1:A:586:C:O3'	10:H:89:PRO:HB2	2.21	0.41
17:O:36:ILE:HA	17:O:59:MET:CE	2.51	0.41
1:A:50:A:H4'	1:A:51:A:H5'	2.02	0.41
7:E:150:ARG:NH1	7:E:150:ARG:HG3	2.36	0.41
1:A:619:U:O2	6:D:133:VAL:HA	2.20	0.41
1:A:916:G:H2'	1:A:917:G:H8	1.86	0.41
21:S:74:PHE:N	21:S:74:PHE:CD1	2.89	0.41
1:A:304:U:O2'	1:A:305:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:C:C4	1:A:1345:U:C5	3.09	0.41
1:A:1068:G:H8	1:A:1068:G:OP2	2.02	0.41
12:J:79:ARG:HG2	12:J:79:ARG:HH11	1.85	0.41
1:A:136:C:H2'	1:A:137:C:H6	1.86	0.41
12:J:24:VAL:HG12	12:J:28:ARG:NE	2.36	0.41
12:J:49:VAL:CG1	16:N:41:ARG:HD2	2.46	0.41
1:A:1300:G:C2'	1:A:1301:U:OP2	2.68	0.41
15:M:15:VAL:HG23	15:M:43:THR:O	2.21	0.41
1:A:1154:G:H2'	1:A:1155:G:C8	2.47	0.41
4:B:64:ARG:NH1	4:B:64:ARG:HB2	2.36	0.41
1:A:1288:A:C6	1:A:1289:A:C5	3.09	0.41
1:A:947:G:H2'	1:A:948:C:O4'	2.21	0.41
14:L:126:LYS:C	14:L:126:LYS:HZ2	2.24	0.41
16:N:11:LYS:HB2	16:N:11:LYS:HE3	1.90	0.41
1:A:1494:G:O2'	1:A:1495:U:H5'	2.21	0.41
18:P:63:GLY:O	18:P:64:ALA:C	2.59	0.41
4:B:228:GLY:O	4:B:229:VAL:C	2.59	0.41
13:K:99:GLN:HG2	13:K:105:VAL:HG21	2.03	0.41
1:A:645:C:H2'	1:A:646:U:H6	1.85	0.41
1:A:166:G:O2'	1:A:167:G:H5'	2.20	0.41
1:A:272:C:O2'	1:A:273:A:H5'	2.21	0.41
1:A:855:G:H2'	1:A:856:C:C6	2.56	0.41
1:A:678:U:H2'	1:A:679:C:C6	2.56	0.41
1:A:1278:U:H4'	1:A:1279:A:H5'	1.99	0.40
5:C:14:ILE:O	5:C:15:THR:C	2.60	0.40
22:T:43:LEU:HD12	22:T:52:ALA:HA	2.03	0.40
6:D:8:VAL:O	6:D:10:ARG:N	2.54	0.40
19:Q:103:GLY:O	19:Q:104:LYS:HD3	2.20	0.40
1:A:204:U:H5'	1:A:216:G:O4'	2.21	0.40
4:B:230:VAL:HG13	4:B:231:GLU:OE2	2.21	0.40
6:D:149:ALA:O	6:D:152:SER:N	2.38	0.40
1:A:523:A:H61	14:L:53:ARG:NH1	2.20	0.40
15:M:63:THR:HG23	15:M:64:TRP:N	2.35	0.40
1:A:180:U:C2'	1:A:181:G:H5'	2.50	0.40
9:G:122:HIS:HD2	9:G:125:MET:HE1	1.84	0.40
16:N:44:LEU:O	16:N:48:ALA:HB2	2.21	0.40
1:A:983:A:C2	1:A:984:C:C6	3.09	0.40
1:A:90:U:H2'	1:A:91:C:C6	2.56	0.40
1:A:1082:G:O2'	1:A:1083:U:H5'	2.21	0.40
1:A:1010:G:O2'	1:A:1011:G:H5'	2.21	0.40
4:B:18:GLY:CA	4:B:41:ILE:HA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:C6	1:A:1446:A:N6	2.88	0.40
15:M:25:ILE:HD11	15:M:60:VAL:HG13	2.03	0.40
8:F:75:LEU:HD13	8:F:75:LEU:O	2.21	0.40
5:C:147:LYS:HE2	5:C:205:GLY:CA	2.52	0.40
22:T:100:ILE:O	22:T:100:ILE:HG22	2.21	0.40
1:A:1125:U:O4	12:J:5:ARG:HG2	2.22	0.40
1:A:1145:C:O2'	1:A:1146:A:O5'	2.32	0.40
1:A:972:C:O2'	12:J:55:LYS:HA	2.22	0.40
1:A:130:A:C8	19:Q:63:ARG:HG3	2.56	0.40
1:A:751:U:H4'	17:O:24:SER:HA	2.02	0.40
4:B:124:SER:O	4:B:127:ILE:HG13	2.20	0.40
14:L:89:ARG:HG2	14:L:97:ARG:HB3	2.02	0.40
1:A:1002:G:N1	1:A:1003:G:C6	2.89	0.40
7:E:102:ALA:HB2	7:E:120:THR:HB	2.03	0.40
7:E:102:ALA:CB	7:E:120:THR:HG21	2.51	0.40
1:A:421:U:C5'	1:A:422:C:OP2	2.65	0.40
5:C:150:LYS:HB2	5:C:169:ALA:HB1	2.02	0.40
16:N:37:PHE:C	16:N:39:LEU:N	2.75	0.40
10:H:65:TYR:HA	10:H:79:VAL:HG23	2.03	0.40
1:A:560:U:O2'	1:A:561:U:OP2	2.30	0.40
22:T:63:ILE:HD13	22:T:80:ARG:HB2	2.04	0.40
18:P:43:LYS:HG2	18:P:48:TRP:CE2	2.56	0.40
8:F:23:LYS:HE2	8:F:23:LYS:HB3	1.97	0.40
1:A:67:C:O2'	1:A:171:A:H1'	2.21	0.40
7:E:126:ARG:HH11	7:E:126:ARG:HG3	1.86	0.40
1:A:739:C:O2'	17:O:42:HIS:ND1	2.46	0.40
