



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2017 – 01:59 AM EDT

PDB ID : 2VQE  
Title : Modified uridines with C5-methylene substituents at the first position of the tRNA anticodon stabilize U-G wobble pairing during decoding  
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino, Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.  
Deposited on : unknown  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

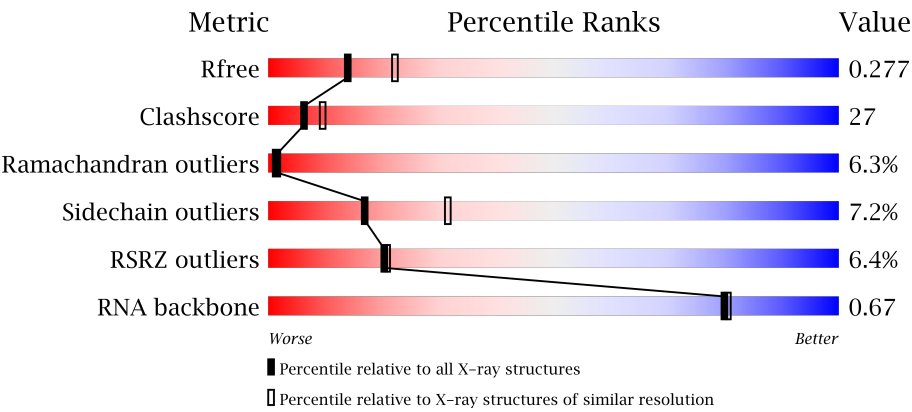
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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





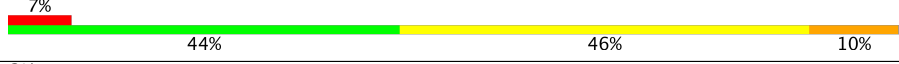
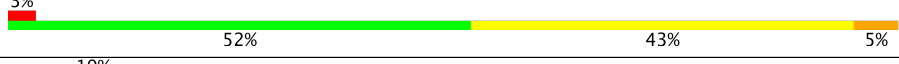
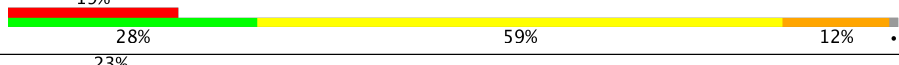
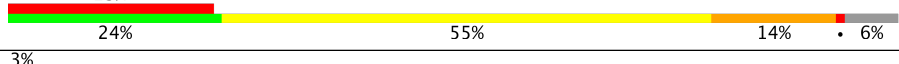
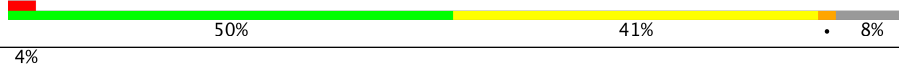
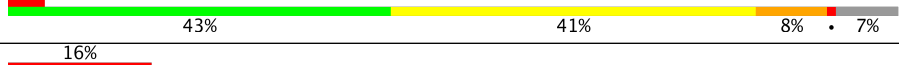
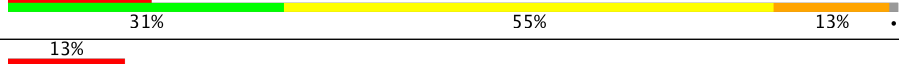
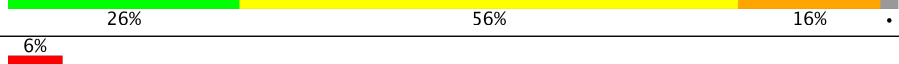


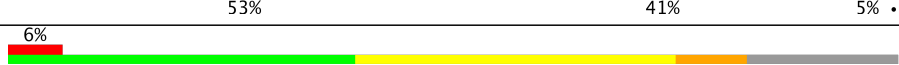
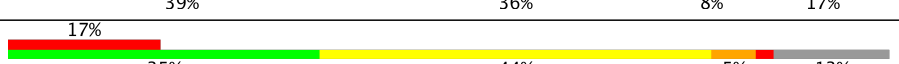

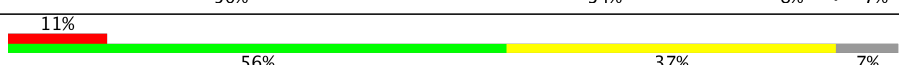
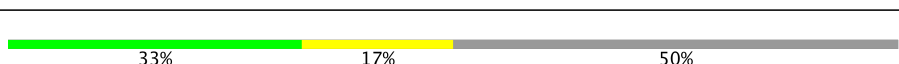
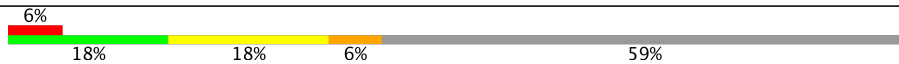

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)
RNA backbone	2435	1019 (2.90-2.10)

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>2%</div><div><div>39%</div><div>48%</div><div>10%</div><div>..</div></div></div>
2	B	256	<div><div>9%</div><div><div>29%</div><div>50%</div><div>12%</div><div>8%</div></div></div>
3	C	239	<div><div>9%</div><div><div>27%</div><div>46%</div><div>13%</div><div>13%</div></div></div>
4	D	209	<div><div>10%</div><div><div>53%</div><div>43%</div><div>..</div></div></div>

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

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
24	MG	A	1626	-	-	-	X
24	MG	A	1636	-	-	-	X
24	MG	A	1637	-	-	-	X
24	MG	A	1641	-	-	-	X
24	MG	A	1647	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1654	-	-	-	X
24	MG	A	1657	-	-	-	X
24	MG	A	1664	-	-	-	X
24	MG	A	1667	-	-	-	X
24	MG	A	1671	-	-	-	X
24	MG	A	1676	-	-	-	X
24	MG	A	1681	-	-	-	X
24	MG	A	1682	-	-	-	X
24	MG	A	1694	-	-	-	X
24	MG	A	1700	-	-	-	X
24	MG	A	1703	-	-	-	X
24	MG	A	1719	-	-	-	X
24	MG	A	1721	-	-	-	X
24	MG	A	1722	-	-	-	X
24	MG	A	1731	-	-	-	X
24	MG	A	1733	-	-	-	X
24	MG	A	1736	-	-	-	X
24	MG	A	1739	-	-	-	X
24	MG	A	1740	-	-	-	X
24	MG	A	1745	-	-	-	X
24	MG	A	1746	-	-	-	X
24	MG	A	1757	-	-	-	X
24	MG	A	1765	-	-	-	X
24	MG	A	1778	-	-	-	X
24	MG	A	1779	-	-	-	X
24	MG	A	1787	-	-	-	X
24	MG	A	1788	-	-	-	X
24	MG	A	1795	-	-	-	X
24	MG	D	302	-	-	-	X
24	MG	I	201	-	-	-	X
25	K	A	1845	-	-	-	X
25	K	N	103	-	-	-	X
25	K	P	101	-	-	-	X
26	PAR	A	1854	-	-	-	X
27	ZN	D	301	-	-	-	X

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52245 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

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

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(\*UP\*UP\*AP\*AP\*AP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	3	Total	C	N	O	P	0	0	0
			59	28	9	20	2			

- Molecule 23 is a RNA chain called 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*A  
P \*AP\*CP\*AP\*UP\*GP\*CP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	S	0	0	0
			153	70	28	48	6	1			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	Q	1	Total	Mg	0	0
			1	1		
24	D	1	Total	Mg	0	0
			1	1		
24	E	1	Total	Mg	0	0
			1	1		
24	B	1	Total	Mg	0	0
			1	1		
24	I	1	Total	Mg	0	0
			1	1		
24	A	199	Total	Mg	0	0
			199	199		
24	N	1	Total	Mg	0	0
			1	1		
24	M	1	Total	Mg	0	0
			1	1		

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	K	0	0
			1	1		
25	E	3	Total	K	0	0
			3	3		

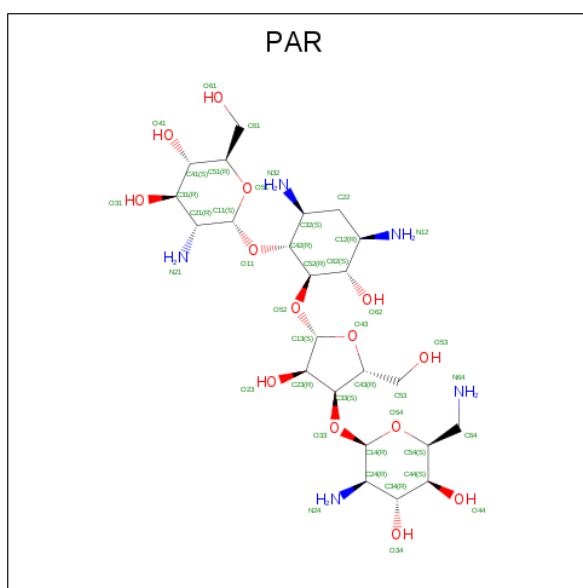
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	I	1	Total K 1 1	0	0
25	A	54	Total K 54 54	0	0
25	T	1	Total K 1 1	0	0
25	N	1	Total K 1 1	0	0
25	R	1	Total K 1 1	0	0

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



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

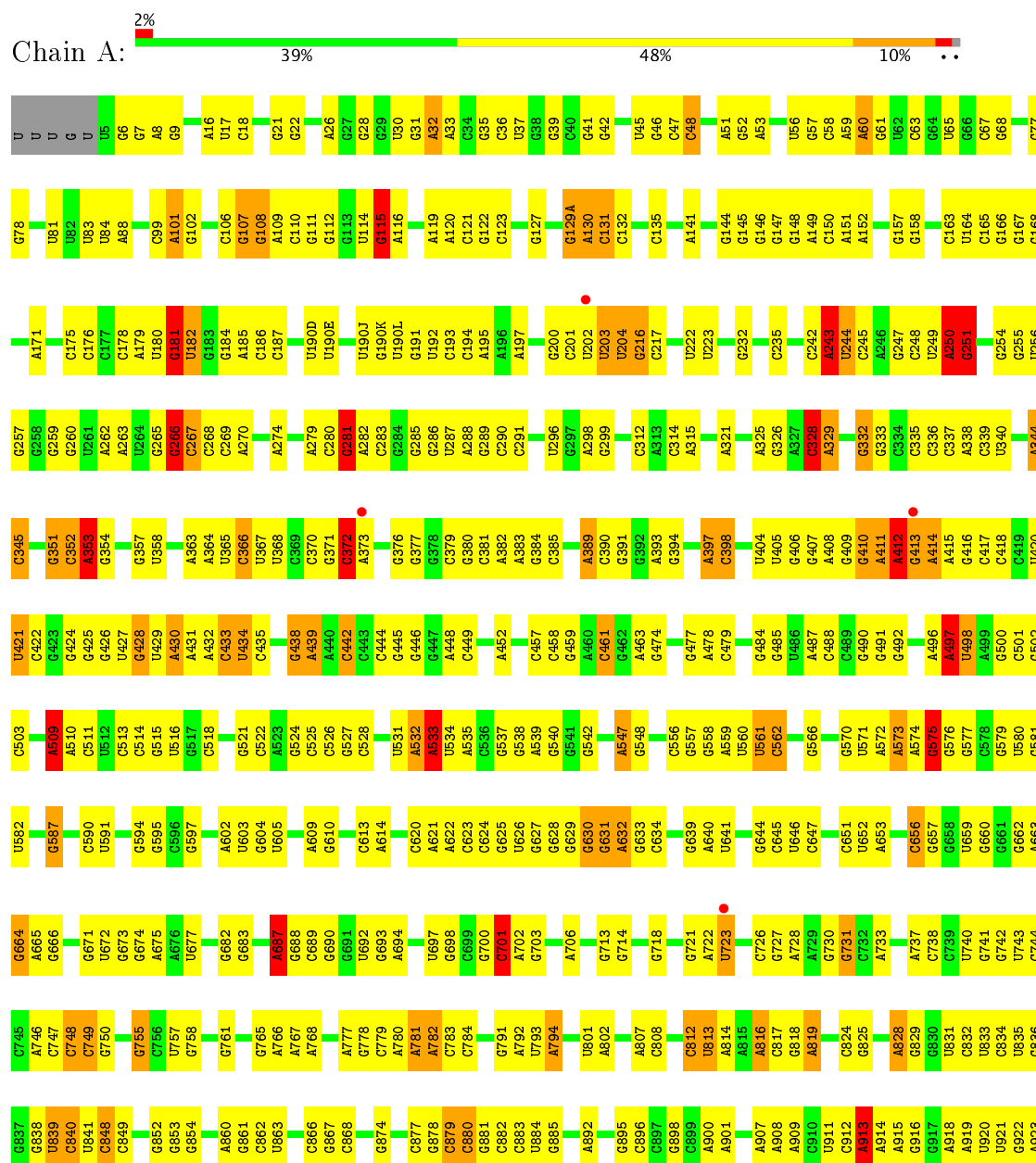
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

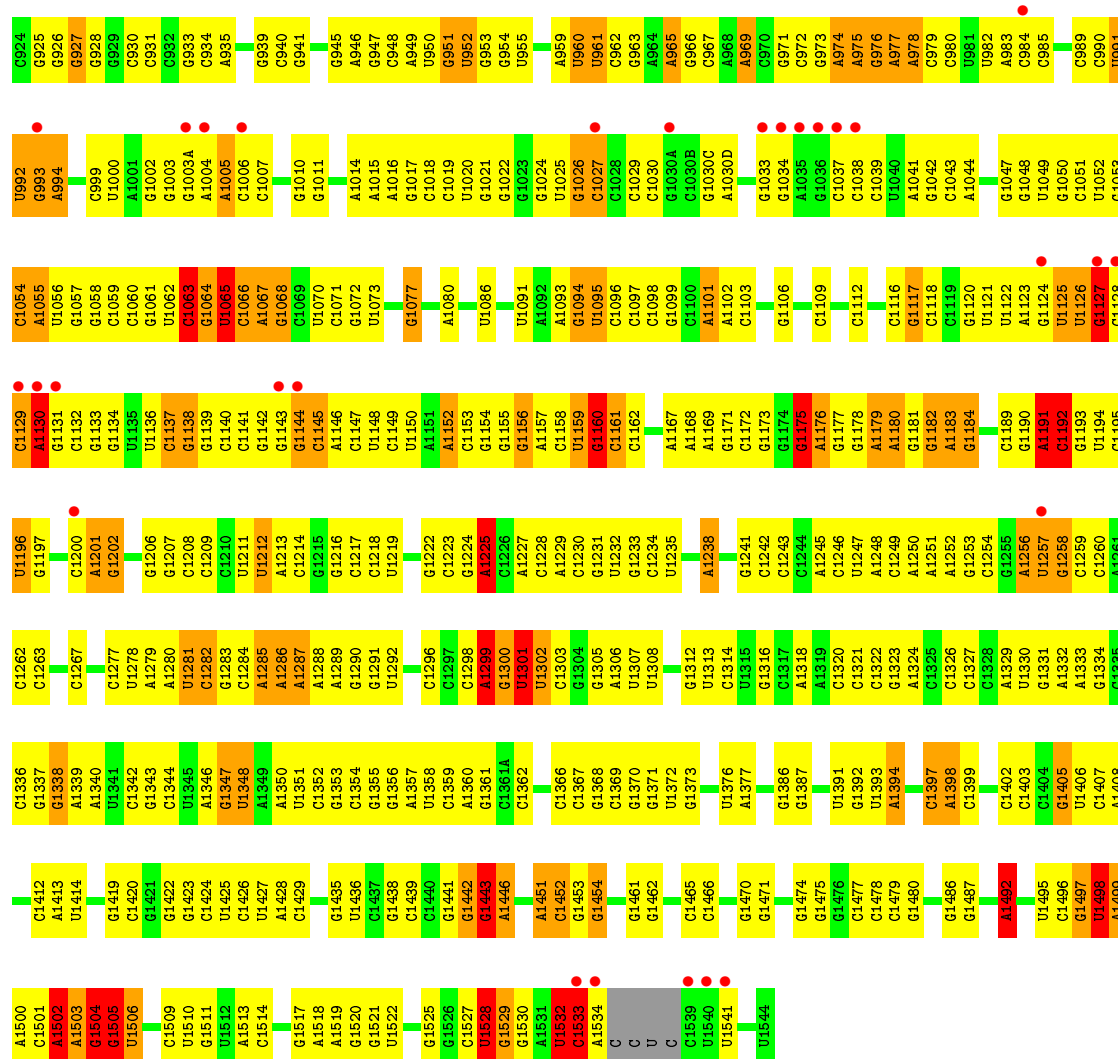
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	D	1	Total Zn 1 1	0	0
27	N	1	Total Zn 1 1	0	0

### 3 Residue-property plots

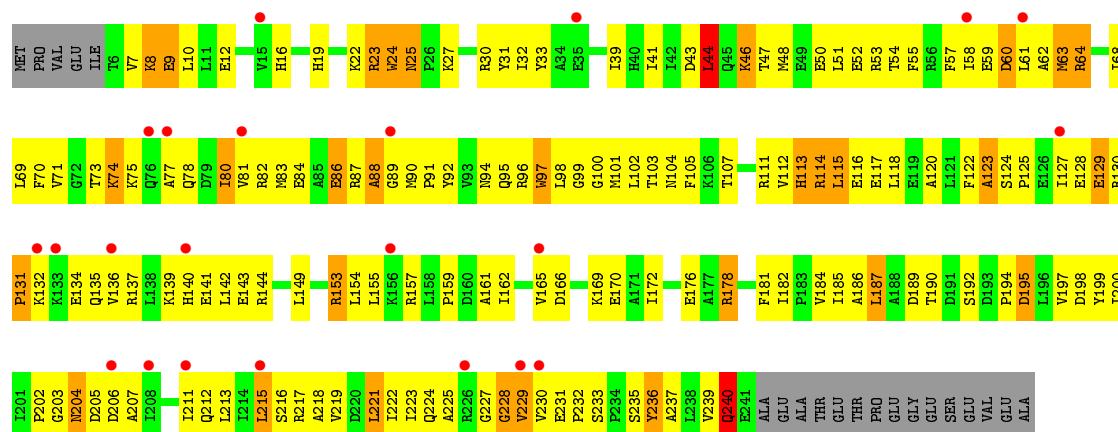
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S rRNA

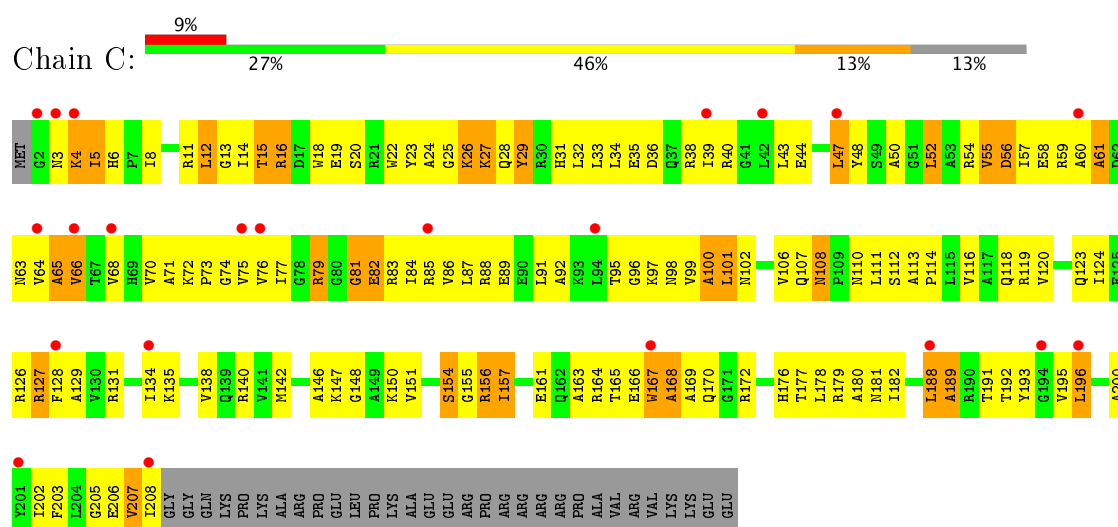




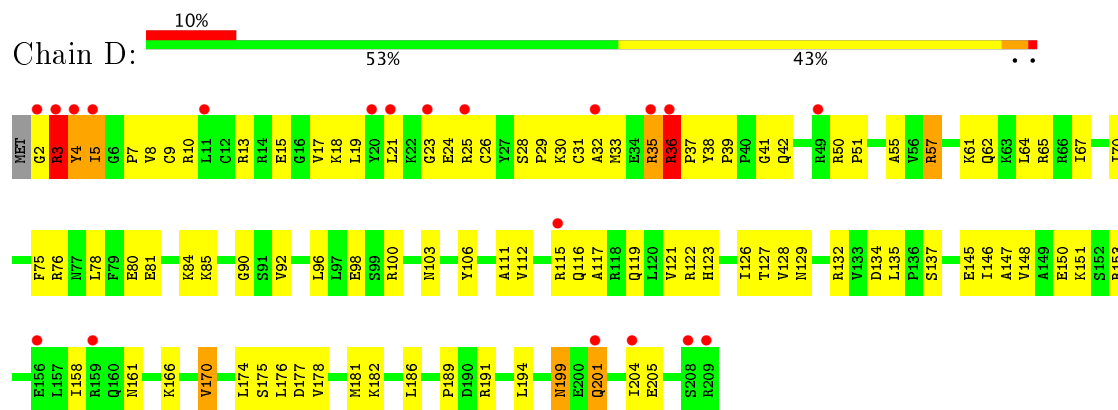
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



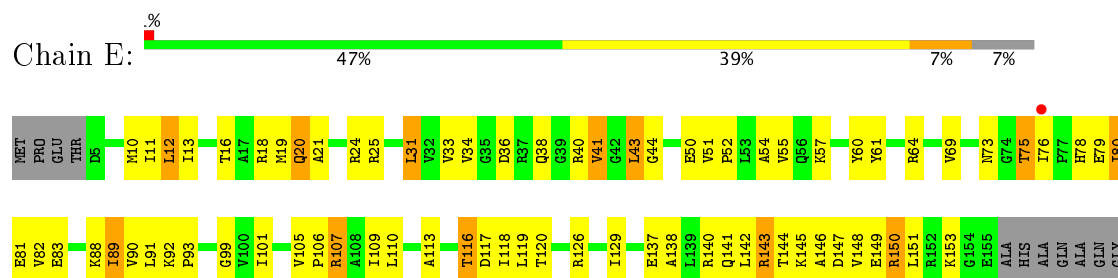
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



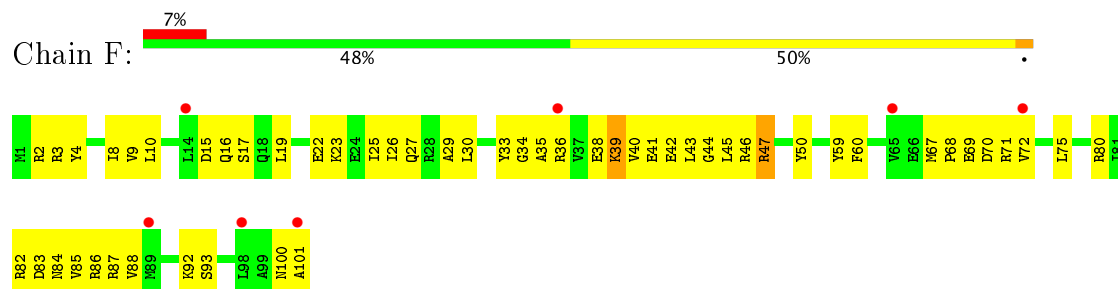
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



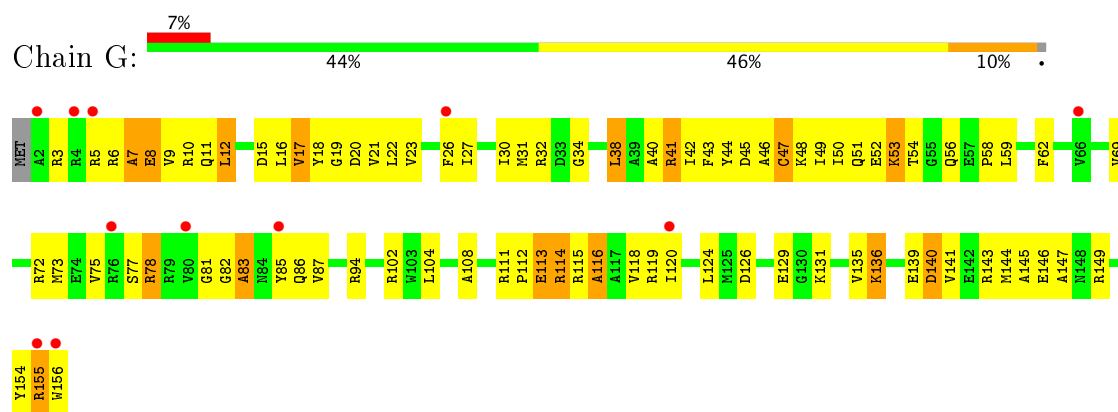
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



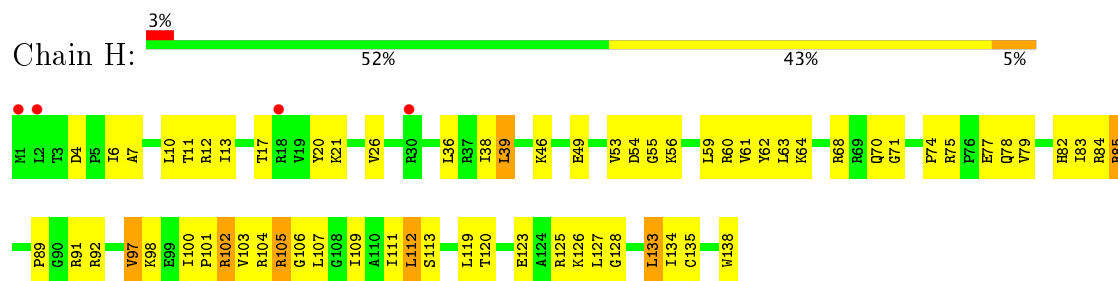
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



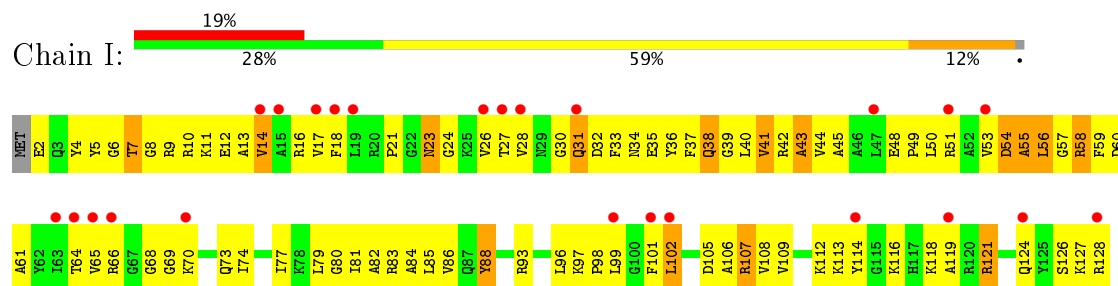
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



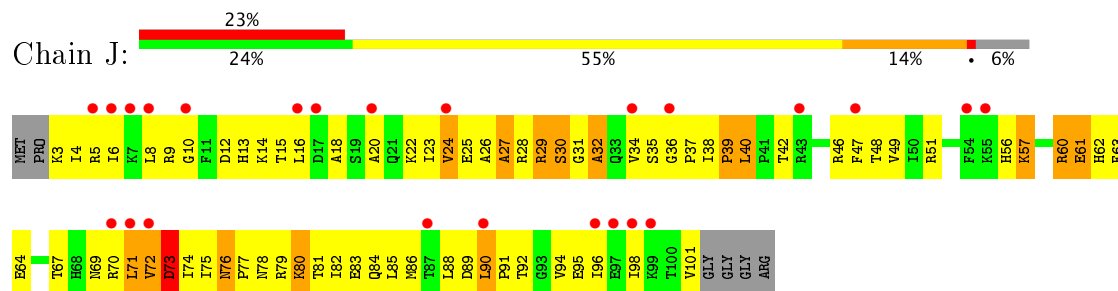
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



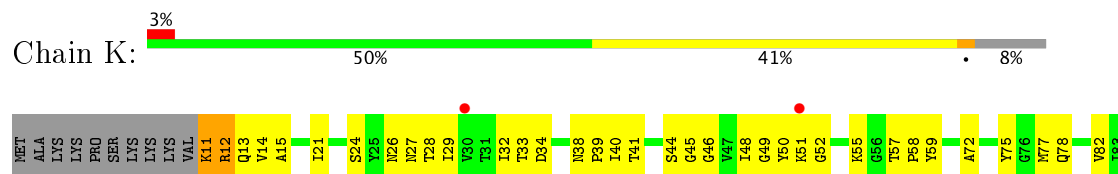
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

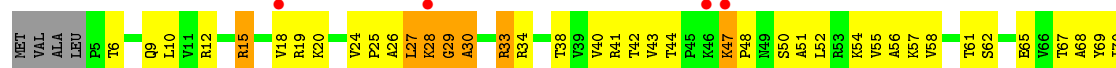


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

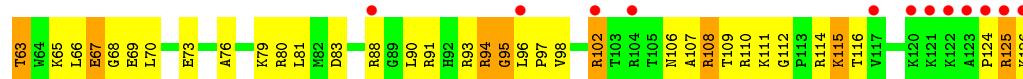
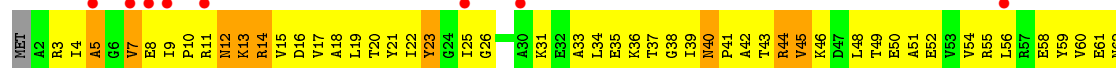




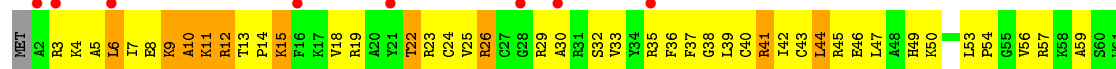
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



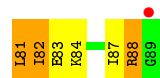
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



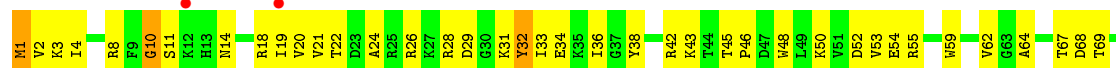
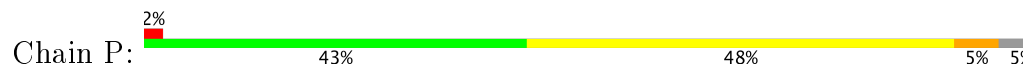
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



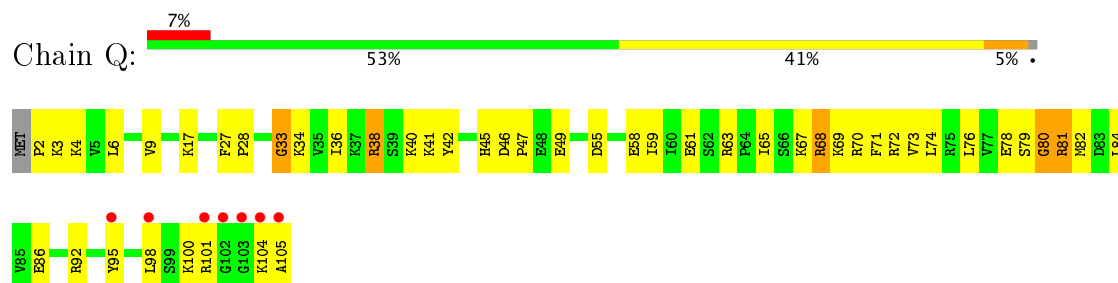
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