4:B:72:GLY:HA3	4:B:81:VAL:HG21	2.04	0.40
12:J:16:LEU:O	12:J:17:ASP:C	2.60	0.40
12:J:23:ILE:CG2	12:J:72:VAL:HG11	2.51	0.40
1:A:1112:C:O2	5:C:179:ARG:HB2	2.21	0.40
4:B:97:TRP:CH2	4:B:176:GLU:CD	2.93	0.40
1:A:1286:A:H2'	1:A:1287:A:O5'	2.21	0.40
9:G:139:GLU:O	9:G:143:ARG:HG3	2.22	0.40
15:M:91:ARG:HD2	15:M:91:ARG:HA	1.97	0.40
1:A:141:A:H2'	1:A:142:G:O4'	2.22	0.40
10:H:25:ASP:OD1	10:H:25:ASP:N	2.54	0.40
9:G:110:GLN:OE1	9:G:110:GLN:HA	2.21	0.40
1:A:426:G:H2'	1:A:427:U:C6	2.57	0.40
1:A:582:U:C2	1:A:760:G:C6	3.10	0.40
4:B:14:GLY:C	4:B:15:VAL:CG2	2.90	0.40
21:S:22:LEU:HD13	21:S:28:LYS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:153:VAL:HG12	5:C:154:SER:N	2.36	0.40
5:C:154:SER:OG	5:C:155:GLY:N	2.53	0.40
14:L:46:LYS:HE3	14:L:47:LYS:HB2	2.03	0.40
4:B:112:VAL:C	4:B:114:ARG:N	2.73	0.40
4:B:140:HIS:O	4:B:141:GLU:C	2.58	0.40
9:G:51:GLN:O	9:G:53:LYS:N	2.54	0.40
1:A:1065:U:O2'	1:A:1066:C:OP2	2.30	0.40
1:A:812:C:O2'	1:A:813:U:OP2	2.19	0.40
1:A:942:G:H2'	1:A:943:U:C6	2.57	0.40
1:A:1342:C:O3'	11:I:125:TYR:CE2	2.74	0.40
15:M:81:LEU:HA	15:M:84:ILE:HG12	2.03	0.40
15:M:59:TYR:O	15:M:62:ASN:O	2.38	0.40
9:G:115:ARG:HB3	9:G:118:VAL:CG2	2.52	0.40
4:B:91:PRO:HG2	4:B:155:LEU:HG	2.03	0.40
5:C:123:GLN:NE2	5:C:140:ARG:HH22	2.20	0.40
1:A:757:U:O2'	1:A:879:C:H1'	2.22	0.40
1:A:154:C:H2'	1:A:155:C:H6	1.87	0.40
1:A:1524:C:OP1	13:K:120:ARG:NH1	2.54	0.40
17:O:85:LEU:HA	17:O:85:LEU:HD23	1.86	0.40
1:A:224:C:H2'	1:A:225:C:H6	1.87	0.40
10:H:75:ARG:HA	10:H:76:PRO:HD3	1.77	0.40
21:S:32:LYS:O	21:S:32:LYS:HG3	2.22	0.40
22:T:14:LYS:O	22:T:18:GLN:HG3	2.21	0.40
1:A:1191:A:H2'	1:A:1192:C:H6	1.85	0.40
1:A:1169:A:H2'	1:A:1171:G:O4'	2.22	0.40
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.40
1:A:373:A:C1'	1:A:481:G:O2'	2.69	0.40
8:F:42:GLU:HG3	8:F:61:LEU:HD23	2.03	0.40
9:G:95:ARG:HG2	9:G:99:LEU:CD1	2.52	0.40
12:J:25:GLU:C	12:J:27:ALA:H	2.25	0.40
1:A:665:A:N3	1:A:732:C:H2'	2.36	0.40
14:L:123:LYS:HG2	14:L:123:LYS:H	1.66	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	232/256 (91%)	159 (68%)	49 (21%)	24 (10%)	1	3
5	C	204/239 (85%)	128 (63%)	44 (22%)	32 (16%)	0	1
6	D	206/208 (99%)	170 (82%)	25 (12%)	11 (5%)	2	14
7	E	148/161 (92%)	132 (89%)	15 (10%)	1 (1%)	26	70
8	F	99/101 (98%)	80 (81%)	16 (16%)	3 (3%)	5	29
9	G	153/155 (99%)	121 (79%)	28 (18%)	4 (3%)	7	33
10	H	136/138 (99%)	117 (86%)	17 (12%)	2 (2%)	13	50
11	I	125/128 (98%)	91 (73%)	24 (19%)	10 (8%)	1	5
12	J	96/104 (92%)	58 (60%)	21 (22%)	17 (18%)	0	1
13	K	117/129 (91%)	95 (81%)	13 (11%)	9 (8%)	1	6
14	L	122/135 (90%)	99 (81%)	16 (13%)	7 (6%)	2	12
15	M	116/126 (92%)	83 (72%)	21 (18%)	12 (10%)	1	3
16	N	58/60 (97%)	33 (57%)	15 (26%)	10 (17%)	0	1
17	O	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	8	36
18	P	81/88 (92%)	64 (79%)	13 (16%)	4 (5%)	3	16
19	Q	102/104 (98%)	85 (83%)	10 (10%)	7 (7%)	1	7
20	R	71/88 (81%)	62 (87%)	5 (7%)	4 (6%)	2	13
21	S	78/92 (85%)	57 (73%)	15 (19%)	6 (8%)	1	6
22	T	97/106 (92%)	73 (75%)	15 (16%)	9 (9%)	1	4
23	V	22/26 (85%)	15 (68%)	6 (27%)	1 (4%)	3	18
All	All	2349/2532 (93%)	1800 (77%)	374 (16%)	175 (7%)	1	6