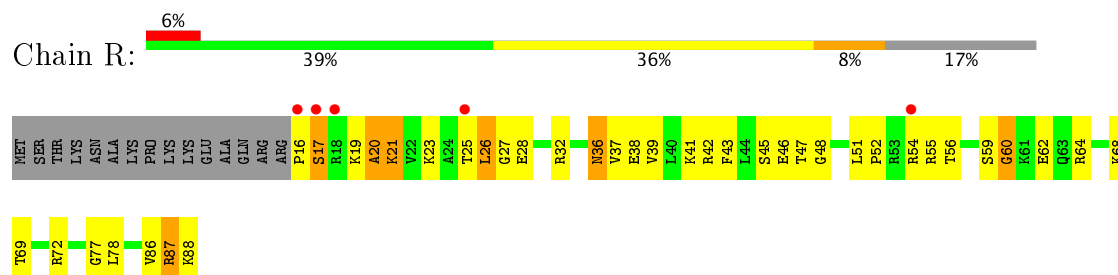
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



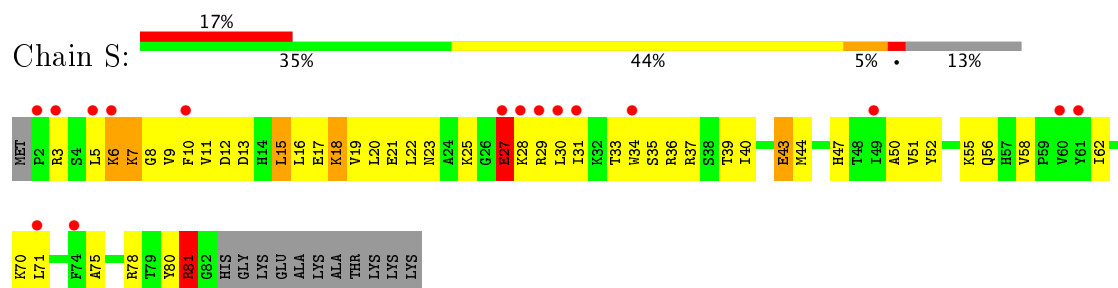
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



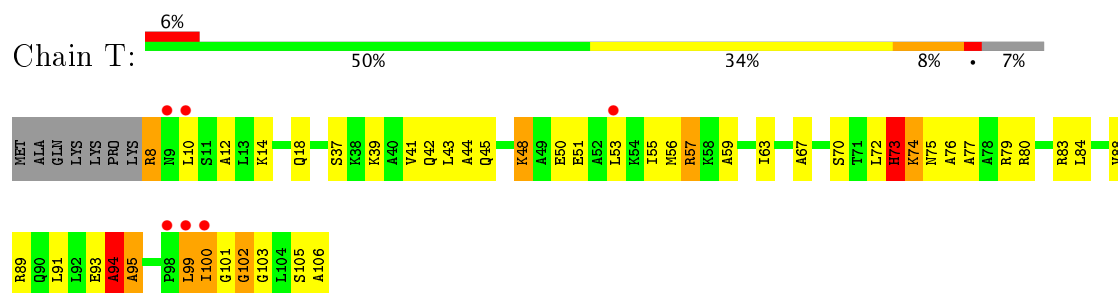
- Molecule 18: 30S RIBOSOMAL PROTEIN S18



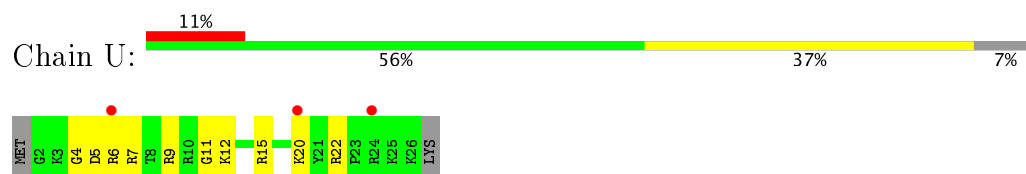
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



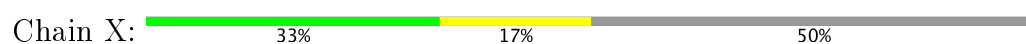
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

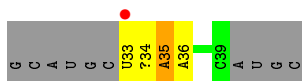
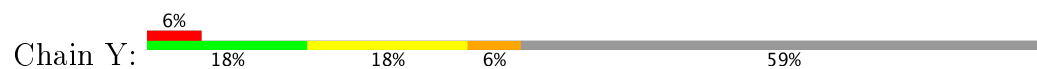


- Molecule 22: 5'-R(\*UP\*UP\*AP\*AP\*AP\*AP)-3'





- Molecule 23: 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*AP \*AP\*CP\*AP\*UP\*GP\*CP)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.00Å 402.00Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.50 284.26 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.50-2.50) 99.0 (284.26-2.35)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.257 , 0.283 0.253 , 0.277	Depositor DCC
$R_{free}$ test set	24518 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	52245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, PAR, ZN, TM2

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	1.17	15/36390 (0.0%)	0.88	71/56793 (0.1%)
2	B	29.07	1/1909 (0.1%)	1.16	2/2579 (0.1%)
3	C	0.35	0/1637	0.59	0/2207
4	D	0.34	0/1733	0.57	0/2318
5	E	0.45	0/1163	0.71	0/1566
6	F	0.32	0/856	0.59	0/1154
7	G	0.33	0/1276	0.63	0/1709
8	H	0.43	0/1136	0.75	0/1527
9	I	0.35	0/1029	0.63	0/1378
10	J	0.37	0/806	0.63	0/1084
11	K	0.38	0/900	0.70	0/1213
12	L	0.43	0/987	0.75	0/1322
13	M	0.33	0/1008	0.60	0/1347
14	N	0.35	0/501	0.62	0/664
15	O	0.36	0/745	0.61	1/992 (0.1%)
16	P	0.45	0/717	0.70	0/965
17	Q	0.42	0/870	0.73	1/1159 (0.1%)
18	R	0.37	0/603	0.61	0/799
19	S	0.33	0/662	0.61	0/892
20	T	0.37	0/764	0.72	1/1006 (0.1%)
21	U	0.48	0/213	0.65	0/279
22	X	0.53	0/65	0.60	0/99
23	Y	0.43	0/140	0.65	0/216
All	All	5.45	16/56110 (0.0%)	0.83	76/83268 (0.1%)

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	11	31
2	B	0	1
16	P	0	1
All	All	11	33

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	240	GLN	CD-OE1	1270.14	29.18	1.24
1	A	1127	G	O3'-P	-95.85	0.46	1.61
1	A	1063	C	O3'-P	-75.59	0.70	1.61
1	A	1160	G	O3'-P	-73.55	0.72	1.61
1	A	1532	U	O3'-P	-64.97	0.83	1.61
1	A	1156	G	O3'-P	-59.43	0.89	1.61
1	A	1191	A	O3'-P	-52.33	0.98	1.61
1	A	1175	G	O3'-P	-51.28	0.99	1.61
1	A	1179	A	O3'-P	-44.13	1.08	1.61
1	A	1192	C	O3'-P	-42.03	1.10	1.61
1	A	1144	G	O3'-P	-30.47	1.24	1.61
1	A	1064	G	O3'-P	-25.75	1.30	1.61
1	A	1533	C	O3'-P	9.56	1.72	1.61
1	A	1541	U	O3'-P	-5.55	1.54	1.61
1	A	1505	G	P-O5'	-5.23	1.54	1.59
1	A	813	U	P-O5'	-5.11	1.54	1.59

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	240	GLN	CG-CD-OE1	-49.40	22.81	121.60
1	A	1160	G	P-O3'-C3'	-45.24	65.41	119.70
1	A	1064	G	OP1-P-O3'	-36.76	24.33	105.20
1	A	1192	C	OP2-P-O3'	-35.85	26.34	105.20
1	A	1144	G	P-O3'-C3'	-33.90	79.02	119.70
1	A	1160	G	O3'-P-O5'	31.41	163.69	104.00
1	A	1179	A	OP2-P-O3'	-28.19	43.18	105.20
1	A	1144	G	OP1-P-O3'	26.60	163.72	105.20
1	A	1179	A	P-O3'-C3'	-23.60	91.38	119.70
1	A	1179	A	O3'-P-O5'	22.44	146.64	104.00
1	A	1533	C	P-O3'-C3'	-21.79	93.55	119.70
1	A	1160	G	OP1-P-O3'	-20.98	59.03	105.20
1	A	1127	G	P-O3'-C3'	20.38	144.15	119.70
1	A	1144	G	O3'-P-O5'	-19.92	66.15	104.00
1	A	1191	A	P-O3'-C3'	19.44	143.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1532	U	OP2-P-O3'	-19.31	62.72	105.20
1	A	1063	C	P-O3'-C3'	17.18	140.31	119.70
1	A	1532	U	O3'-P-O5'	15.76	133.94	104.00
1	A	1156	G	P-O3'-C3'	14.91	137.59	119.70
1	A	1144	G	OP2-P-O3'	-13.77	74.90	105.20
1	A	1064	G	OP2-P-O3'	13.43	134.75	105.20
1	A	1533	C	O3'-P-O5'	12.94	128.58	104.00
1	A	1175	G	O3'-P-O5'	12.42	127.61	104.00
1	A	1498	U	C2'-C3'-O3'	10.61	132.84	109.50
1	A	1179	A	OP1-P-O3'	-10.35	82.43	105.20
1	A	115	G	C2'-C3'-O3'	9.98	131.45	109.50
1	A	1192	C	OP1-P-O3'	9.79	126.75	105.20
1	A	1503	A	C2'-C3'-O3'	9.65	130.74	109.50
1	A	1443	G	C2'-C3'-O3'	9.42	130.22	109.50
1	A	1192	C	O3'-P-O5'	9.40	121.86	104.00
1	A	243	A	C2'-C3'-O3'	9.32	130.01	109.50
1	A	1301	U	C2'-C3'-O3'	9.28	129.93	109.50
1	A	1127	G	OP1-P-O3'	9.17	125.38	105.20
1	A	701	C	C2'-C3'-O3'	9.05	129.41	109.50
1	A	1528	U	C2'-C3'-O3'	8.97	129.23	109.50
1	A	575	G	C2'-C3'-O3'	8.93	129.14	109.50
1	A	1175	G	OP2-P-O3'	-8.93	85.56	105.20
1	A	281	G	C2'-C3'-O3'	8.74	128.74	109.50
1	A	1160	G	OP2-P-O3'	-8.54	86.40	105.20
1	A	1532	U	P-O3'-C3'	-8.53	109.46	119.70
2	B	240	GLN	OE1-CD-NE2	-8.37	102.66	121.90
1	A	812	C	C2'-C3'-O3'	8.21	127.55	109.50
1	A	412	A	N9-C1'-C2'	8.16	124.60	114.00
1	A	687	A	C2'-C3'-O3'	7.93	126.96	109.50
1	A	60	A	C2'-C3'-O3'	7.64	126.31	109.50
1	A	328	C	C2'-C3'-O3'	7.55	126.11	109.50
1	A	1191	A	O3'-P-O5'	-7.50	89.74	104.00
1	A	410	G	C2'-C3'-O3'	7.46	125.91	109.50
1	A	181	G	C2'-C3'-O3'	7.24	125.43	109.50
1	A	497	A	C2'-C3'-O3'	7.16	125.24	109.50
1	A	266	G	C2'-C3'-O3'	7.13	125.19	109.50
1	A	372	C	C2'-C3'-O3'	7.08	125.07	109.50
1	A	1505	G	C2'-C3'-O3'	7.06	125.03	109.50
1	A	366	C	C2'-C3'-O3'	7.05	125.01	109.50
1	A	533	A	C2'-C3'-O3'	6.85	124.67	113.70
1	A	1299	A	N9-C1'-C2'	6.76	122.79	114.00
1	A	965	A	C2'-C3'-O3'	6.68	124.39	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	913	A	C2'-C3'-O3'	6.59	124.24	113.70
1	A	1502	A	N9-C1'-C2'	6.35	122.25	114.00
1	A	1191	A	OP1-P-O3'	6.25	118.96	105.20
1	A	353	A	C5'-C4'-O4'	-6.21	101.65	109.10
1	A	1065	U	C2'-C3'-O3'	6.05	123.38	113.70
1	A	428	G	C2'-C3'-O3'	5.74	122.89	113.70
1	A	509	A	C2'-C3'-O3'	5.71	122.84	113.70
1	A	281	G	C4'-C3'-O3'	5.67	124.34	113.00
1	A	63	C	C5'-C4'-C3'	-5.59	107.06	116.00
1	A	328	C	O4'-C1'-N1	-5.47	103.83	108.20
17	Q	98	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	748	C	C2'-C3'-O3'	5.26	122.12	113.70
1	A	1504	G	C2'-C3'-O3'	5.24	122.09	113.70
1	A	1533	C	OP1-P-O3'	-5.22	93.72	105.20
1	A	575	G	O4'-C1'-N9	-5.22	104.03	108.20
15	O	45	VAL	N-CA-C	-5.09	97.25	111.00
1	A	1225	A	N9-C1'-C2'	5.07	120.58	114.00
1	A	389	A	C5'-C4'-C3'	5.06	124.09	116.00
20	T	94	ALA	N-CA-C	-5.02	97.44	111.00

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	243	A	C3'
1	A	281	G	C3'
1	A	410	G	C3'
1	A	412	A	C1'
1	A	701	C	C3'
1	A	812	C	C3'
1	A	1443	G	C3'
1	A	1498	U	C3'
1	A	1503	A	C3'
1	A	1528	U	C3'