All (175) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	15	VAL
4	B	17	PHE
4	B	21	ARG
4	B	23	ARG
4	B	24	TRP
4	B	123	ALA
4	B	142	LEU

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Mol	Chain	Res	Type
4	B	143	GLU
4	B	190	THR
4	B	229	VAL
4	B	232	PRO
5	C	15	THR
5	C	16	ARG
5	C	26	LYS
5	C	82	GLU
5	C	84	ILE
5	C	98	ASN
5	C	100	ALA
5	C	101	LEU
5	C	156	ARG
5	C	187	ALA
5	C	189	ALA
6	D	36	ARG
7	E	16	THR
8	F	36	ARG
10	H	91	ARG
11	I	41	VAL
11	I	127	LYS
12	J	34	VAL
12	J	61	GLU
12	J	79	ARG
13	K	13	GLN
13	K	127	LYS
14	L	27	LEU
14	L	28	LYS
14	L	47	LYS
15	M	6	GLY
15	M	23	TYR
15	M	24	GLY
15	M	27	LYS
15	M	67	GLU
15	M	86	CYS
16	N	22	THR
17	O	88	ARG
18	P	52	ASP
18	P	64	ALA
19	Q	14	LYS
19	Q	80	GLY
19	Q	81	ARG

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Mol	Chain	Res	Type
19	Q	96	GLN
20	R	19	LYS
20	R	87	ARG
21	S	5	LEU
22	T	9	ASN
22	T	11	SER
4	B	8	LYS
4	B	18	GLY
4	B	95	GLN
4	B	195	ASP
4	B	228	GLY
5	C	66	VAL
5	C	127	ARG
5	C	154	SER
5	C	171	GLY
5	C	179	ARG
6	D	31	CYS
6	D	44	GLY
8	F	35	ALA
9	G	4	ARG
9	G	80	VAL
10	H	105	ARG
11	I	11	LYS
11	I	46	ALA
11	I	55	ALA
11	I	58	ARG
11	I	78	LYS
12	J	27	ALA
12	J	30	SER
12	J	32	ALA
12	J	54	PHE
12	J	55	LYS
12	J	72	VAL
13	K	90	GLY
14	L	79	GLU
14	L	116	SER
15	M	63	THR
15	M	106	ASN
16	N	15	LYS
16	N	36	PHE
16	N	56	VAL
18	P	10	GLY

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Mol	Chain	Res	Type
19	Q	103	GLY
20	R	48	GLY
22	T	74	LYS
22	T	96	GLY
22	T	102	GLY
4	B	20	GLU
4	B	74	LYS
5	C	102	ASN
5	C	181	ASN
5	C	205	GLY
6	D	4	TYR
6	D	42	GLN
12	J	65	LEU
12	J	90	LEU
12	J	99	LYS
13	K	15	ALA
13	K	27	ASN
13	K	117	ASN
14	L	48	PRO
14	L	126	LYS
15	M	3	ARG
15	M	21	TYR
16	N	12	ARG
16	N	14	PRO
19	Q	68	ARG
19	Q	98	LEU
21	S	6	LYS
21	S	32	LYS
22	T	73	HIS
22	T	103	GLY
23	V	9	ARG
4	B	9	GLU
4	B	16	HIS
4	B	39	ILE
4	B	90	MET
5	C	12	LEU
5	C	108	ASN
5	C	146	ALA
5	C	188	LEU
6	D	5	ILE
6	D	7	PRO
6	D	9	CYS

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Mol	Chain	Res	Type
6	D	88	VAL
8	F	98	LEU
9	G	41	ARG
11	I	105	ASP
12	J	39	PRO
12	J	40	LEU
12	J	73	ASP
12	J	86	MET
15	M	4	ILE
16	N	26	ARG
20	R	38	GLU
21	S	17	GLU
21	S	30	LEU
5	C	4	LYS
5	C	14	ILE
5	C	29	TYR
11	I	121	ARG
13	K	69	ALA
16	N	4	LYS
17	O	75	PRO
22	T	94	ALA
4	B	130	ARG
5	C	53	ALA
5	C	168	ALA
6	D	91	SER
11	I	12	GLU
13	K	70	LYS
16	N	23	ARG
21	S	9	VAL
22	T	97	ALA
6	D	87	GLY
12	J	4	ILE
18	P	51	VAL
4	B	227	GLY
5	C	81	GLY
15	M	97	PRO
5	C	55	VAL
5	C	57	ILE
9	G	42	ILE
13	K	48	ILE
16	N	25	VAL
5	C	13	GLY

### 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%)	175 (87%)	27 (13%)	5	21
5	C	160/188 (85%)	144 (90%)	16 (10%)	9	34
6	D	180/180 (100%)	167 (93%)	13 (7%)	18	53
7	E	115/122 (94%)	99 (86%)	16 (14%)	4	19
8	F	90/90 (100%)	80 (89%)	10 (11%)	8	29
9	G	126/126 (100%)	120 (95%)	6 (5%)	31	71
10	H	119/119 (100%)	106 (89%)	13 (11%)	8	30
11	I	98/99 (99%)	87 (89%)	11 (11%)	7	29
12	J	87/91 (96%)	79 (91%)	8 (9%)	11	40
13	K	90/99 (91%)	83 (92%)	7 (8%)	16	49
14	L	104/111 (94%)	94 (90%)	10 (10%)	10	38
15	M	94/101 (93%)	83 (88%)	11 (12%)	7	27
16	N	49/49 (100%)	43 (88%)	6 (12%)	6	25
17	O	79/79 (100%)	73 (92%)	6 (8%)	16	51
18	P	72/74 (97%)	68 (94%)	4 (6%)	26	65
19	Q	96/96 (100%)	87 (91%)	9 (9%)	11	39
20	R	64/77 (83%)	61 (95%)	3 (5%)	32	72
21	S	71/79 (90%)	62 (87%)	9 (13%)	5	23
22	T	76/82 (93%)	70 (92%)	6 (8%)	15	48
23	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1991/2103 (95%)	1800 (90%)	191 (10%)	10	38

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	10	LEU
4	B	15	VAL

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Mol	Chain	Res	Type
4	B	23	ARG
4	B	24	TRP
4	B	25	ASN
4	B	82	ARG
4	B	87	ARG
4	B	90	MET
4	B	98	LEU
4	B	117	GLU
4	B	121	LEU
4	B	129	GLU
4	B	141	GLU
4	B	156	LYS
4	B	162	ILE
4	B	163	PHE
4	B	165	VAL
4	B	169	LYS
4	B	170	GLU
4	B	178	ARG
4	B	187	LEU
4	B	204	ASN
4	B	208	ILE
4	B	231	GLU
4	B	232	PRO
4	B	236	TYR
5	C	3	ASN
5	C	5	ILE
5	C	14	ILE
5	C	26	LYS
5	C	35	GLU
5	C	44	GLU
5	C	52	LEU
5	C	56	ASP
5	C	99	VAL
5	C	139	GLN
5	C	162	GLN
5	C	166	GLU
5	C	167	TRP
5	C	184	TYR
5	C	188	LEU
5	C	204	LEU
6	D	9	CYS
6	D	15	GLU

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Mol	Chain	Res	Type
6	D	33	MET
6	D	36	ARG
6	D	57	ARG
6	D	58	LEU
6	D	72	GLU
6	D	96	LEU
6	D	122	ARG
6	D	127	THR
6	D	157	LEU
6	D	192	GLU
6	D	193	ASP
7	E	12	LEU
7	E	15	ARG
7	E	25	ARG
7	E	26	PHE
7	E	31	LEU
7	E	33	VAL
7	E	41	VAL
7	E	43	LEU
7	E	53	LEU
7	E	73	ASN
7	E	79	GLU
7	E	80	ILE
7	E	89	ILE
7	E	120	THR
7	E	144	THR
7	E	150	ARG
8	F	1	MET
8	F	10	LEU
8	F	24	GLU
8	F	55	ASP
8	F	63	TYR
8	F	69	GLU
8	F	74	ASP
8	F	86	ARG
8	F	89	MET
8	F	95	GLU
9	G	11	GLN
9	G	37	ASN
9	G	38	LEU
9	G	84	ASN
9	G	149	ARG

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Mol	Chain	Res	Type
9	G	156	TRP
10	H	24	THR
10	H	26	VAL
10	H	52	ASP
10	H	63	LEU
10	H	81	HIS
10	H	84	ARG
10	H	85	ARG
10	H	91	ARG
10	H	92	ARG
10	H	112	LEU
10	H	125	ARG
10	H	127	LEU
10	H	133	LEU
11	I	2	GLU
11	I	16	ARG
11	I	38	GLN
11	I	41	VAL
11	I	58	ARG
11	I	65	VAL
11	I	75	ASP
11	I	79	LEU
11	I	92	TYR
11	I	111	ARG
11	I	121	ARG
12	J	29	ARG
12	J	45	ARG
12	J	57	LYS
12	J	60	ARG
12	J	66	ARG
12	J	73	ASP
12	J	83	GLU
12	J	89	ASP
13	K	24	SER
13	K	29	ILE
13	K	30	VAL
13	K	35	PRO
13	K	54	ARG
13	K	57	THR
13	K	73	MET
14	L	33	ARG
14	L	41	ARG

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Mol	Chain	Res	Type
14	L	48	PRO
14	L	53	ARG
14	L	59	ARG
14	L	60	LEU
14	L	79	GLU
14	L	113	ARG
14	L	114	LYS
14	L	126	LYS
15	M	40	ASN
15	M	44	ARG
15	M	56	LEU
15	M	59	TYR
15	M	70	LEU
15	M	81	LEU
15	M	102	ARG
15	M	105	THR
15	M	106	ASN
15	M	110	ARG
15	M	115	LYS
16	N	12	ARG
16	N	14	PRO
16	N	22	THR
16	N	31	ARG
16	N	41	ARG
16	N	44	LEU
17	O	10	LYS
17	O	31	LEU
17	O	34	LEU
17	O	39	LEU
17	O	70	LEU
17	O	81	LEU
18	P	2	VAL
18	P	8	ARG
18	P	53	VAL
18	P	62	VAL
19	Q	9	VAL
19	Q	38	ARG
19	Q	48	GLU
19	Q	53	LEU
19	Q	60	ILE
19	Q	68	ARG
19	Q	74	LEU

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Mol	Chain	Res	Type
19	Q	76	LEU
19	Q	101	ARG
20	R	36	ASN
20	R	54	ARG
20	R	55	ARG
21	S	5	LEU
21	S	7	LYS
21	S	12	ASP
21	S	15	LEU
21	S	36	ARG
21	S	61	TYR
21	S	62	ILE
21	S	65	ASN
21	S	81	ARG
22	T	13	LEU
22	T	42	GLN
22	T	57	ARG
22	T	73	HIS
22	T	75	ASN
22	T	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	19	HIS
4	B	25	ASN
4	B	40	HIS
4	B	94	ASN
4	B	204	ASN
4	B	212	GLN
4	B	240	GLN
5	C	3	ASN
5	C	6	HIS
5	C	37	GLN
5	C	107	GLN
5	C	108	ASN
5	C	110	ASN
5	C	123	GLN
5	C	139	GLN
5	C	170	GLN
5	C	176	HIS
5	C	181	ASN

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Mol	Chain	Res	Type
6	D	42	GLN
6	D	62	GLN
6	D	123	HIS
6	D	161	ASN
7	E	20	GLN
7	E	73	ASN
8	F	18	GLN
8	F	32	ASN
8	F	57	GLN
8	F	73	ASN
8	F	94	GLN
8	F	100	ASN
9	G	37	ASN
9	G	51	GLN
9	G	56	GLN
9	G	64	GLN
9	G	68	ASN
9	G	96	GLN
9	G	106	GLN
9	G	122	HIS
11	I	31	GLN
11	I	73	GLN
12	J	62	HIS
12	J	78	ASN
13	K	38	ASN
13	K	93	GLN
13	K	117	ASN
14	L	49	ASN
14	L	75	HIS
15	M	40	ASN
17	O	37	ASN
17	O	46	HIS
18	P	16	HIS
19	Q	16	GLN
20	R	36	ASN
21	S	14	HIS
21	S	23	ASN
21	S	47	HIS
21	S	56	GLN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	211 (13%)	69 (4%)
2	Y	14/17 (82%)	1 (7%)	0
3	Z	3/6 (50%)	0	0
All	All	1528/1545 (98%)	212 (13%)	69 (4%)

All (212) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	81	U
1	A	82	U
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	130	A
1	A	131	C
1	A	163	C
1	A	181	G
1	A	182	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	282	A

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Mol	Chain	Res	Type
1	A	289	G
1	A	316	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	461	C
1	A	462	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A

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Mol	Chain	Res	Type
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	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	721	G
1	A	723	U
1	A	724	G
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	794	A
1	A	813	U
1	A	815	A
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
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	965	A

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Mol	Chain	Res	Type
1	A	966	G
1	A	968	A
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	1004	A
1	A	1005	A
1	A	1026	G
1	A	1031	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1085	U
1	A	1086	U
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	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1152	A

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1160	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1250	A
1	A	1257	U
1	A	1279	A
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	1303	C
1	A	1305	G
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1379	G
1	A	1398	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A

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Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
2	Y	34	G

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	48	C
1	A	51	A
1	A	60	A
1	A	64	G
1	A	81	U
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	202	U
1	A	204	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
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	421	U
1	A	428	G
1	A	438	G
1	A	484	G
1	A	485	G

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Mol	Chain	Res	Type
1	A	496	A
1	A	497	A
1	A	509	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	722	A
1	A	793	U
1	A	812	C
1	A	913	A
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	1085	U
1	A	1101	A
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1224	G
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1346	A
1	A	1347	G
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1528	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	PSU	Y	38	2	13,21,22	1.68	2 (15%)	18,30,33	6.01	7 (38%)

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
2	PSU	Y	38	2	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	38	PSU	C6-N1	3.30	1.41	1.34
2	Y	38	PSU	C4-N3	4.74	1.41	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	38	PSU	N1-C2-N3	-20.95	114.96	128.33
2	Y	38	PSU	C4-C5-C1'	-3.72	114.45	121.23
2	Y	38	PSU	C5-C6-N1	-2.15	121.36	124.39
2	Y	38	PSU	C5-C1'-C2'	-2.12	111.75	115.52
2	Y	38	PSU	O4'-C1'-C2'	3.31	108.11	104.73
2	Y	38	PSU	C6-N1-C2	3.52	121.12	115.47
2	Y	38	PSU	C4-N3-C2	12.70	126.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	38	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 160 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	1.59	12 (26%)	59,67,67	1.12	4 (6%)