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	1077	G	Sidechain
1	A	108	G	Sidechain
1	A	1130	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1299	A	Sidechain
1	A	1405	G	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	1492	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	274	A	Sidechain
1	A	37	U	Sidechain
1	A	380	G	Sidechain
1	A	561	U	Sidechain
1	A	566	G	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	597	G	Sidechain
1	A	656	C	Sidechain
1	A	664	G	Sidechain
1	A	682	G	Sidechain
1	A	727	G	Sidechain
1	A	733	A	Sidechain
1	A	852	G	Sidechain
1	A	879	C	Sidechain
1	A	880	C	Sidechain
1	A	898	G	Sidechain
1	A	951	G	Sidechain
1	A	952	U	Sidechain
1	A	982	U	Sidechain
2	B	240	GLN	Sidechain
16	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	32511	0	16411	950	0
2	B	1874	0	1887	190	0
3	C	1613	0	1677	200	0
4	D	1703	0	1767	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	85	0
6	F	843	0	857	58	0
7	G	1257	0	1296	102	0
8	H	1116	0	1177	54	0
9	I	1011	0	1041	120	0
10	J	793	0	835	127	1
11	K	885	0	904	51	0
12	L	971	0	1057	79	0
13	M	997	0	1072	122	0
14	N	492	0	531	66	0
15	O	734	0	771	44	0
16	P	701	0	720	45	0
17	Q	857	0	930	56	0
18	R	597	0	668	47	0
19	S	648	0	673	57	0
20	T	762	0	859	61	0
21	U	209	0	221	15	0
22	X	59	0	33	1	0
23	Y	153	0	83	8	0
24	A	199	0	0	0	0
24	B	1	0	0	0	0
24	D	1	0	0	0	0
24	E	1	0	0	0	0
24	I	1	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
24	Q	1	0	0	0	0
25	A	54	0	0	0	0
25	E	3	0	0	0	0
25	I	1	0	0	0	0
25	N	1	0	0	0	0
25	P	1	0	0	0	0
25	R	1	0	0	0	0
25	T	1	0	0	0	0
26	A	42	0	45	1	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	52245	0	36722	2401	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (2401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:C:O3'	1:A:1193:G:P	1.10	1.49
1:A:1175:G:O3'	1:A:1176:A:P	0.99	1.39
1:A:1191:A:O3'	1:A:1192:C:P	0.98	1.37
1:A:1175:G:C3'	1:A:1176:A:P	2.14	1.34
1:A:1156:G:C3'	1:A:1157:A:P	2.17	1.32
1:A:1118:C:O2	1:A:1179:A:C6	1.83	1.32
1:A:1533:C:O2'	1:A:1534:A:H5'	1.25	1.31
1:A:1156:G:O3'	1:A:1157:A:P	0.89	1.29
1:A:1532:U:O2	1:A:1534:A:OP2	1.52	1.27
1:A:1191:A:HO3'	1:A:1192:C:P	0.89	1.26
1:A:1192:C:HO3'	1:A:1193:G:P	1.10	1.19
1:A:1191:A:C3'	1:A:1192:C:P	2.31	1.18
1:A:1192:C:C4'	1:A:1193:G:OP2	1.95	1.13
1:A:1192:C:C3'	1:A:1193:G:OP2	0.79	1.09
1:A:243:A:H4'	1:A:244:U:H5'	1.34	1.08
19:S:33:THR:HG22	19:S:35:SER:H	1.21	1.03
1:A:1533:C:O2'	1:A:1534:A:C5'	2.07	1.03
1:A:1192:C:H3'	1:A:1193:G:OP2	1.22	1.01
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.26	1.00
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.23	1.00
1:A:1356:G:H2'	1:A:1357:A:C8	1.98	0.99
14:N:26:ARG:HH21	14:N:47:LEU:HG	1.26	0.99
1:A:1175:G:O3'	1:A:1176:A:OP2	1.72	0.98
1:A:1192:C:C2'	1:A:1193:G:OP2	2.11	0.98
1:A:266:G:H5''	1:A:268:C:H41	1.28	0.98
19:S:28:LYS:HG2	19:S:29:ARG:H	1.26	0.98
1:A:1118:C:O2	1:A:1179:A:C5	2.17	0.97
1:A:1065:U:H5''	1:A:1190:G:N2	1.78	0.97
3:C:14:ILE:HG22	3:C:15:THR:H	1.29	0.97
14:N:6:LEU:HD12	14:N:23:ARG:HH21	1.26	0.97
13:M:49:THR:HG22	13:M:51:ALA:H	1.28	0.96
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.43	0.96
1:A:1152:A:H5''	10:J:13:HIS:HD2	1.28	0.96
1:A:1190:G:H3'	3:C:3:ASN:ND2	1.80	0.96
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.47	0.96
1:A:1156:G:O3'	1:A:1157:A:OP2	1.83	0.95
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.47	0.95
1:A:975:A:H5'	1:A:975:A:H8	1.32	0.94
2:B:132:LYS:HD2	2:B:135:GLN:HB2	1.46	0.94
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.49	0.94
1:A:1086:U:H3	1:A:1099:G:H22	1.10	0.93
1:A:1533:C:HO2'	1:A:1534:A:H5'	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.49	0.92
1:A:1128:C:C5'	9:I:16:ARG:HH12	1.83	0.92
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.52	0.92
1:A:1026:G:H3'	1:A:1027:C:H5''	1.52	0.91
1:A:664:G:H22	1:A:741:G:H1	1.18	0.91
13:M:108:ARG:HE	13:M:108:ARG:HA	1.35	0.91
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.50	0.91
1:A:1175:G:O2'	1:A:1176:A:H5'	1.72	0.90
3:C:6:HIS:HD2	3:C:8:ILE:H	1.18	0.90
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.53	0.90
1:A:1156:G:HO3'	1:A:1157:A:P	1.10	0.90
18:R:17:SER:HB3	18:R:54:ARG:HH11	1.36	0.89
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.72	0.89
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.54	0.89
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.54	0.89
10:J:32:ALA:HB2	10:J:76:ASN:HD22	1.37	0.89
1:A:1250:A:H4'	9:I:68:GLY:H	1.37	0.89
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.07	0.89
1:A:1533:C:H2'	1:A:1534:A:O5'	1.73	0.89
1:A:1367:C:H5'	10:J:60:ARG:NH1	1.88	0.89
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.03	0.88
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.56	0.88
1:A:328:C:O2	1:A:328:C:H2'	1.74	0.88
7:G:54:THR:HG22	7:G:56:GLN:H	1.37	0.88
2:B:48:MET:HA	2:B:51:LEU:HD12	1.55	0.88
20:T:8:ARG:HH11	20:T:8:ARG:HB3	1.37	0.88
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.56	0.87
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.57	0.87
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.40	0.87
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.57	0.87
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.56	0.87
19:S:5:LEU:O	19:S:6:LYS:HB2	1.75	0.87
5:E:150:ARG:HH11	5:E:150:ARG:HG3	1.40	0.86
1:A:1532:U:O2'	1:A:1533:C:O5'	1.66	0.86
12:L:111:LYS:HE3	12:L:112:ASP:H	1.40	0.86
2:B:118:LEU:HB2	2:B:142:LEU:HD21	1.57	0.86
2:B:83:MET:HA	2:B:86:GLU:HB2	1.56	0.86
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.58	0.85
2:B:103:THR:HG23	2:B:176:GLU:HB2	1.56	0.85
1:A:1137:C:H4'	1:A:1138:G:C2	2.12	0.85
1:A:1532:U:H2'	1:A:1533:C:C5'	2.02	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.90	0.85
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.57	0.85
2:B:44:LEU:H	2:B:44:LEU:HD12	1.42	0.85
7:G:136:LYS:HA	7:G:136:LYS:HE2	1.57	0.85
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.59	0.85
1:A:1250:A:H4'	9:I:68:GLY:N	1.91	0.84
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.42	0.84
12:L:55:VAL:HG12	12:L:56:ALA:H	1.42	0.84
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.42	0.84
9:I:93:ARG:HB3	9:I:93:ARG:NH1	1.92	0.84
1:A:1116:C:H2'	1:A:1117:G:H5''	1.60	0.84
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.58	0.84
1:A:1190:G:OP1	3:C:4:LYS:HA	1.78	0.84
2:B:211:ILE:O	2:B:215:LEU:HB2	1.75	0.84
11:K:57:THR:HG22	11:K:59:TYR:H	1.43	0.84
1:A:1369:C:H2'	1:A:1370:G:C8	2.13	0.83
2:B:46:LYS:HE3	2:B:46:LYS:HA	1.59	0.83
1:A:975:A:H4'	1:A:976:G:H5''	1.58	0.83
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.60	0.83
6:F:80:ARG:NH1	6:F:88:VAL:HB	1.93	0.83
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.58	0.83
1:A:432:A:H3'	1:A:433:C:H5''	1.60	0.83
7:G:155:ARG:HA	7:G:155:ARG:HH11	1.42	0.83
19:S:17:GLU:HA	19:S:20:LEU:HG	1.61	0.82
1:A:1178:G:N2	1:A:1180:A:C8	2.47	0.82
1:A:203:U:H5''	1:A:204:U:OP1	1.78	0.82
1:A:1160:G:O2'	1:A:1161:C:H5'	1.79	0.82
1:A:250:A:H4'	1:A:251:G:O5'	1.78	0.82
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.61	0.82
18:R:32:ARG:HA	18:R:69:THR:HG21	1.60	0.82
5:E:144:THR:O	5:E:148:VAL:HG23	1.79	0.81
12:L:111:LYS:HA	12:L:111:LYS:HE3	1.59	0.81
1:A:946:A:H2'	1:A:947:G:C8	2.15	0.81
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.45	0.81
20:T:74:LYS:HZ3	20:T:74:LYS:HA	1.44	0.81
3:C:14:ILE:HG22	3:C:15:THR:N	1.96	0.81
1:A:1128:C:H5'	9:I:16:ARG:NH1	1.95	0.81
13:M:4:ILE:HG22	13:M:5:ALA:H	1.45	0.81
2:B:114:ARG:HA	2:B:117:GLU:HB3	1.62	0.81
12:L:111:LYS:CE	12:L:112:ASP:H	1.93	0.81
4:D:24:GLU:HG2	4:D:25:ARG:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.62	0.81
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.63	0.80
13:M:11:ARG:HG3	13:M:12:ASN:N	1.97	0.80
1:A:1118:C:O2	1:A:1179:A:N1	2.13	0.80
1:A:243:A:C4'	1:A:244:U:H5'	2.09	0.80
12:L:27:LEU:O	12:L:29:GLY:N	2.13	0.80
1:A:1477:C:H2'	1:A:1478:C:H6	1.46	0.80
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.62	0.80
13:M:4:ILE:HG22	13:M:5:ALA:N	1.97	0.80
1:A:975:A:H5'	1:A:975:A:C8	2.16	0.80
1:A:1292:U:P	7:G:41:ARG:HH22	2.05	0.80
15:O:8:LYS:O	15:O:11:VAL:HG12	1.81	0.80
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.62	0.80
1:A:1175:G:O2'	1:A:1176:A:C5'	2.31	0.79
1:A:1192:C:C3'	1:A:1193:G:P	2.13	0.79
2:B:25:ASN:HD22	2:B:27:LYS:H	1.29	0.79
1:A:1281:U:H5'	1:A:1282:C:H5	1.46	0.79
1:A:972:C:H4'	10:J:57:LYS:HG2	1.65	0.79
9:I:106:ALA:O	9:I:108:VAL:HG23	1.81	0.79
13:M:11:ARG:O	13:M:13:LYS:HG2	1.81	0.79
1:A:1435:G:H2'	1:A:1436:U:C6	2.17	0.79
1:A:579:G:H5'	1:A:728:A:H1'	1.64	0.79
4:D:150:GLU:CD	4:D:150:GLU:H	1.85	0.79
3:C:147:LYS:HE2	3:C:205:GLY:HA2	1.65	0.79
1:A:1175:G:H2'	1:A:1176:A:H8	1.48	0.78
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.65	0.78
9:I:6:GLY:H	9:I:84:ALA:HB2	1.48	0.78
1:A:1116:C:C2'	1:A:1117:G:H5''	2.13	0.78
1:A:1057:G:H5''	3:C:154:SER:HB2	1.65	0.78
1:A:1179:A:N6	1:A:1180:A:C2	2.52	0.78
3:C:34:LEU:HD23	3:C:34:LEU:O	1.83	0.78
12:L:28:LYS:C	12:L:30:ALA:H	1.85	0.78
9:I:6:GLY:N	9:I:84:ALA:HB2	1.99	0.78
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.66	0.78
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.65	0.77
1:A:1175:G:O3'	1:A:1176:A:OP1	2.01	0.77
12:L:28:LYS:O	12:L:30:ALA:N	2.15	0.77
9:I:48:GLU:HG2	9:I:51:ARG:NH2	2.00	0.77
1:A:1175:G:HO3'	1:A:1176:A:P	1.24	0.77
5:E:144:THR:HG22	5:E:146:ALA:H	1.49	0.77
1:A:1191:A:O3'	1:A:1192:C:OP2	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:U:C2	1:A:1534:A:OP2	2.38	0.77
1:A:35:G:H2'	1:A:36:C:C6	2.20	0.77
2:B:103:THR:CG2	2:B:176:GLU:HB2	2.14	0.77
2:B:223:ILE:HD12	2:B:224:GLN:N	1.99	0.77
6:F:46:ARG:HB3	6:F:46:ARG:NH1	2.00	0.77
1:A:1127:G:H21	1:A:1146:A:N6	1.83	0.76
1:A:1502:A:H2	1:A:1505:G:H1	1.32	0.76
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.66	0.76
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.65	0.76
14:N:6:LEU:HD12	14:N:23:ARG:NH2	2.00	0.76
1:A:1160:G:O2'	1:A:1161:C:C5'	2.28	0.76
14:N:12:ARG:HD3	14:N:12:ARG:H	1.51	0.76
1:A:1175:G:C2'	1:A:1176:A:P	2.73	0.76
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.67	0.76
1:A:1352:C:H2'	1:A:1353:G:C8	2.20	0.76
1:A:1080:A:H5''	5:E:16:THR:HG21	1.68	0.76
1:A:1532:U:HO2'	1:A:1533:C:H6	1.31	0.75
1:A:1127:G:N2	1:A:1146:A:H62	1.85	0.75
2:B:124:SER:O	2:B:127:ILE:HG13	1.85	0.75
1:A:1189:C:P	10:J:51:ARG:HH22	2.09	0.75
1:A:1443:G:H4'	1:A:1446:A:H5'	1.68	0.75
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.86	0.75
1:A:1127:G:H21	1:A:1146:A:H62	1.35	0.75
1:A:1356:G:H2'	1:A:1357:A:H8	1.46	0.75
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.68	0.75
1:A:1060:C:H2'	1:A:1061:G:H8	1.52	0.75
11:K:87:THR:HA	11:K:91:ARG:HH21	1.52	0.75
16:P:67:THR:HG22	16:P:69:THR:H	1.51	0.75
1:A:371:G:O2'	1:A:372:C:H5'	1.87	0.75
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.68	0.75