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	-	-	0/18/94/94	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C44-C34	2.03	1.57	1.52
24	A	1545	PAR	C52-C42	2.10	1.56	1.52
24	A	1545	PAR	C44-C54	2.11	1.57	1.53
24	A	1545	PAR	O44-C44	2.16	1.48	1.43
24	A	1545	PAR	O51-C11	2.17	1.47	1.41
24	A	1545	PAR	O33-C33	2.20	1.49	1.43
24	A	1545	PAR	C41-C51	2.23	1.57	1.53
24	A	1545	PAR	C11-C21	2.32	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C31-C21	2.46	1.56	1.53
24	A	1545	PAR	O33-C14	2.85	1.49	1.41
24	A	1545	PAR	C64-C54	3.10	1.59	1.52
24	A	1545	PAR	O54-C14	3.97	1.52	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O11-C11-C21	2.15	111.93	107.96
24	A	1545	PAR	C14-O54-C54	2.87	119.32	113.75
24	A	1545	PAR	O52-C13-C23	3.21	114.42	107.75
24	A	1545	PAR	O54-C54-C64	3.26	112.47	106.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	1513/1522 (99%)	1.19	179 (11%) 6 2	25, 57, 134, 201	0
2	Y	14/17 (82%)	1.00	0 100 100	60, 113, 163, 179	0
3	Z	4/6 (66%)	1.27	1 (25%) 1 1	65, 69, 85, 179	0
4	B	234/256 (91%)	0.18	11 (4%) 35 14	38, 96, 154, 190	0
5	C	206/239 (86%)	0.39	11 (5%) 30 12	44, 83, 144, 182	0
6	D	208/208 (100%)	0.16	8 (3%) 44 18	39, 64, 115, 166	0
7	E	150/161 (93%)	0.06	1 (0%) 89 70	27, 50, 86, 155	0
8	F	101/101 (100%)	0.44	5 (4%) 32 13	51, 87, 132, 156	0
9	G	155/155 (100%)	-0.03	1 (0%) 90 73	38, 71, 130, 175	0
10	H	138/138 (100%)	0.00	2 (1%) 78 51	25, 46, 90, 127	0
11	I	127/128 (99%)	0.65	13 (10%) 9 3	39, 86, 135, 161	0
12	J	98/104 (94%)	1.51	30 (30%) 1 0	42, 110, 178, 201	0
13	K	119/129 (92%)	0.20	3 (2%) 61 30	27, 61, 104, 180	0
14	L	124/135 (91%)	0.17	1 (0%) 87 67	22, 61, 114, 166	0
15	M	118/126 (93%)	0.20	6 (5%) 32 12	41, 73, 119, 146	0
16	N	60/60 (100%)	0.78	8 (13%) 4 1	49, 80, 123, 174	0
17	O	88/88 (100%)	0.42	4 (4%) 37 15	34, 60, 109, 178	0
18	P	83/88 (94%)	0.07	1 (1%) 81 55	28, 48, 70, 146	0
19	Q	104/104 (100%)	0.52	8 (7%) 16 6	28, 48, 149, 201	0
20	R	73/88 (82%)	0.35	2 (2%) 58 28	41, 70, 152, 186	0
21	S	80/92 (86%)	1.00	14 (17%) 2 1	53, 101, 164, 180	0
22	T	99/106 (93%)	0.02	1 (1%) 84 60	30, 55, 105, 159	0
23	V	24/26 (92%)	0.46	2 (8%) 14 5	42, 64, 114, 151	0
All	All	3920/4077 (96%)	0.66	312 (7%) 15 5	22, 65, 141, 201	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Q	102	GLY	10.1
1	A	1534	A	9.1
19	Q	105	ALA	8.2
19	Q	104	LYS	8.1
21	S	3	ARG	8.0
1	A	1129	C	7.8
1	A	1540	U	7.6
1	A	1541	U	7.2
19	Q	103	GLY	5.9
1	A	1034	G	5.8
1	A	1144	G	5.8
1	A	1024	G	5.7
12	J	72	VAL	5.5
6	D	23	GLY	5.2
1	A	1004	A	5.1
1	A	1006	C	5.0
1	A	1025	U	4.9
1	A	993	G	4.9
1	A	1277	C	4.8
10	H	1	MET	4.7
1	A	1027	C	4.6
1	A	1030(A)	G	4.6
1	A	1539	C	4.6
12	J	10	GLY	4.5
16	N	6	LEU	4.5
16	N	3	ARG	4.5
12	J	37	PRO	4.4
1	A	992	U	4.3
11	I	17	VAL	4.3
12	J	36	GLY	4.3
1	A	1221	G	4.3
11	I	15	ALA	4.2
1	A	1003(A)	G	4.2
1	A	1030(B)	C	4.2
1	A	1001	A	4.1
1	A	1421	G	4.0
1	A	1276	G	4.0
17	O	22	THR	4.0
6	D	2	GLY	4.0
21	S	4	SER	3.9
19	Q	96	GLN	3.9
23	V	6	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
12	J	70	ARG	3.9
21	S	27	GLU	3.8
1	A	1023	G	3.8
16	N	18	VAL	3.8
1	A	1124	G	3.8
1	A	841	U	3.8
1	A	1022	G	3.8
12	J	74	ILE	3.7
1	A	1174	G	3.7
13	K	128	ALA	3.7
5	C	63	ASN	3.7
1	A	438	G	3.7
1	A	1019	C	3.7
12	J	93	GLY	3.6
1	A	1029	C	3.6
11	I	102	LEU	3.6
1	A	1283	G	3.6
1	A	1131	G	3.6
16	N	30	ALA	3.6
1	A	1002	G	3.5
1	A	1282	C	3.5
11	I	19	LEU	3.5
6	D	3	ARG	3.5
1	A	1128	C	3.5
1	A	1182	G	3.5
1	A	266	G	3.5
12	J	31	GLY	3.5
12	J	34	VAL	3.5
1	A	1011	G	3.5
1	A	1278	U	3.5
1	A	437	U	3.4
1	A	1135	U	3.4
1	A	978	A	3.4
1	A	1255	G	3.4
12	J	78	ASN	3.4
1	A	1010	G	3.3
1	A	1220	G	3.3
21	S	26	GLY	3.3
1	A	1287	A	3.3
1	A	1140	C	3.3
1	A	959	A	3.3
1	A	1005	A	3.3

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Mol	Chain	Res	Type	RSRZ
19	Q	97	SER	3.3
1	A	723	U	3.2
1	A	1268	A	3.2
1	A	410	G	3.2
1	A	1017	G	3.2
1	A	530	G	3.2
1	A	1269	A	3.2
11	I	128	ARG	3.2
1	A	1137	C	3.2
1	A	1139	G	3.2
18	P	83	GLU	3.2
11	I	7	THR	3.2
1	A	413	G	3.2
12	J	89	ASP	3.1
1	A	160	A	3.1
4	B	238	LEU	3.1
1	A	1467	G	3.1
15	M	106	ASN	3.1
21	S	53	ASN	3.1
1	A	1030(C)	G	3.0
1	A	1222	G	3.0
12	J	79	ARG	3.0
1	A	1035	A	3.0
1	A	161	A	3.0
1	A	426	G	3.0
12	J	38	ILE	3.0
21	S	37	ARG	3.0
1	A	1143	G	3.0
17	O	23	GLY	3.0
21	S	54	GLY	3.0
1	A	1016	A	3.0
20	R	25	THR	3.0
1	A	1041	A	3.0
1	A	1146	A	2.9
12	J	7	LYS	2.9
21	S	34	TRP	2.9
1	A	1503	A	2.9
1	A	1133	G	2.9
1	A	1200	C	2.9
1	A	1127	G	2.9
11	I	18	PHE	2.9
1	A	1181	G	2.9