13:M:11:ARG:HG3	13:M:12:ASN:H	1.52	0.75
1:A:438:G:H4'	1:A:439:A:OP1	1.87	0.74
7:G:62:PHE:HD1	7:G:124:LEU:HD11	1.49	0.74
13:M:14:ARG:HB3	13:M:16:ASP:OD1	1.86	0.74
19:S:52:TYR:HA	19:S:56:GLN:O	1.87	0.74
1:A:141:A:H1'	1:A:182:U:O2	1.87	0.74
1:A:984:C:H2'	1:A:985:C:H6	1.51	0.74
13:M:88:ARG:HD2	19:S:3:ARG:NH2	2.03	0.74
19:S:7:LYS:HD2	19:S:7:LYS:O	1.87	0.74
19:S:33:THR:HG22	19:S:35:SER:N	2.02	0.74
16:P:81:ARG:HG2	16:P:83:GLU:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:H	2:B:44:LEU:CD1	1.99	0.74
7:G:136:LYS:NZ	7:G:143:ARG:HH12	1.85	0.74
1:A:629:G:H2'	1:A:630:G:O4'	1.88	0.74
15:O:87:ILE:HG22	15:O:88:ARG:N	2.03	0.74
1:A:1190:G:H3'	3:C:3:ASN:HD22	1.49	0.74
1:A:351:G:H4'	1:A:352:C:OP1	1.88	0.74
12:L:38:THR:O	12:L:79:GLU:HG3	1.87	0.74
3:C:91:LEU:HD21	3:C:99:VAL:H	1.52	0.73
10:J:46:ARG:NH1	10:J:64:GLU:HB3	2.03	0.73
7:G:155:ARG:HA	7:G:155:ARG:NH1	2.02	0.73
6:F:46:ARG:HB3	6:F:46:ARG:HH11	1.52	0.73
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.71	0.73
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.00	0.73
1:A:390:C:H2'	1:A:391:G:H8	1.53	0.73
5:E:107:ARG:HH11	5:E:107:ARG:HB2	1.54	0.73
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.52	0.73
1:A:1193:G:O2'	1:A:1194:U:H5'	1.88	0.73
1:A:1533:C:C2'	1:A:1534:A:O5'	2.36	0.73
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.23	0.73
1:A:1133:G:H2'	1:A:1134:G:H8	1.52	0.73
20:T:8:ARG:NH1	20:T:8:ARG:HB3	2.04	0.73
1:A:382:A:H2'	1:A:383:A:C8	2.23	0.73
23:Y:33:U:H2'	23:Y:34:TM2:H3'	1.69	0.73
2:B:88:ALA:CB	2:B:90:MET:HG2	2.19	0.73
1:A:390:C:H2'	1:A:391:G:C8	2.24	0.73
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.71	0.73
14:N:44:LEU:O	14:N:44:LEU:HD12	1.87	0.73
14:N:12:ARG:H	14:N:12:ARG:CD	2.02	0.72
1:A:1016:A:H2'	1:A:1017:G:O4'	1.89	0.72
2:B:218:ALA:O	2:B:222:ILE:HG13	1.88	0.72
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.71	0.72
3:C:70:VAL:HG12	3:C:72:LYS:H	1.54	0.72
5:E:144:THR:HG22	5:E:146:ALA:N	2.04	0.72
19:S:50:ALA:HA	19:S:58:VAL:O	1.89	0.72
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.72	0.72
10:J:90:LEU:H	10:J:91:PRO:CD	2.03	0.72
1:A:1286:A:H2'	1:A:1287:A:H4'	1.70	0.72
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.70	0.72
10:J:35:SER:HB2	10:J:72:VAL:O	1.89	0.72
15:O:25:THR:HG21	15:O:70:LEU:HG	1.72	0.72
2:B:84:GLU:OE1	2:B:216:SER:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASP:O	2:B:64:ARG:HG3	1.89	0.72
3:C:101:LEU:HD23	3:C:102:ASN:N	2.04	0.72
1:A:496:A:H4'	1:A:497:A:O5'	1.89	0.71
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.53	0.71
1:A:1497:G:O2'	1:A:1498:U:H5'	1.90	0.71
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.90	0.71
1:A:434:U:H2'	1:A:435:C:C6	2.25	0.71
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.72	0.71
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.24	0.71
1:A:1156:G:C3'	1:A:1157:A:OP2	2.38	0.71
1:A:1191:A:P	3:C:3:ASN:HD21	2.12	0.71
9:I:128:ARG:HG2	13:M:126:LYS:HZ3	1.55	0.71
1:A:1054:C:H3'	1:A:1054:C:O2	1.90	0.71
1:A:1086:U:H3	1:A:1099:G:N2	1.87	0.71
1:A:1504:G:H3'	1:A:1504:G:OP2	1.90	0.71
3:C:79:ARG:HG2	3:C:82:GLU:HG2	1.73	0.71
10:J:38:ILE:HB	10:J:71:LEU:CB	2.20	0.71
1:A:1281:U:H5'	1:A:1282:C:C5	2.25	0.71
2:B:166:ASP:OD2	2:B:169:LYS:HB2	1.91	0.71
7:G:140:ASP:HA	7:G:143:ARG:HH22	1.54	0.71
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.56	0.71
9:I:70:LYS:O	9:I:74:ILE:HG13	1.91	0.71
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.72	0.71
18:R:88:LYS:HG2	18:R:88:LYS:OXT	1.90	0.71
2:B:139:LYS:O	2:B:139:LYS:HD3	1.90	0.71
15:O:87:ILE:HG22	15:O:88:ARG:H	1.56	0.71
18:R:36:ASN:HD21	18:R:38:GLU:HG2	1.55	0.70
1:A:524:G:H2'	1:A:525:C:C6	2.26	0.70
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.56	0.70
19:S:22:LEU:HD11	19:S:31:ILE:HD11	1.72	0.70
1:A:1095:U:H2'	1:A:1096:C:C6	2.25	0.70
2:B:204:ASN:ND2	2:B:206:ASP:H	1.89	0.70
2:B:116:GLU:HB3	2:B:153:ARG:HH22	1.56	0.70
4:D:35:ARG:O	4:D:36:ARG:HB2	1.90	0.70
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.39	0.70
3:C:110:ASN:O	3:C:111:LEU:HD23	1.90	0.70
1:A:1178:G:N2	1:A:1180:A:H8	1.89	0.70
1:A:1492:A:OP1	12:L:47:LYS:N	2.19	0.70
1:A:353:A:H5'	1:A:353:A:H8	1.57	0.70
1:A:1366:C:H2'	1:A:1367:C:H6	1.54	0.70
4:D:24:GLU:HG2	4:D:25:ARG:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:120:ILE:O	7:G:124:LEU:HD23	1.91	0.70
2:B:88:ALA:C	2:B:90:MET:H	1.95	0.70
16:P:52:ASP:OD1	16:P:54:GLU:HG2	1.92	0.70
10:J:24:VAL:O	10:J:28:ARG:HG3	1.92	0.70
1:A:187:C:O2	20:T:105:SER:HB3	1.91	0.70
9:I:55:ALA:O	9:I:56:LEU:HB2	1.92	0.70
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.72	0.69
10:J:39:PRO:O	10:J:40:LEU:HB2	1.91	0.69
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.73	0.69
20:T:53:LEU:O	20:T:57:ARG:HD2	1.92	0.69
3:C:14:ILE:CG2	3:C:15:THR:H	2.04	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.69
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.25	0.69
2:B:178:ARG:HB3	2:B:178:ARG:HH11	1.56	0.69
2:B:64:ARG:HH11	2:B:64:ARG:HB3	1.58	0.69
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.05	0.69
12:L:111:LYS:HE3	12:L:112:ASP:N	2.07	0.69
13:M:17:VAL:O	13:M:20:THR:HB	1.92	0.69
19:S:15:LEU:O	19:S:19:VAL:HG12	1.93	0.69
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.75	0.69
1:A:1160:G:O6	1:A:1181:G:O6	2.10	0.69
1:A:254:G:OP1	17:Q:67:LYS:O	2.09	0.69
1:A:1477:C:H2'	1:A:1478:C:C6	2.28	0.69
5:E:10:MET:SD	5:E:13:ILE:HD11	2.33	0.69
1:A:1497:G:C2'	1:A:1498:U:H5'	2.23	0.69
9:I:27:THR:HG23	9:I:30:GLY:O	1.93	0.69
1:A:1529:G:H3'	1:A:1529:G:OP2	1.93	0.69
2:B:25:ASN:ND2	2:B:27:LYS:H	1.91	0.69
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.58	0.69
7:G:149:ARG:HB3	7:G:149:ARG:NH2	2.08	0.69
10:J:6:ILE:HA	10:J:98:ILE:HG12	1.75	0.68
7:G:140:ASP:HA	7:G:143:ARG:NH2	2.09	0.68
14:N:32:SER:HB3	14:N:41:ARG:HB3	1.74	0.68
19:S:28:LYS:HG2	19:S:29:ARG:N	2.05	0.68
6:F:26:ILE:O	6:F:30:LEU:HG	1.94	0.68
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.75	0.68
10:J:23:ILE:O	10:J:23:ILE:HG22	1.92	0.68
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.59	0.68
9:I:102:LEU:HD12	9:I:102:LEU:H	1.59	0.68
1:A:433:C:H5''	1:A:433:C:H6	1.59	0.68
13:M:15:VAL:HG23	13:M:43:THR:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:C:H2'	1:A:1150:U:C6	2.29	0.68
1:A:1366:C:H2'	1:A:1367:C:C6	2.28	0.68
2:B:115:LEU:HG	2:B:153:ARG:HH21	1.56	0.68
12:L:25:PRO:C	12:L:27:LEU:H	1.95	0.68
1:A:1142:G:H2'	1:A:1143:G:O4'	1.93	0.68
1:A:1175:G:C3'	1:A:1176:A:OP2	2.33	0.68
1:A:731:G:OP1	1:A:766:A:H1'	1.94	0.68
2:B:22:LYS:HG3	2:B:23:ARG:N	2.08	0.68
11:K:15:ALA:HA	11:K:77:MET:HA	1.76	0.68
21:U:6:ARG:HG3	21:U:15:ARG:NH1	2.09	0.68
1:A:1026:G:H3'	1:A:1027:C:C5'	2.22	0.67
1:A:35:G:H2'	1:A:36:C:H6	1.59	0.67
13:M:22:ILE:HB	13:M:25:ILE:HB	1.75	0.67
15:O:79:ARG:CZ	15:O:83:GLU:HB2	2.24	0.67
6:F:60:PHE:CE2	18:R:78:LEU:HD21	2.28	0.67
10:J:57:LYS:O	10:J:57:LYS:HD2	1.94	0.67
13:M:11:ARG:CG	13:M:12:ASN:H	2.07	0.67
20:T:74:LYS:HB3	20:T:74:LYS:HZ2	1.59	0.67
1:A:1062:U:H2'	1:A:1063:C:C6	2.29	0.67
1:A:1211:U:H5'	1:A:1212:U:OP1	1.94	0.67
1:A:364:A:N6	12:L:28:LYS:HE3	2.09	0.67
9:I:118:LYS:O	9:I:119:ALA:HB3	1.93	0.67
1:A:1057:G:H5''	3:C:154:SER:CB	2.24	0.67
11:K:57:THR:HG22	11:K:59:TYR:N	2.09	0.67
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.43	0.67
3:C:155:GLY:O	3:C:156:ARG:HB2	1.94	0.67
1:A:1257:U:H4'	1:A:1258:G:OP2	1.95	0.67
1:A:1521:G:H2'	1:A:1522:U:C6	2.30	0.67
1:A:1502:A:H2	1:A:1505:G:N1	1.93	0.67
9:I:21:PRO:HA	9:I:58:ARG:O	1.94	0.67
1:A:1117:G:N2	1:A:1180:A:H1'	2.09	0.67
1:A:1521:G:H2'	1:A:1522:U:H6	1.60	0.67
1:A:1080:A:C5'	5:E:16:THR:HG21	2.25	0.67
2:B:98:LEU:O	2:B:101:MET:HG3	1.95	0.67
2:B:215:LEU:O	2:B:219:VAL:HG23	1.94	0.67
4:D:80:GLU:O	4:D:84:LYS:HG3	1.95	0.67
10:J:49:VAL:O	10:J:60:ARG:O	2.13	0.67
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.74	0.67
1:A:1250:A:H4'	9:I:68:GLY:CA	2.24	0.66
2:B:77:ALA:HB2	2:B:211:ILE:HG21	1.75	0.66
3:C:119:ARG:HG2	3:C:140:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:GLY:HA2	9:I:59:PHE:O	1.95	0.66
11:K:33:THR:HG22	11:K:39:PRO:HA	1.77	0.66
1:A:1126:U:H2'	1:A:1127:G:C8	2.30	0.66
1:A:664:G:OP1	18:R:64:ARG:HD2	1.94	0.66
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.77	0.66
3:C:195:VAL:C	3:C:196:LEU:HD22	2.15	0.66
1:A:127:G:HO2'	17:Q:2:PRO:N	1.94	0.66
1:A:853:G:O2'	1:A:854:G:H5'	1.95	0.66
1:A:1412:C:H2'	1:A:1413:A:C8	2.31	0.66
1:A:1392:G:O2'	1:A:1502:A:H5''	1.96	0.66
12:L:55:VAL:HG12	12:L:56:ALA:N	2.11	0.66
10:J:10:GLY:N	10:J:16:LEU:HD11	2.11	0.66
13:M:37:THR:O	13:M:37:THR:HG22	1.95	0.66
2:B:239:VAL:O	2:B:240:GLN:HG3	1.96	0.66
3:C:180:ALA:O	3:C:181:ASN:HB3	1.96	0.66
1:A:1062:U:H2'	1:A:1063:C:C5	2.30	0.66
1:A:1068:G:H8	1:A:1068:G:OP2	1.80	0.65
1:A:1527:C:O2'	1:A:1528:U:H5'	1.96	0.65
3:C:23:TYR:CD2	3:C:24:ALA:N	2.63	0.65
10:J:15:THR:HG22	10:J:94:VAL:HG23	1.78	0.65
9:I:128:ARG:HA	13:M:126:LYS:NZ	2.10	0.65
18:R:38:GLU:CD	18:R:38:GLU:H	1.99	0.65
21:U:5:ASP:O	21:U:11:GLY:HA3	1.96	0.65
1:A:575:G:OP1	1:A:575:G:H4'	1.97	0.65
13:M:62:ASN:O	13:M:63:THR:HB	1.97	0.65
1:A:780:A:O2'	1:A:781:A:H5''	1.96	0.65
3:C:3:ASN:O	3:C:4:LYS:HB2	1.96	0.65
3:C:84:ILE:HD11	3:C:88:ARG:HH21	1.61	0.65
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.29	0.65
1:A:1347:G:N2	1:A:1373:G:H2'	2.12	0.65
1:A:1443:G:H4'	1:A:1446:A:C5'	2.25	0.65
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.12	0.65
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.77	0.65
10:J:15:THR:HG22	10:J:94:VAL:CG2	2.27	0.65
13:M:4:ILE:CG2	13:M:5:ALA:H	2.10	0.65
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.79	0.65
1:A:1128:C:O2'	1:A:1130:A:C8	2.50	0.65
1:A:1256:A:O2'	1:A:1257:U:H5'	1.97	0.65
1:A:556:C:O2'	1:A:557:G:H5'	1.95	0.65
1:A:163:C:O2'	1:A:164:U:H5'	1.97	0.65
1:A:537:G:H2'	1:A:538:G:H8	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.79	0.65
9:I:53:VAL:CG1	9:I:96:LEU:HD11	2.27	0.65
18:R:36:ASN:ND2	18:R:38:GLU:HG2	2.11	0.65
18:R:46:GLU:CD	18:R:46:GLU:H	2.00	0.65
2:B:139:LYS:C	2:B:139:LYS:HD3	2.17	0.65
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.30	0.65
1:A:1066:C:O2'	1:A:1067:A:H5'	1.97	0.65
1:A:683:G:H21	11:K:38:ASN:HD22	1.43	0.65
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.31	0.65
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.78	0.65
1:A:1156:G:O3'	1:A:1157:A:OP1	2.03	0.64
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.78	0.64
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.78	0.64
6:F:33:TYR:HA	6:F:71:ARG:CZ	2.27	0.64
1:A:1152:A:C5'	10:J:13:HIS:HD2	2.07	0.64
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.97	0.64
1:A:421:U:H5'	1:A:422:C:C5	2.32	0.64
1:A:840:C:H4'	1:A:848:C:O2	1.97	0.64
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.78	0.64
12:L:79:GLU:O	12:L:79:GLU:HG2	1.97	0.64
16:P:22:THR:HA	16:P:33:ILE:HG13	1.79	0.64