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Mol	Chain	Res	Type	RSRZ
21	S	14	HIS	2.9
12	J	80	LYS	2.8
12	J	27	ALA	2.8
1	A	548	G	2.8
1	A	1026	G	2.8
5	C	78	GLY	2.8
1	A	1030	C	2.8
1	A	1048	G	2.8
16	N	32	SER	2.8
5	C	76	VAL	2.8
4	B	19	HIS	2.8
21	S	2	PRO	2.8
1	A	1145	C	2.8
4	B	16	HIS	2.8
1	A	1279	A	2.8
23	V	24	ARG	2.8
4	B	35	GLU	2.8
1	A	427	U	2.8
14	L	28	LYS	2.8
1	A	1141	C	2.8
1	A	1003	G	2.8
1	A	1130	A	2.8
4	B	122	PHE	2.7
16	N	60	SER	2.7
1	A	1147	C	2.7
1	A	1248	A	2.7
11	I	70	LYS	2.7
1	A	1007	C	2.7
17	O	89	GLY	2.7
1	A	750	G	2.7
5	C	21	ARG	2.7
1	A	991	U	2.7
1	A	1313	U	2.7
1	A	428	G	2.7
19	Q	101	ARG	2.7
1	A	1014	A	2.7
1	A	1013	G	2.7
1	A	1134	G	2.7
1	A	1000	U	2.7
11	I	65	VAL	2.7
1	A	1260	C	2.7
12	J	85	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
17	O	39	LEU	2.7
15	M	7	VAL	2.7
16	N	61	TRP	2.6
12	J	8	LEU	2.6
1	A	532	A	2.6
12	J	75	ILE	2.6
1	A	1442	G	2.6
22	T	103	GLY	2.6
8	F	75	LEU	2.6
1	A	1020	U	2.6
1	A	406	G	2.6
1	A	1288	A	2.6
7	E	5	ASP	2.6
11	I	92	TYR	2.6
1	A	1482	G	2.6
12	J	81	THR	2.6
12	J	6	ILE	2.5
1	A	989	C	2.5
12	J	24	VAL	2.5
15	M	81	LEU	2.5
12	J	56	HIS	2.5
1	A	758	G	2.5
12	J	35	SER	2.5
1	A	255	G	2.5
1	A	1474	G	2.5
1	A	411	A	2.5
1	A	1213	A	2.5
20	R	17	SER	2.4
1	A	1030(D)	A	2.4
1	A	1159	U	2.4
1	A	159	G	2.4
1	A	960	U	2.4
21	S	52	TYR	2.4
12	J	28	ARG	2.4
1	A	373	A	2.4
1	A	701	C	2.4
1	A	409	G	2.4
1	A	1219	U	2.4
1	A	1318	A	2.4
15	M	9	ILE	2.4
11	I	111	ARG	2.4
16	N	29	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	481	G	2.4
1	A	1053	G	2.4
1	A	1371	G	2.4
12	J	76	ASN	2.4
11	I	11	LYS	2.4
1	A	1323	G	2.4
1	A	1355	G	2.4
8	F	64	GLN	2.4
1	A	371	G	2.3
1	A	1171	G	2.3
1	A	1334	G	2.3
1	A	439	A	2.3
1	A	494	G	2.3
4	B	18	GLY	2.3
4	B	131	PRO	2.3
13	K	42	TRP	2.3
19	Q	16	GLN	2.3
6	D	32	ALA	2.3
9	G	2	ALA	2.3
5	C	23	TYR	2.3
1	A	1015	A	2.3
5	C	178	LEU	2.3
6	D	25	ARG	2.3
12	J	54	PHE	2.3
1	A	1259	C	2.3
1	A	1175	G	2.3
1	A	1370	G	2.3
4	B	235	SER	2.3
1	A	1361(A)	C	2.3
1	A	1198	G	2.3
1	A	1349	A	2.3
6	D	9	CYS	2.3
5	C	77	ILE	2.3
1	A	975	A	2.3
1	A	1178	G	2.3
3	Z	4	U	2.2
21	S	49	ILE	2.2
5	C	95	THR	2.2
1	A	251	G	2.2
1	A	254	G	2.2
1	A	529	G	2.2
1	A	1046	A	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	121	LEU	2.2
1	A	1028	C	2.2
12	J	71	LEU	2.2
1	A	837	G	2.2
5	C	59	ARG	2.2
15	M	88	ARG	2.2
1	A	1363	A	2.2
1	A	1441	G	2.2
1	A	264	U	2.2
1	A	797	C	2.2
10	H	2	LEU	2.2
6	D	21	LEU	2.2
1	A	1033	G	2.2
1	A	418	C	2.2
1	A	840	C	2.2
1	A	1285	A	2.2
1	A	1038	C	2.2
1	A	1018	C	2.2
8	F	65	VAL	2.2
1	A	1037	C	2.2
1	A	1132	C	2.2
1	A	666	G	2.2
1	A	497	A	2.1
15	M	6	GLY	2.1
4	B	81	VAL	2.1
21	S	28	LYS	2.1
1	A	1249	C	2.1
1	A	253	U	2.1
1	A	581	G	2.1
1	A	1031	G	2.1
1	A	1271	G	2.1
1	A	1475	G	2.1
1	A	1067	A	2.1
1	A	984	C	2.1
1	A	1036	G	2.1
4	B	118	LEU	2.1
6	D	42	GLN	2.1
12	J	29	ARG	2.1
8	F	101	ALA	2.1
1	A	657	G	2.1
1	A	1361	G	2.1
11	I	85	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	C	53	ALA	2.1
8	F	84	ASN	2.1
13	K	14	VAL	2.1
1	A	1304	G	2.1
1	A	1275	A	2.1
1	A	492	G	2.1
1	A	1169	A	2.0
1	A	1289	A	2.0
1	A	1502	A	2.0
21	S	15	LEU	2.0
1	A	1274	G	2.0
1	A	1422	G	2.0
5	C	60	ALA	2.0
1	A	484	G	2.0
1	A	1142	G	2.0
1	A	1434	A	2.0
12	J	11	PHE	2.0
1	A	1223	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PSU	Y	38	20/21	0.92	0.17	-	24,24,24,24	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1650	1/1	0.86	1.80	20.46	24,24,24,24	1
25	MG	A	1615	1/1	0.71	0.72	19.43	24,24,24,24	1
25	MG	A	1632	1/1	0.80	0.60	12.98	24,24,24,24	1
25	MG	A	1665	1/1	0.92	0.51	8.60	24,24,24,24	1
25	MG	A	1561	1/1	0.96	0.28	6.69	24,24,24,24	0
25	MG	A	1600	1/1	0.94	0.33	5.62	24,24,24,24	0