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.32	0.64
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.79	0.64
19:S:28:LYS:CG	19:S:29:ARG:H	2.06	0.64
1:A:1300:G:O2'	1:A:1301:U:H6	1.80	0.64
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.61	0.64
3:C:64:VAL:H	3:C:99:VAL:HB	1.61	0.64
1:A:1021:G:O2'	1:A:1022:G:H5'	1.96	0.64
2:B:74:LYS:NZ	2:B:206:ASP:HA	2.12	0.64
8:H:112:LEU:HD23	8:H:112:LEU:N	2.13	0.64
12:L:54:LYS:HD2	12:L:54:LYS:N	2.12	0.64
13:M:9:ILE:N	13:M:9:ILE:HD12	2.13	0.64
14:N:29:ARG:HH11	14:N:29:ARG:HG2	1.61	0.64
1:A:99:C:H2'	1:A:101:A:C8	2.33	0.64
1:A:1026:G:C3'	1:A:1027:C:H5''	2.26	0.64
1:A:1286:A:C8	1:A:1287:A:H4'	2.31	0.64
3:C:127:ARG:HG2	3:C:127:ARG:HH11	1.62	0.64
6:F:47:ARG:N	6:F:47:ARG:HD3	2.13	0.64
1:A:1147:C:H4'	9:I:5:TYR:HE2	1.63	0.64
1:A:1392:G:N2	1:A:1502:A:H8	1.96	0.64
1:A:397:A:H5'	1:A:398:C:OP1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:THR:HG22	9:I:8:GLY:N	2.12	0.64
1:A:946:A:H2'	1:A:947:G:H8	1.63	0.64
2:B:129:GLU:O	2:B:130:ARG:HB2	1.97	0.64
1:A:363:A:H62	12:L:28:LYS:HE2	1.61	0.64
19:S:17:GLU:O	19:S:21:GLU:HG3	1.97	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.46	0.63
3:C:58:GLU:HB3	10:J:92:THR:CG2	2.28	0.63
10:J:32:ALA:H	10:J:78:ASN:HD21	1.44	0.63
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.80	0.63
19:S:17:GLU:HA	19:S:20:LEU:CG	2.29	0.63
19:S:6:LYS:HG2	19:S:7:LYS:HG3	1.79	0.63
20:T:10:LEU:HG	20:T:12:ALA:HB3	1.80	0.63
1:A:1251:A:H1'	1:A:1369:C:HO2'	1.62	0.63
2:B:114:ARG:CA	2:B:117:GLU:HB3	2.29	0.63
2:B:185:ILE:H	2:B:185:ILE:HD12	1.63	0.63
2:B:88:ALA:HB3	2:B:90:MET:HG2	1.80	0.63
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.13	0.63
7:G:38:LEU:HD12	7:G:38:LEU:O	1.98	0.63
16:P:67:THR:HG22	16:P:68:ASP:N	2.13	0.63
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.28	0.63
1:A:948:C:OP1	13:M:109:THR:HG22	1.98	0.63
5:E:149:GLU:O	5:E:153:LYS:HG2	1.99	0.63
10:J:32:ALA:CB	10:J:76:ASN:HD22	2.11	0.63
1:A:109:A:H2'	1:A:326:G:N2	2.13	0.63
2:B:77:ALA:CB	2:B:211:ILE:HG21	2.28	0.63
1:A:1161:C:H2'	1:A:1162:C:C6	2.33	0.63
1:A:1435:G:H2'	1:A:1436:U:H6	1.64	0.63
15:O:36:ILE:HG12	15:O:59:MET:HE3	1.81	0.63
1:A:1407:C:O2'	1:A:1408:A:H5'	1.99	0.63
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.63	0.63
3:C:52:LEU:H	3:C:52:LEU:CD2	2.11	0.63
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.34	0.63
7:G:50:ILE:O	7:G:54:THR:HB	1.99	0.63
10:J:49:VAL:HG22	14:N:41:ARG:HD2	1.81	0.63
15:O:8:LYS:O	15:O:12:ILE:HG13	1.99	0.63
1:A:1053:G:C3'	1:A:1054:C:H5'	2.29	0.63
5:E:101:ILE:HD12	5:E:119:LEU:HD23	1.79	0.63
1:A:1121:U:H2'	1:A:1122:U:H6	1.64	0.63
1:A:1125:U:H5'	1:A:1126:U:H5	1.63	0.63
1:A:991:U:O4	1:A:1212:U:H1'	1.98	0.63
1:A:1250:A:H2'	1:A:1251:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.81	0.63
3:C:15:THR:O	3:C:16:ARG:HB2	1.97	0.63
10:J:32:ALA:H	10:J:78:ASN:ND2	1.97	0.63
12:L:111:LYS:HE3	12:L:111:LYS:CA	2.29	0.63
1:A:1141:C:H2'	1:A:1142:G:H8	1.64	0.62
1:A:1533:C:C2'	1:A:1534:A:C5'	2.76	0.62
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.81	0.62
1:A:537:G:H2'	1:A:538:G:C8	2.34	0.62
3:C:70:VAL:HG12	3:C:71:ALA:N	2.13	0.62
5:E:24:ARG:HH11	5:E:24:ARG:HG2	1.63	0.62
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.17	0.62
10:J:30:SER:CB	10:J:84:GLN:HE21	2.11	0.62
10:J:90:LEU:H	10:J:91:PRO:HD2	1.64	0.62
19:S:51:VAL:O	19:S:58:VAL:HG22	1.98	0.62
1:A:1305:G:N2	1:A:1331:G:O2'	2.33	0.62
4:D:17:VAL:HG12	4:D:18:LYS:N	2.14	0.62
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.15	0.62
10:J:94:VAL:HG12	10:J:95:GLU:N	2.14	0.62
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.82	0.62
19:S:5:LEU:O	19:S:6:LYS:CB	2.47	0.62
1:A:107:G:C2'	1:A:108:G:H5'	2.29	0.62
1:A:1132:C:H2'	1:A:1133:G:C8	2.34	0.62
1:A:839:U:O2	1:A:839:U:H2'	1.97	0.62
1:A:1014:A:C2	1:A:1219:U:H1'	2.34	0.62
1:A:1369:C:H2'	1:A:1370:G:H8	1.61	0.62
1:A:314:C:O2'	1:A:315:A:H5'	1.99	0.62
1:A:287:U:O2'	1:A:288:A:H5'	2.00	0.62
1:A:421:U:H5'	1:A:422:C:H5	1.64	0.62
1:A:657:G:H4'	15:O:28:GLN:HG2	1.82	0.62
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.65	0.62
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.28	0.62
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.33	0.62
13:M:25:ILE:HD11	13:M:60:VAL:HG11	1.82	0.62
2:B:54:THR:O	2:B:57:PHE:HB3	2.00	0.62
9:I:58:ARG:HD2	9:I:59:PHE:CE1	2.34	0.62
16:P:74:LEU:O	16:P:79:VAL:HG23	1.98	0.62
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.81	0.62
12:L:33:ARG:HG2	12:L:62:SER:HB2	1.82	0.62
14:N:9:LYS:HD2	14:N:9:LYS:C	2.19	0.62
1:A:192:U:C1'	20:T:103:GLY:HA2	2.30	0.62
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:VAL:O	3:C:106:VAL:HG23	1.99	0.62
3:C:19:GLU:HA	3:C:54:ARG:HH21	1.65	0.62
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.34	0.62
4:D:176:LEU:HD12	4:D:177:ASP:H	1.64	0.62
13:M:31:LYS:O	13:M:35:GLU:HB2	2.00	0.62
15:O:6:GLU:CD	15:O:6:GLU:H	2.04	0.62
1:A:266:G:C8	1:A:266:G:H5'	2.35	0.61
1:A:562:C:H1'	12:L:15:ARG:HG3	1.81	0.61
1:A:1128:C:C4'	9:I:16:ARG:HH12	2.11	0.61
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.00	0.61
1:A:1160:G:C6	1:A:1181:G:O6	2.53	0.61
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.64	0.61
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.82	0.61
10:J:90:LEU:N	10:J:91:PRO:HD2	2.15	0.61
1:A:371:G:C2'	1:A:372:C:H5'	2.29	0.61
1:A:828:A:H2'	1:A:829:G:O4'	2.00	0.61
7:G:43:PHE:O	7:G:47:CYS:HB2	2.00	0.61
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.25	0.61
1:A:1251:A:H2'	1:A:1252:A:C8	2.36	0.61
1:A:112:G:H4'	1:A:389:A:H5''	1.82	0.61
7:G:51:GLN:O	7:G:52:GLU:HG2	2.01	0.61
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.35	0.61
13:M:50:GLU:O	13:M:54:VAL:HG23	1.99	0.61
1:A:1241:G:H2'	1:A:1242:C:C6	2.34	0.61
1:A:631:G:H5'	1:A:632:A:OP1	2.00	0.61
9:I:108:VAL:HG12	9:I:109:VAL:N	2.16	0.61
1:A:969:A:H61	13:M:126:LYS:HB2	1.65	0.61
13:M:22:ILE:HG13	13:M:25:ILE:HD12	1.83	0.61
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.81	0.61
1:A:1128:C:O2'	1:A:1130:A:H8	1.84	0.61
1:A:1286:A:H8	1:A:1287:A:H4'	1.65	0.61
1:A:1300:G:HO2'	1:A:1301:U:H6	1.46	0.61
1:A:983:A:H5'	1:A:984:C:OP2	2.00	0.61
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.81	0.61
12:L:24:VAL:O	12:L:26:ALA:N	2.32	0.61
3:C:107:GLN:O	3:C:108:ASN:HB3	2.01	0.61
4:D:146:ILE:HD12	4:D:146:ILE:N	2.15	0.61
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.29	0.61
2:B:195:ASP:O	8:H:74:PRO:HG3	2.00	0.61
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.15	0.61
10:J:71:LEU:O	10:J:72:VAL:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:C:H5''	1:A:703:G:O4'	2.00	0.61
13:M:102:ARG:HH11	13:M:102:ARG:HB2	1.66	0.61
1:A:243:A:H4'	1:A:244:U:C5'	2.20	0.61
1:A:376:G:OP2	16:P:67:THR:HG21	2.01	0.61
1:A:818:G:C3'	1:A:819:A:H5''	2.30	0.61
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.82	0.61
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.82	0.61
1:A:538:G:OP2	12:L:115:LYS:HG3	1.99	0.61
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.16	0.61
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.82	0.61
12:L:24:VAL:HG12	12:L:24:VAL:O	2.01	0.61
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.66	0.61
7:G:12:LEU:N	7:G:12:LEU:HD12	2.15	0.60
9:I:82:ALA:O	9:I:86:VAL:HG23	2.01	0.60
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.16	0.60
1:A:1343:G:H2'	1:A:1344:C:C6	2.35	0.60
12:L:126:LYS:HG3	12:L:127:GLU:H	1.66	0.60
1:A:364:A:H61	12:L:28:LYS:HE3	1.65	0.60
1:A:818:G:O2'	1:A:819:A:H5''	2.01	0.60
6:F:38:GLU:O	6:F:39:LYS:HB3	2.00	0.60
13:M:49:THR:HB	13:M:52:GLU:HG3	1.83	0.60
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.83	0.60
1:A:539:A:H2'	1:A:540:G:C8	2.36	0.60
10:J:9:ARG:C	10:J:16:LEU:HD11	2.22	0.60
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.82	0.60
12:L:40:VAL:HG11	12:L:77:LEU:O	2.01	0.60
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.32	0.60
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.15	0.60
1:A:1132:C:H2'	1:A:1133:G:H8	1.66	0.60
1:A:433:C:C5'	1:A:433:C:H6	2.14	0.60
1:A:539:A:H2'	1:A:540:G:H8	1.66	0.60
1:A:973:G:H3'	1:A:974:A:H5''	1.84	0.60
10:J:49:VAL:O	10:J:60:ARG:HA	2.01	0.60
10:J:90:LEU:N	10:J:91:PRO:CD	2.63	0.60
3:C:188:LEU:O	3:C:189:ALA:HB2	2.02	0.60
1:A:405:U:H3'	1:A:406:G:H5'	1.84	0.60
10:J:36:GLY:O	10:J:72:VAL:HA	2.01	0.60
1:A:26:A:N6	1:A:558:G:H1'	2.17	0.60
1:A:427:U:OP1	4:D:13:ARG:NH2	2.35	0.60
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.84	0.60
10:J:23:ILE:N	10:J:23:ILE:HD12	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.22	0.60
19:S:18:LYS:HD3	19:S:18:LYS:O	2.02	0.60
1:A:1298:C:H2'	7:G:114:ARG:NH1	2.17	0.60
1:A:1305:G:H22	1:A:1331:G:C2'	2.15	0.60
13:M:125:ARG:HD2	13:M:125:ARG:C	2.22	0.60
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.59
9:I:93:ARG:CB	9:I:93:ARG:HH11	2.13	0.59
1:A:1323:G:H2'	1:A:1324:A:C8	2.37	0.59
1:A:353:A:H5'	1:A:353:A:C8	2.37	0.59
10:J:6:ILE:HG23	10:J:98:ILE:HD11	1.84	0.59
11:K:126:ARG:O	11:K:127:LYS:HB2	2.03	0.59
1:A:1156:G:H3'	1:A:1157:A:P	2.34	0.59
1:A:639:G:O2'	1:A:640:A:H5'	2.02	0.59
1:A:382:A:H2'	1:A:383:A:H8	1.63	0.59
2:B:88:ALA:HB1	2:B:90:MET:HG2	1.84	0.59
1:A:412:A:N6	4:D:35:ARG:HB2	2.17	0.59
11:K:108:ILE:N	11:K:108:ILE:HD12	2.17	0.59
2:B:204:ASN:HD22	2:B:206:ASP:H	1.50	0.59
3:C:82:GLU:O	3:C:85:ARG:HB3	2.03	0.59
1:A:1063:C:H3'	1:A:1064:G:H2'	1.84	0.59
1:A:107:G:H2'	1:A:108:G:H5'	1.84	0.59
3:C:156:ARG:NH2	3:C:161:GLU:HA	2.17	0.59
12:L:124:LYS:HD3	12:L:125:PRO:HD2	1.85	0.59
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.84	0.59
17:Q:59:ILE:HG22	17:Q:71:PHE:HD1	1.65	0.59
12:L:28:LYS:C	12:L:30:ALA:N	2.53	0.59
20:T:43:LEU:CD1	20:T:55:ILE:HD12	2.33	0.59
1:A:1176:A:H2'	1:A:1177:G:C8	2.38	0.59
6:F:45:LEU:HD12	6:F:45:LEU:O	2.03	0.59
9:I:126:SER:O	9:I:127:LYS:HB3	2.02	0.59
1:A:1148:U:H2'	1:A:1149:C:O4'	2.03	0.59
1:A:818:G:C2'	1:A:819:A:H5''	2.33	0.59
12:L:43:VAL:HG12	12:L:44:THR:N	2.18	0.59
13:M:90:LEU:HA	13:M:93:ARG:HB2	1.85	0.59
1:A:1190:G:H3'	3:C:3:ASN:HD21	1.62	0.59
1:A:860:A:H2'	1:A:861:G:O4'	2.03	0.59
2:B:129:GLU:N	2:B:129:GLU:OE2	2.36	0.59
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.30	0.59
1:A:1153:C:P	10:J:13:HIS:HE2	2.26	0.59
10:J:76:ASN:O	10:J:78:ASN:N	2.33	0.59
10:J:5:ARG:O	10:J:98:ILE:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:O2'	1:A:1348:U:P	2.60	0.58
1:A:1479:C:H2'	1:A:1480:G:H8	1.66	0.58
1:A:984:C:H2'	1:A:985:C:C6	2.37	0.58
2:B:53:ARG:HH12	2:B:199:TYR:HA	1.67	0.58
2:B:88:ALA:O	2:B:90:MET:N	2.36	0.58
4:D:126:ILE:HG22	4:D:127:THR:N	2.18	0.58
5:E:150:ARG:NH1	5:E:150:ARG:HG3	2.09	0.58
1:A:1128:C:C5'	9:I:16:ARG:NH1	2.59	0.58
1:A:1168:A:H2'	1:A:1169:A:C8	2.37	0.58
1:A:908:A:H2'	1:A:909:A:C8	2.39	0.58
2:B:204:ASN:HD22	2:B:204:ASN:C	2.04	0.58
2:B:74:LYS:HZ2	2:B:206:ASP:HA	1.68	0.58
3:C:123:GLN:O	3:C:126:ARG:HG2	2.02	0.58
6:F:100:ASN:HB3	18:R:27:GLY:O	2.03	0.58
1:A:961:U:C2'	1:A:962:C:H5'	2.34	0.58
8:H:120:THR:OG1	8:H:123:GLU:HG3	2.03	0.58
9:I:48:GLU:HA	9:I:51:ARG:HE	1.68	0.58
1:A:1038:C:H2'	1:A:1039:C:C6	2.39	0.58
1:A:1247:U:O2'	1:A:1248:A:H5'	2.03	0.58
1:A:1330:U:OP1	13:M:23:TYR:O	2.21	0.58
1:A:269:C:H2'	1:A:270:A:C8	2.39	0.58
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.84	0.58
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.03	0.58
7:G:136:LYS:NZ	7:G:143:ARG:NH1	2.51	0.58
8:H:83:ILE:O	8:H:83:ILE:HG23	2.03	0.58
1:A:1125:U:H3	10:J:5:ARG:HH21	1.50	0.58
14:N:9:LYS:O	14:N:11:LYS:N	2.36	0.58
19:S:33:THR:HG22	19:S:34:TRP:N	2.19	0.58
1:A:1029:C:H2'	1:A:1030:C:C6	2.39	0.58
1:A:1277:C:HO2'	1:A:1279:A:H8	1.51	0.58
4:D:10:ARG:HG3	4:D:10:ARG:HH11	1.69	0.58
1:A:1368:G:OP2	9:I:112:LYS:HD2	2.04	0.58
9:I:48:GLU:N	9:I:49:PRO:CD	2.67	0.58
13:M:40:ASN:ND2	13:M:42:ALA:H	2.01	0.58
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.38	0.58
1:A:1042:G:O2'	1:A:1043:C:H5'	2.03	0.58
1:A:1316:G:N2	1:A:1318:A:H3'	2.18	0.58
1:A:1391:U:H2'	1:A:1392:G:C8	2.39	0.58
2:B:114:ARG:HA	2:B:117:GLU:CB	2.33	0.58
2:B:223:ILE:HD12	2:B:224:GLN:H	1.68	0.58
1:A:1250:A:C4'	9:I:68:GLY:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.68	0.58
1:A:1118:C:H1'	1:A:1179:A:C4	2.39	0.58
1:A:192:U:H1'	20:T:103:GLY:HA2	1.85	0.58
1:A:1190:G:C3'	3:C:3:ASN:ND2	2.64	0.58
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.31	0.58
4:D:199:ASN:HD21	4:D:201:GLN:HB2	1.68	0.58
14:N:3:ARG:HB2	14:N:3:ARG:HH11	1.68	0.58
1:A:1175:G:H3'	1:A:1176:A:OP2	2.03	0.58
1:A:1232:U:P	9:I:124:GLN:HE21	2.27	0.58
3:C:27:LYS:HD3	3:C:27:LYS:N	2.19	0.58
6:F:46:ARG:HH11	6:F:46:ARG:CB	2.16	0.58
23:Y:34:TM2:H2'	23:Y:35:A:C8	2.39	0.58
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.03	0.58
1:A:407:G:O2'	4:D:116:GLN:HG3	2.03	0.58
1:A:939:G:H2'	1:A:940:C:C6	2.39	0.58
3:C:32:LEU:HD22	3:C:59:ARG:HH11	1.69	0.58
5:E:76:ILE:HG13	5:E:142:LEU:CD1	2.34	0.58
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.25	0.58
6:F:3:ARG:HG2	6:F:93:SER:OG	2.04	0.58
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.35	0.58
10:J:27:ALA:HA	10:J:81:THR:HG23	1.86	0.58
14:N:26:ARG:HH21	14:N:47:LEU:CG	2.11	0.58
3:C:29:TYR:OH	14:N:54:PRO:HG2	2.03	0.58
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.86	0.58
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.18	0.58
1:A:1137:C:H4'	1:A:1138:G:N1	2.19	0.57
2:B:141:GLU:O	2:B:144:ARG:HG3	2.04	0.57
3:C:34:LEU:HD21	3:C:38:ARG:NE	2.19	0.57
7:G:31:MET:HG2	7:G:32:ARG:H	1.68	0.57
7:G:5:ARG:NE	7:G:7:ALA:HA	2.19	0.57
1:A:1251:A:H1'	1:A:1369:C:O2'	2.02	0.57
1:A:1397:C:H4'	1:A:1398:A:OP2	2.04	0.57
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.86	0.57
3:C:91:LEU:HD23	3:C:92:ALA:N	2.17	0.57
1:A:972:C:P	10:J:57:LYS:HE2	2.44	0.57
12:L:57:LYS:HD3	12:L:67:THR:HG23	1.86	0.57
15:O:87:ILE:CG2	15:O:88:ARG:H	2.17	0.57
19:S:80:TYR:CZ	19:S:81:ARG:HD3	2.39	0.57
1:A:1160:G:HO2'	1:A:1161:C:H5'	1.70	0.57
3:C:79:ARG:HG2	3:C:82:GLU:CG	2.34	0.57
1:A:620:C:N1	4:D:135:LEU:HD13	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:CYS:O	4:D:31:CYS:SG	2.62	0.57
1:A:666:G:H5'	1:A:726:C:H1'	1.86	0.57
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.39	0.57
12:L:34:ARG:O	12:L:61:THR:HG23	2.05	0.57
13:M:8:GLU:OE1	13:M:22:ILE:HG23	2.04	0.57
1:A:1320:C:O2'	1:A:1321:C:H5'	2.05	0.57
9:I:107:ARG:HH11	9:I:107:ARG:HB3	1.68	0.57
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.39	0.57
1:A:1157:A:C5	1:A:1180:A:N6	2.73	0.57
1:A:457:C:H2'	1:A:458:C:H6	1.69	0.57
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.85	0.57
6:F:100:ASN:ND2	18:R:23:LYS:HG2	2.20	0.57
12:L:113:ARG:NH1	12:L:116:SER:H	2.02	0.57
12:L:58:VAL:O	12:L:65:GLU:HA	2.04	0.57
3:C:6:HIS:CD2	3:C:8:ILE:H	2.09	0.57
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.03	0.57
12:L:89:ARG:HA	12:L:97:ARG:HA	1.86	0.57
13:M:3:ARG:HB2	13:M:9:ILE:HG13	1.86	0.57
1:A:337:C:H2'	1:A:338:A:H8	1.69	0.57
1:A:832:C:O2'	1:A:833:U:H5'	2.04	0.57
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.20	0.57
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.40	0.57
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.87	0.57
9:I:45:ALA:O	9:I:48:GLU:HB2	2.04	0.57
12:L:27:LEU:HG	12:L:28:LYS:H	1.70	0.57
1:A:1024:G:C3'	1:A:1025:U:H5''	2.34	0.57
1:A:746:A:O2'	1:A:747:C:H5'	2.05	0.57
3:C:154:SER:OG	3:C:155:GLY:N	2.37	0.57
10:J:84:GLN:O	10:J:88:LEU:HD12	2.05	0.57
12:L:83:VAL:HG13	12:L:100:ILE:HG23	1.86	0.57
1:A:1175:G:C2'	1:A:1176:A:O5'	2.53	0.57
1:A:646:U:H2'	1:A:647:C:C6	2.39	0.57
1:A:918:A:H2'	1:A:919:A:C8	2.40	0.57
3:C:126:ARG:NH2	3:C:128:PHE:CD1	2.73	0.57
5:E:146:ALA:O	5:E:150:ARG:HB2	2.05	0.57
16:P:38:TYR:CE2	16:P:50:LYS:HE2	2.39	0.57
19:S:5:LEU:HD11	19:S:70:LYS:NZ	2.20	0.57
1:A:1112:C:C4	3:C:178:LEU:HD23	2.40	0.56
1:A:1121:U:H2'	1:A:1122:U:C6	2.39	0.56
1:A:895:G:H2'	1:A:896:C:H6	1.70	0.56
4:D:17:VAL:CG1	4:D:18:LYS:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:VAL:HG21	8:H:109:ILE:O	2.05	0.56
19:S:40:ILE:CG2	19:S:62:ILE:HD11	2.35	0.56
1:A:834:C:H2'	1:A:835:U:H6	1.70	0.56
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.86	0.56
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.87	0.56
1:A:1424:C:O2'	1:A:1425:U:H5'	2.05	0.56
1:A:344:A:H4'	1:A:345:C:OP2	2.06	0.56
2:B:87:ARG:O	2:B:88:ALA:CB	2.52	0.56
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.22	0.56
13:M:79:LYS:HE2	13:M:83:ASP:OD2	2.06	0.56
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.20	0.56
20:T:74:LYS:CB	20:T:74:LYS:NZ	2.68	0.56
23:Y:34:TM2:H2'	23:Y:35:A:H8	1.70	0.56
7:G:31:MET:HG2	7:G:32:ARG:N	2.20	0.56
1:A:1101:A:H8	2:B:172:ILE:HD13	1.71	0.56
5:E:60:TYR:CE1	5:E:64:ARG:NH2	2.73	0.56
11:K:57:THR:HG23	11:K:58:PRO:HD2	1.87	0.56
16:P:10:GLY:HA3	16:P:14:ASN:O	2.05	0.56
19:S:47:HIS:O	19:S:62:ILE:HG22	2.06	0.56
1:A:1065:U:H5''	1:A:1190:G:H21	1.64	0.56
1:A:1347:G:H2'	1:A:1373:G:H1	1.70	0.56
4:D:62:GLN:HE22	4:D:65:ARG:NH1	2.03	0.56
17:Q:4:LYS:HD2	17:Q:6:LEU:HD21	1.87	0.56
1:A:1161:C:H2'	1:A:1162:C:C5	2.40	0.56
1:A:409:G:H1	1:A:433:C:H42	1.54	0.56
13:M:65:LYS:O	13:M:66:LEU:HD23	2.05	0.56
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.87	0.56
1:A:1496:C:H2'	1:A:1497:G:C8	2.41	0.56
2:B:130:ARG:CB	2:B:131:PRO:HD2	2.36	0.56
2:B:207:ALA:O	2:B:211:ILE:HG13	2.05	0.56
3:C:131:ARG:O	3:C:135:LYS:HB2	2.06	0.56
3:C:11:ARG:O	3:C:14:ILE:O	2.23	0.56
13:M:90:LEU:O	13:M:94:ARG:HD2	2.05	0.56
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.15	0.56
19:S:13:ASP:HA	19:S:16:LEU:CB	2.32	0.56
20:T:74:LYS:HB3	20:T:74:LYS:NZ	2.20	0.56
1:A:1118:C:C2	1:A:1179:A:N1	2.74	0.56
1:A:1427:U:H2'	1:A:1428:A:C8	2.41	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.56
1:A:895:G:H2'	1:A:896:C:C6	2.40	0.56
18:R:17:SER:HB3	18:R:54:ARG:NH1	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:A:H2'	1:A:916:G:H5'	1.88	0.56
2:B:204:ASN:HD21	2:B:206:ASP:HB3	1.68	0.56
3:C:73:PRO:O	3:C:76:VAL:HG22	2.06	0.56
6:F:25:ILE:HD12	6:F:82:ARG:HD2	1.88	0.56
11:K:33:THR:HG22	11:K:39:PRO:CA	2.36	0.56
13:M:66:LEU:O	13:M:69:GLU:HB2	2.05	0.56
20:T:67:ALA:HA	20:T:73:HIS:H	1.71	0.56
1:A:1015:A:H2'	1:A:1016:A:C8	2.41	0.55
1:A:1041:A:H2'	1:A:1042:G:C8	2.41	0.55
1:A:1126:U:H2'	1:A:1127:G:H8	1.67	0.55
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.88	0.55
5:E:75:THR:HG23	5:E:76:ILE:N	2.21	0.55
7:G:135:VAL:O	7:G:139:GLU:HG3	2.06	0.55
10:J:4:ILE:HG12	10:J:74:ILE:HB	1.87	0.55
1:A:1159:U:C4	1:A:1182:G:C6	2.94	0.55
1:A:807:A:H2'	1:A:808:C:C6	2.41	0.55
14:N:24:CYS:SG	14:N:40:CYS:N	2.79	0.55
14:N:6:LEU:C	14:N:8:GLU:H	2.07	0.55
18:R:47:THR:HG22	18:R:48:GLY:H	1.70	0.55
1:A:1072:G:H2'	1:A:1073:U:C6	2.42	0.55
1:A:1370:G:O2'	1:A:1371:G:H5'	2.07	0.55
13:M:59:TYR:O	13:M:63:THR:HG22	2.06	0.55
15:O:87:ILE:CG2	15:O:88:ARG:N	2.69	0.55
18:R:47:THR:HG22	18:R:48:GLY:N	2.20	0.55
1:A:1038:C:H2'	1:A:1039:C:H6	1.70	0.55
2:B:70:PHE:HB3	2:B:81:VAL:HG13	1.87	0.55
9:I:126:SER:HB2	9:I:128:ARG:O	2.07	0.55
1:A:269:C:H2'	1:A:270:A:H8	1.72	0.55
1:A:357:G:O2'	1:A:358:U:H5'	2.06	0.55
1:A:478:A:O2'	1:A:479:C:H5'	2.07	0.55
1:A:834:C:H2'	1:A:835:U:C6	2.41	0.55
1:A:1206:G:H1'	3:C:193:TYR:O	2.06	0.55
3:C:56:ASP:O	3:C:57:ILE:HG13	2.06	0.55
7:G:120:ILE:H	7:G:120:ILE:HD12	1.71	0.55
1:A:953:G:H1'	13:M:125:ARG:CB	2.36	0.55
13:M:40:ASN:HD22	13:M:41:PRO:N	2.05	0.55
19:S:19:VAL:HG13	19:S:20:LEU:N	2.21	0.55
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.40	0.55
1:A:1160:G:N2	1:A:1161:C:C1'	2.66	0.55
1:A:1216:G:H5''	14:N:5:ALA:CB	2.37	0.55
1:A:1258:G:O2'	1:A:1259:C:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:G:H2'	1:A:1439:C:C6	2.42	0.55
1:A:21:G:H2'	1:A:22:G:C8	2.42	0.55
1:A:268:C:H2'	1:A:269:C:H6	1.72	0.55
1:A:337:C:H2'	1:A:338:A:C8	2.42	0.55
1:A:862:C:O2'	1:A:863:U:H5'	2.06	0.55
3:C:60:ALA:O	3:C:61:ALA:HB2	2.06	0.55
12:L:126:LYS:C	12:L:127:GLU:HG3	2.27	0.55
9:I:128:ARG:HA	13:M:126:LYS:HZ3	1.71	0.55
13:M:25:ILE:HD11	13:M:60:VAL:CG1	2.37	0.55
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.06	0.55
1:A:1175:G:H2'	1:A:1176:A:C8	2.36	0.55
1:A:328:C:O2	1:A:328:C:C2'	2.47	0.55
3:C:79:ARG:HG3	3:C:79:ARG:O	2.07	0.55
18:R:19:LYS:O	18:R:20:ALA:HB2	2.07	0.55
3:C:107:GLN:H	3:C:107:GLN:CD	2.10	0.55
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.37	0.55
1:A:411:A:O2'	1:A:412:A:H5'	2.06	0.55
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.71	0.55
1:A:1091:U:O2	1:A:1093:A:C8	2.60	0.55
1:A:268:C:O2'	1:A:269:C:H5'	2.07	0.55
1:A:991:U:C4	1:A:1212:U:H1'	2.42	0.55
3:C:110:ASN:HD21	3:C:140:ARG:HB3	1.71	0.55
18:R:87:ARG:O	18:R:88:LYS:HB3	2.06	0.55
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.42	0.54
12:L:68:ALA:HB3	12:L:100:ILE:HD11	1.89	0.54
20:T:100:ILE:O	20:T:101:GLY:C	2.45	0.54
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.23	0.54
2:B:113:HIS:O	2:B:117:GLU:HB2	2.07	0.54
1:A:921:U:O2	5:E:19:MET:HB2	2.07	0.54
1:A:1123:A:H2	10:J:39:PRO:HG2	1.71	0.54
20:T:76:ALA:O	20:T:80:ARG:HG3	2.07	0.54
22:X:3:A:N1	23:Y:34:TM2:O4	2.39	0.54
1:A:1024:G:H3'	1:A:1025:U:H5''	1.90	0.54
1:A:1159:U:C5	1:A:1182:G:C5	2.96	0.54
1:A:1218:C:H2'	1:A:1219:U:C6	2.42	0.54
1:A:431:A:O2'	1:A:432:A:H5'	2.07	0.54
1:A:594:G:C2'	1:A:595:G:H5'	2.37	0.54
1:A:818:G:H3'	1:A:819:A:C5'	2.37	0.54
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.88	0.54
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.41	0.54
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.89	0.54
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.90	0.54
1:A:755:G:OP2	15:O:65:ARG:HD2	2.08	0.54
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.42	0.54
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.88	0.54
1:A:1192:C:C2'	1:A:1193:G:P	2.89	0.54
1:A:1228:C:H4'	13:M:116:THR:HA	1.90	0.54