25	MG	A	1572	1/1	0.49	0.68	5.46	24,24,24,24	1
25	MG	A	1626	1/1	0.94	0.41	5.39	24,24,24,24	0
25	MG	A	1624	1/1	0.73	0.42	4.76	24,24,24,24	1
25	MG	A	1636	1/1	0.81	0.58	4.65	24,24,24,24	1
25	MG	A	1644	1/1	0.77	0.68	4.40	24,24,24,24	1
25	MG	A	1601	1/1	0.94	0.40	3.74	24,24,24,24	0
25	MG	A	1659	1/1	0.81	0.34	3.33	24,24,24,24	1
25	MG	A	464	1/1	0.63	0.26	1.46	24,24,24,24	1
25	MG	A	1666	1/1	0.81	0.33	0.98	24,24,24,24	1
25	MG	A	1606	1/1	0.95	0.27	0.87	24,24,24,24	0
25	MG	A	1594	1/1	0.97	0.26	0.55	24,24,24,24	0
24	PAR	A	1545	42/42	0.92	0.25	0.43	24,24,24,24	0
25	MG	A	214	1/1	0.89	0.30	0.37	24,24,24,24	1
25	MG	D	215	1/1	0.89	0.25	0.35	24,24,24,24	1
25	MG	A	1660	1/1	0.94	0.26	0.24	24,24,24,24	0
25	MG	A	1597	1/1	0.92	0.26	0.15	24,24,24,24	0
25	MG	A	1556	1/1	0.94	0.24	-0.32	24,24,24,24	0
25	MG	A	1587	1/1	0.95	0.26	-0.34	24,24,24,24	0
25	MG	A	1552	1/1	0.94	0.27	-0.48	24,24,24,24	0
26	ZN	N	307	1/1	0.99	0.19	-0.55	24,24,24,24	1
25	MG	A	1589	1/1	0.97	0.23	-0.67	24,24,24,24	0
25	MG	A	1565	1/1	0.91	0.24	-0.80	24,24,24,24	0
25	MG	A	1646	1/1	0.77	0.22	-0.98	24,24,24,24	0
25	MG	A	1640	1/1	0.86	0.23	-1.16	24,24,24,24	0
25	MG	M	475	1/1	0.98	0.17	-1.23	24,24,24,24	1
25	MG	A	1573	1/1	0.86	0.18	-1.25	24,24,24,24	1
25	MG	A	1582	1/1	0.90	0.23	-1.27	24,24,24,24	0
25	MG	A	1581	1/1	0.90	0.23	-1.30	24,24,24,24	0
25	MG	A	1559	1/1	0.97	0.23	-1.32	24,24,24,24	0
25	MG	E	468	1/1	0.91	0.23	-1.34	24,24,24,24	1
25	MG	A	441	1/1	0.54	0.21	-1.34	24,24,24,24	1
25	MG	A	211	1/1	0.93	0.25	-1.79	24,24,24,24	0
25	MG	A	467	1/1	0.90	0.20	-1.99	24,24,24,24	1
25	MG	A	1599	1/1	0.94	0.18	-2.57	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1609	1/1	0.67	0.17	-2.65	24,24,24,24	1
25	MG	A	1623	1/1	0.85	0.22	-2.69	24,24,24,24	1
25	MG	A	1562	1/1	0.90	0.18	-2.78	24,24,24,24	1
25	MG	A	1546	1/1	0.98	0.19	-2.78	24,24,24,24	0
25	MG	A	1605	1/1	0.77	0.17	-2.80	24,24,24,24	1
25	MG	A	1648	1/1	0.83	0.19	-2.81	24,24,24,24	1
25	MG	A	1637	1/1	0.88	0.18	-2.92	24,24,24,24	0
25	MG	A	1593	1/1	0.98	0.20	-3.13	24,24,24,24	0
25	MG	A	1574	1/1	0.93	0.16	-3.23	24,24,24,24	0
25	MG	A	1595	1/1	0.95	0.09	-4.08	24,24,24,24	0
25	MG	A	1598	1/1	0.97	0.09	-4.60	24,24,24,24	1
25	MG	A	1610	1/1	0.61	0.16	-6.18	24,24,24,24	0
25	MG	A	1639	1/1	0.90	0.14	-6.97	24,24,24,24	0
25	MG	A	1576	1/1	0.93	0.16	-7.09	24,24,24,24	1
25	MG	A	1608	1/1	0.97	0.14	-8.30	24,24,24,24	1
25	MG	A	210	1/1	0.88	0.18	-9.29	24,24,24,24	1
25	MG	A	1657	1/1	0.97	0.12	-10.24	24,24,24,24	1
25	MG	A	1586	1/1	0.93	0.10	-11.22	24,24,24,24	0
25	MG	A	1669	1/1	0.93	0.12	-	24,24,24,24	1
25	MG	A	469	1/1	0.94	0.20	-	24,24,24,24	1
25	MG	A	1663	1/1	0.75	0.39	-	24,24,24,24	1
25	MG	A	1668	1/1	0.74	0.18	-	24,24,24,24	1
25	MG	A	1571	1/1	0.93	0.25	-	24,24,24,24	1
25	MG	A	1619	1/1	0.78	0.48	-	24,24,24,24	1
25	MG	A	1617	1/1	0.63	0.45	-	24,24,24,24	1
25	MG	A	1580	1/1	0.98	0.20	-	24,24,24,24	1
25	MG	A	1555	1/1	0.76	0.23	-	24,24,24,24	0
25	MG	A	1652	1/1	0.96	0.29	-	24,24,24,24	0
25	MG	A	1591	1/1	0.94	0.21	-	24,24,24,24	1
25	MG	A	1575	1/1	0.81	0.16	-	24,24,24,24	1
25	MG	A	1621	1/1	0.85	0.54	-	24,24,24,24	1
25	MG	A	1590	1/1	0.87	0.50	-	24,24,24,24	1
25	MG	A	1577	1/1	0.94	0.23	-	24,24,24,24	0
25	MG	A	1550	1/1	0.96	0.38	-	24,24,24,24	0
25	MG	A	1584	1/1	0.91	0.25	-	24,24,24,24	1
25	MG	A	1653	1/1	0.93	0.31	-	24,24,24,24	1
25	MG	A	1583	1/1	0.96	0.35	-	24,24,24,24	1
25	MG	A	1670	1/1	0.99	0.27	-	24,24,24,24	1
25	MG	A	1557	1/1	0.95	0.28	-	24,24,24,24	0
25	MG	A	1551	1/1	0.88	0.16	-	24,24,24,24	1
25	MG	A	1673	1/1	0.78	0.37	-	24,24,24,24	1
25	MG	A	1634	1/1	0.98	0.25	-	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1674	1/1	0.87	0.18	-	24,24,24,24	1
25	MG	A	1558	1/1	0.97	0.25	-	24,24,24,24	0
25	MG	A	1633	1/1	0.89	0.21	-	24,24,24,24	1
25	MG	A	1677	1/1	0.91	0.22	-	24,24,24,24	1
25	MG	Y	500	1/1	0.83	0.35	-	24,24,24,24	1
25	MG	J	449	1/1	0.81	0.23	-	24,24,24,24	1
25	MG	A	1662	1/1	0.87	0.56	-	24,24,24,24	1
25	MG	A	1603	1/1	0.82	0.30	-	24,24,24,24	1
25	MG	A	1667	1/1	0.93	0.24	-	24,24,24,24	1
25	MG	A	1592	1/1	0.94	0.38	-	24,24,24,24	1
25	MG	A	1620	1/1	0.79	0.24	-	24,24,24,24	1
25	MG	A	1679	1/1	0.93	0.62	-	24,24,24,24	1
25	MG	A	1566	1/1	0.96	0.34	-	24,24,24,24	0
25	MG	A	1613	1/1	0.96	0.38	-	24,24,24,24	1
25	MG	A	1579	1/1	0.73	0.34	-	24,24,24,24	1
25	MG	A	1604	1/1	0.88	0.18	-	24,24,24,24	1
25	MG	A	1547	1/1	0.88	0.30	-	24,24,24,24	0
25	MG	A	1607	1/1	0.80	0.36	-	24,24,24,24	1
25	MG	A	1635	1/1	0.78	0.28	-	24,24,24,24	1
25	MG	A	470	1/1	0.91	0.27	-	24,24,24,24	1
25	MG	A	1553	1/1	0.96	0.19	-	24,24,24,24	0
25	MG	A	493	1/1	0.79	0.27	-	24,24,24,24	1
25	MG	A	1681	1/1	0.83	0.72	-	24,24,24,24	1
25	MG	A	466	1/1	0.81	0.54	-	24,24,24,24	1
25	MG	A	1678	1/1	0.70	0.48	-	24,24,24,24	1
25	MG	A	1649	1/1	0.82	0.23	-	24,24,24,24	1
25	MG	A	1570	1/1	0.97	0.37	-	24,24,24,24	1
25	MG	A	1630	1/1	0.84	0.28	-	24,24,24,24	1
25	MG	A	1628	1/1	0.83	0.19	-	24,24,24,24	0
25	MG	A	1614	1/1	0.85	0.15	-	24,24,24,24	1
25	MG	A	1641	1/1	0.59	0.57	-	24,24,24,24	1
25	MG	A	1625	1/1	0.77	0.20	-	24,24,24,24	1
25	MG	A	1564	1/1	0.97	0.52	-	24,24,24,24	1
25	MG	A	1661	1/1	0.87	0.49	-	24,24,24,24	1
25	MG	A	1616	1/1	0.70	0.30	-	24,24,24,24	1
25	MG	A	1658	1/1	0.89	0.22	-	24,24,24,24	1
25	MG	A	87	1/1	0.94	0.26	-	24,24,24,24	1
25	MG	A	1642	1/1	0.93	0.13	-	24,24,24,24	1
25	MG	A	1596	1/1	0.93	0.34	-	24,24,24,24	0
25	MG	A	1611	1/1	0.94	0.39	-	24,24,24,24	1
25	MG	A	1588	1/1	0.97	0.24	-	24,24,24,24	0
25	MG	A	1675	1/1	0.59	0.42	-	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1656	1/1	0.94	0.21	-	24,24,24,24	0
25	MG	A	1643	1/1	0.80	0.17	-	24,24,24,24	1
25	MG	A	1568	1/1	0.94	0.23	-	24,24,24,24	0
25	MG	A	1676	1/1	0.91	0.20	-	24,24,24,24	1
25	MG	A	465	1/1	0.79	0.21	-	24,24,24,24	1
25	MG	A	1612	1/1	0.93	0.45	-	24,24,24,24	1
25	MG	A	1651	1/1	0.94	0.45	-	24,24,24,24	1
25	MG	A	71	1/1	0.81	0.51	-	24,24,24,24	1
25	MG	A	1680	1/1	0.77	0.64	-	24,24,24,24	1
25	MG	A	1563	1/1	0.86	0.27	-	24,24,24,24	0
25	MG	A	1567	1/1	0.78	0.49	-	24,24,24,24	1
25	MG	A	1578	1/1	0.98	0.21	-	24,24,24,24	0
25	MG	A	213	1/1	0.90	0.49	-	24,24,24,24	1
25	MG	A	1671	1/1	0.88	0.29	-	24,24,24,24	1
25	MG	A	1585	1/1	0.80	0.48	-	24,24,24,24	1
25	MG	A	1672	1/1	0.96	0.57	-	24,24,24,24	1
25	MG	A	1645	1/1	0.62	0.73	-	24,24,24,24	1
25	MG	A	1638	1/1	0.91	0.52	-	24,24,24,24	1
25	MG	A	1647	1/1	0.28	0.28	-	24,24,24,24	1
25	MG	A	1655	1/1	0.56	0.39	-	24,24,24,24	1
25	MG	A	1618	1/1	0.42	0.73	-	24,24,24,24	1
25	MG	A	1629	1/1	0.90	0.64	-	24,24,24,24	1
25	MG	A	1664	1/1	0.84	0.84	-	24,24,24,24	1
25	MG	A	471	1/1	0.90	0.41	-	24,24,24,24	1
25	MG	A	1627	1/1	0.96	0.30	-	24,24,24,24	1
25	MG	A	1569	1/1	0.93	0.65	-	24,24,24,24	1
25	MG	A	1560	1/1	0.90	0.48	-	24,24,24,24	0
25	MG	A	86	1/1	0.98	0.24	-	24,24,24,24	0
25	MG	A	1602	1/1	0.92	0.21	-	24,24,24,24	1
25	MG	A	1654	1/1	0.91	0.39	-	24,24,24,24	1
25	MG	A	1549	1/1	0.80	0.68	-	24,24,24,24	1
25	MG	A	473	1/1	0.93	0.14	-	24,24,24,24	1
25	MG	A	1548	1/1	0.91	0.18	-	24,24,24,24	0
25	MG	A	1554	1/1	0.98	0.23	-	24,24,24,24	0
25	MG	A	1631	1/1	0.87	0.22	-	24,24,24,24	1
26	ZN	D	306	1/1	0.98	0.32	-	24,24,24,24	1
25	MG	A	1622	1/1	0.99	0.56	-	24,24,24,24	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.