1:A:1283:G:O2'	1:A:1284:C:H5'	2.07	0.54
1:A:1498:U:H4'	1:A:1519:A:C2	2.42	0.54
2:B:83:MET:SD	2:B:235:SER:HB3	2.47	0.54
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.37	0.54
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.90	0.54
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.42	0.54
1:A:1060:C:H2'	1:A:1061:G:C8	2.40	0.54
1:A:1054:C:H5	1:A:1196:U:C5	2.26	0.54
1:A:1479:C:H2'	1:A:1480:G:C8	2.41	0.54
1:A:954:G:H2'	1:A:955:U:C6	2.42	0.54
3:C:147:LYS:HE2	3:C:205:GLY:CA	2.37	0.54
10:J:63:PHE:HE1	14:N:45:ARG:HG3	1.71	0.54
10:J:4:ILE:CG1	10:J:74:ILE:HB	2.37	0.54
1:A:1118:C:C2	1:A:1179:A:C2	2.96	0.54
1:A:1201:A:H4'	1:A:1202:G:O5'	2.07	0.54
1:A:424:G:O2'	1:A:425:G:H5'	2.06	0.54
1:A:838:G:H2'	1:A:839:U:H5''	1.89	0.54
1:A:912:C:O2'	1:A:913:A:H5'	2.07	0.54
2:B:224:GLN:O	2:B:224:GLN:HG2	2.08	0.54
4:D:201:GLN:HA	4:D:201:GLN:HE21	1.73	0.54
1:A:1059:C:O2'	1:A:1060:C:H5'	2.07	0.54
1:A:1253:G:H2'	1:A:1254:C:C6	2.42	0.54
1:A:1392:G:N2	1:A:1502:A:C8	2.75	0.54
2:B:187:LEU:HD21	2:B:203:GLY:HA3	1.90	0.54
2:B:22:LYS:C	2:B:24:TRP:H	2.09	0.54
3:C:91:LEU:HD11	3:C:99:VAL:HG23	1.88	0.54
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.38	0.54
1:A:430:A:OP1	4:D:9:CYS:HB2	2.08	0.54
6:F:22:GLU:HA	6:F:22:GLU:OE2	2.08	0.54
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.87	0.54
1:A:106:C:O2	1:A:379:C:H4'	2.08	0.54
1:A:1147:C:H4'	9:I:5:TYR:CE2	2.42	0.54
1:A:1154:G:H2'	1:A:1155:G:H8	1.73	0.54
1:A:547:A:H4'	1:A:548:G:O5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:TRP:O	3:C:168:ALA:HB3	2.07	0.54
10:J:18:ALA:C	10:J:20:ALA:H	2.11	0.54
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.89	0.54
1:A:45:U:H2'	1:A:46:G:C8	2.43	0.54
1:A:740:U:O2'	1:A:741:G:H5'	2.08	0.54
2:B:88:ALA:C	2:B:90:MET:N	2.60	0.54
5:E:116:THR:HG22	5:E:117:ASP:OD2	2.08	0.54
9:I:107:ARG:HH11	9:I:107:ARG:CB	2.21	0.54
13:M:108:ARG:NE	13:M:108:ARG:HA	2.16	0.54
14:N:18:VAL:HG23	14:N:19:ARG:H	1.73	0.54
5:E:137:GLU:O	5:E:141:GLN:HG3	2.07	0.54
12:L:83:VAL:HG11	12:L:100:ILE:HG13	1.88	0.54
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.71	0.54
1:A:1306:A:N6	1:A:1331:G:H1'	2.24	0.53
1:A:1425:U:H2'	1:A:1426:C:C6	2.44	0.53
1:A:167:G:O2'	1:A:168:G:H5'	2.08	0.53
1:A:77:G:O2'	1:A:78:G:H5'	2.08	0.53
1:A:791:G:C6	1:A:792:A:N7	2.76	0.53
3:C:95:THR:C	3:C:97:LYS:H	2.11	0.53
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.23	0.53
12:L:75:HIS:HD2	12:L:77:LEU:H	1.55	0.53
14:N:12:ARG:N	14:N:12:ARG:CD	2.71	0.53
17:Q:81:ARG:O	17:Q:81:ARG:HG3	2.07	0.53
1:A:1053:G:H3'	1:A:1054:C:H5'	1.90	0.53
1:A:1167:A:H2'	1:A:1168:A:C8	2.44	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.55	0.53
1:A:1419:G:O2'	1:A:1420:C:H5'	2.08	0.53
1:A:542:G:OP1	4:D:10:ARG:NH2	2.41	0.53
1:A:975:A:H4'	1:A:976:G:C5'	2.33	0.53
2:B:162:ILE:HD11	2:B:184:VAL:HG22	1.91	0.53
3:C:142:MET:HG3	3:C:170:GLN:HB2	1.90	0.53
5:E:76:ILE:CG2	5:E:78:HIS:O	2.57	0.53
1:A:1230:C:H1'	13:M:126:LYS:HA	1.90	0.53
1:A:1054:C:C3'	1:A:1054:C:O2	2.57	0.53
5:E:36:ASP:OD1	5:E:38:GLN:N	2.36	0.53
6:F:100:ASN:HD22	18:R:23:LYS:HG2	1.72	0.53
8:H:54:ASP:CG	8:H:55:GLY:N	2.62	0.53
2:B:230:VAL:HG12	2:B:231:GLU:N	2.23	0.53
4:D:4:TYR:O	4:D:5:ILE:HB	2.07	0.53
6:F:19:LEU:HD23	6:F:19:LEU:C	2.29	0.53
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.27	0.53
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.44	0.53
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.74	0.53
1:A:1532:U:O2'	1:A:1533:C:H6	1.91	0.53
2:B:27:LYS:HD3	2:B:195:ASP:OD2	2.08	0.53
3:C:77:ILE:C	3:C:83:ARG:HB3	2.29	0.53
7:G:15:ASP:O	7:G:19:GLY:HA2	2.08	0.53
9:I:48:GLU:HG2	9:I:51:ARG:HH21	1.71	0.53
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.28	0.53
9:I:128:ARG:CG	13:M:126:LYS:HZ3	2.21	0.53
1:A:1004:A:N7	1:A:1037:C:N3	2.56	0.53
13:M:49:THR:HG22	13:M:51:ALA:N	2.10	0.53
14:N:46:GLU:O	14:N:49:HIS:HB2	2.08	0.53
20:T:72:LEU:O	20:T:73:HIS:O	2.26	0.53
1:A:1101:A:H4'	1:A:1102:A:O5'	2.09	0.53
1:A:831:U:OP1	2:B:22:LYS:HE3	2.08	0.53
3:C:134:ILE:HG21	3:C:167:TRP:O	2.09	0.53
3:C:54:ARG:CG	3:C:55:VAL:H	2.22	0.53
5:E:82:VAL:HG21	5:E:138:ALA:CA	2.39	0.53
15:O:45:VAL:HG12	15:O:46:HIS:N	2.24	0.53
17:Q:68:ARG:HH11	17:Q:68:ARG:HG2	1.73	0.53
1:A:1326:C:C5	21:U:6:ARG:NH2	2.77	0.53
1:A:32:A:H2'	1:A:33:A:C8	2.44	0.53
3:C:52:LEU:H	3:C:52:LEU:HD23	1.73	0.53
7:G:5:ARG:HG3	7:G:7:ALA:H	1.74	0.53
1:A:1260:C:O5'	1:A:1284:C:H4'	2.08	0.53
1:A:1238:A:OP1	1:A:1336:C:H5	1.92	0.53
2:B:132:LYS:HG3	2:B:136:VAL:HG23	1.89	0.53
7:G:16:LEU:N	7:G:16:LEU:HD22	2.24	0.53
19:S:17:GLU:CA	19:S:20:LEU:HG	2.37	0.53
1:A:1181:G:O2'	1:A:1184:G:H5'	2.09	0.53
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.42	0.53
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.41	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.44	0.53
1:A:570:G:H2'	1:A:571:U:C6	2.44	0.53
1:A:625:G:H2'	1:A:626:U:C6	2.44	0.53
1:A:833:U:H2'	1:A:834:C:C6	2.44	0.53
3:C:126:ARG:C	3:C:127:ARG:HD2	2.28	0.53
7:G:44:TYR:HE1	9:I:41:VAL:HG11	1.73	0.53
12:L:54:LYS:CD	12:L:54:LYS:N	2.72	0.53
19:S:22:LEU:CD1	19:S:31:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:G:O2'	1:A:296:U:OP1	2.25	0.52
1:A:961:U:H2'	1:A:962:C:H5'	1.91	0.52
3:C:207:VAL:HG12	3:C:207:VAL:O	2.08	0.52
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.90	0.52
1:A:1486:G:H2'	1:A:1487:G:O4'	2.09	0.52
2:B:115:LEU:HG	2:B:153:ARG:NH2	2.22	0.52
4:D:28:SER:C	4:D:30:LYS:H	2.12	0.52
4:D:36:ARG:HG3	4:D:38:TYR:CZ	2.44	0.52
8:H:111:ILE:O	8:H:134:ILE:HB	2.08	0.52
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.92	0.52
1:A:1342:C:O2'	1:A:1343:G:H5'	2.09	0.52
1:A:1372:U:H2'	1:A:1373:G:O4'	2.10	0.52
2:B:44:LEU:HD12	2:B:44:LEU:N	2.18	0.52
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.74	0.52
10:J:6:ILE:HB	10:J:72:VAL:HB	1.90	0.52
1:A:1116:C:H2'	1:A:1117:G:C5'	2.36	0.52
2:B:185:ILE:HD12	2:B:185:ILE:N	2.24	0.52
3:C:44:GLU:HG2	3:C:52:LEU:HD11	1.91	0.52
3:C:54:ARG:CG	3:C:55:VAL:N	2.72	0.52
11:K:78:GLN:O	11:K:103:LEU:HA	2.08	0.52
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.90	0.52
1:A:1005:A:H2'	1:A:1006:C:H5'	1.92	0.52
1:A:1393:U:O4'	1:A:1502:A:H5'	2.08	0.52
1:A:178:C:O2'	1:A:179:A:H5'	2.08	0.52
2:B:64:ARG:NH1	2:B:64:ARG:HB3	2.23	0.52
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.40	0.52
8:H:36:LEU:CD1	8:H:59:LEU:HD13	2.40	0.52
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.10	0.52
18:R:54:ARG:HH21	18:R:54:ARG:HG2	1.75	0.52
18:R:86:VAL:O	18:R:87:ARG:HB2	2.09	0.52
1:A:1123:A:C2	10:J:39:PRO:HG2	2.44	0.52
1:A:1405:G:O2'	1:A:1406:U:H5'	2.09	0.52
1:A:187:C:C2	20:T:105:SER:HB3	2.44	0.52
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.44	0.52
3:C:72:LYS:O	3:C:75:VAL:HG23	2.09	0.52
15:O:79:ARG:O	15:O:79:ARG:HD2	2.10	0.52
1:A:1156:G:O3'	1:A:1157:A:O5'	2.06	0.52
1:A:1329:A:O2'	1:A:1330:U:H5'	2.09	0.52
14:N:14:PRO:O	14:N:15:LYS:CB	2.58	0.52
14:N:47:LEU:HD23	14:N:50:LYS:HD3	1.91	0.52
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG23	16:P:36:ILE:HD11	1.92	0.52
20:T:67:ALA:O	20:T:73:HIS:ND1	2.43	0.52
1:A:1161:C:N4	1:A:1182:G:H22	2.08	0.52
1:A:824:C:H2'	1:A:825:G:H8	1.75	0.52
8:H:101:PRO:HA	8:H:102:ARG:HE	1.74	0.52
13:M:98:VAL:O	13:M:98:VAL:HG12	2.09	0.52
1:A:1190:G:C3'	3:C:3:ASN:HD21	2.22	0.52
1:A:67:C:O2'	1:A:171:A:H1'	2.10	0.52
1:A:640:A:O2'	1:A:641:U:H5'	2.09	0.52
3:C:54:ARG:HG2	3:C:55:VAL:N	2.25	0.52
7:G:136:LYS:HD3	7:G:140:ASP:OD1	2.09	0.52
9:I:10:ARG:HD2	9:I:11:LYS:N	2.25	0.52
10:J:49:VAL:HG21	14:N:41:ARG:O	2.10	0.52
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.40	0.52
18:R:87:ARG:O	18:R:88:LYS:CB	2.58	0.52
1:A:1497:G:H2'	1:A:1498:U:H5'	1.92	0.52
1:A:627:G:H2'	1:A:628:G:H8	1.74	0.52
1:A:761:G:O2'	17:Q:105:ALA:HB2	2.10	0.52
1:A:977:A:H2'	1:A:978:A:H5'	1.92	0.52
2:B:122:PHE:HE2	2:B:139:LYS:HG2	1.75	0.52
10:J:60:ARG:O	10:J:61:GLU:HB3	2.10	0.52
17:Q:4:LYS:HD2	17:Q:6:LEU:CD2	2.40	0.52
18:R:59:SER:H	18:R:62:GLU:HB2	1.75	0.52
1:A:1003(A):G:N3	1:A:1004:A:H1'	2.25	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.44	0.51
1:A:332:G:O2'	1:A:333:G:H5'	2.10	0.51
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.91	0.51
11:K:107:SER:C	11:K:108:ILE:HD12	2.31	0.51
12:L:125:PRO:O	12:L:126:LYS:O	2.27	0.51
1:A:1305:G:H5''	21:U:4:GLY:C	2.30	0.51
1:A:1292:U:P	7:G:41:ARG:NH2	2.80	0.51
4:D:36:ARG:H	4:D:37:PRO:CD	2.23	0.51
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.46	0.51
7:G:45:ASP:O	7:G:48:LYS:HG2	2.10	0.51
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.75	0.51
7:G:113:GLU:CG	7:G:119:ARG:HG3	2.39	0.51
7:G:23:VAL:O	7:G:27:ILE:HG12	2.10	0.51
8:H:7:ALA:HB2	8:H:85:ARG:HD2	1.92	0.51
12:L:126:LYS:O	12:L:127:GLU:OE1	2.28	0.51
17:Q:55:ASP:HB3	17:Q:76:LEU:CD1	2.40	0.51
20:T:94:ALA:O	20:T:95:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:A:C8	2:B:172:ILE:HD13	2.44	0.51
1:A:1118:C:O2	1:A:1179:A:C2	2.63	0.51
1:A:1510:U:H2'	1:A:1511:G:C8	2.46	0.51
1:A:526:C:OP2	12:L:91:LYS:HE3	2.10	0.51
1:A:814:A:H2'	1:A:816:A:H5''	1.92	0.51
2:B:78:GLN:O	2:B:94:ASN:OD1	2.28	0.51
3:C:48:TYR:HE1	3:C:118:GLN:HE21	1.58	0.51
14:N:29:ARG:NH1	14:N:29:ARG:HG2	2.24	0.51
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.25	0.51
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.41	0.51
1:A:961:U:O2'	1:A:962:C:H5'	2.10	0.51
1:A:992:U:H4'	1:A:993:G:O5'	2.10	0.51
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.51
11:K:99:GLN:CG	11:K:105:VAL:HG21	2.39	0.51
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.10	0.51
12:L:113:ARG:NH1	12:L:115:LYS:HB2	2.25	0.51
13:M:4:ILE:O	13:M:5:ALA:C	2.48	0.51
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.40	0.51
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.93	0.51
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.64	0.51
11:K:110:ASP:OD1	18:R:88:LYS:NZ	2.41	0.51
10:J:64:GLU:CG	14:N:59:ALA:HB2	2.36	0.51
20:T:70:SER:HA	20:T:73:HIS:CD2	2.46	0.51
1:A:1179:A:O2'	1:A:1180:A:H5'	2.10	0.51
1:A:908:A:H2'	1:A:909:A:H8	1.74	0.51
2:B:213:LEU:C	2:B:213:LEU:HD23	2.30	0.51
4:D:24:GLU:O	4:D:25:ARG:HB3	2.11	0.51
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.92	0.51
12:L:29:GLY:O	12:L:30:ALA:O	2.29	0.51
10:J:61:GLU:OE1	14:N:45:ARG:HD2	2.10	0.51
1:A:1208:C:H2'	1:A:1209:C:C6	2.46	0.51
1:A:1208:C:H2'	1:A:1209:C:H6	1.76	0.51
1:A:959:A:C2	1:A:1222:G:O4'	2.64	0.51
1:A:1238:A:N7	1:A:1303:C:H1'	2.25	0.51
1:A:1307:U:H5'	13:M:109:THR:HG21	1.93	0.51
1:A:532:A:O2'	1:A:533:A:P	2.69	0.51
1:A:976:G:C8	1:A:1358:U:O2	2.64	0.51
3:C:73:PRO:C	3:C:75:VAL:H	2.14	0.51
5:E:51:VAL:HB	5:E:52:PRO:CD	2.38	0.51
7:G:113:GLU:HG2	7:G:119:ARG:HG3	1.92	0.51
14:N:44:LEU:C	14:N:44:LEU:HD12	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:VAL:O	3:C:124:ILE:HG13	2.11	0.51
4:D:191:ARG:O	4:D:191:ARG:HD2	2.11	0.51
7:G:5:ARG:CZ	7:G:7:ALA:HA	2.40	0.51
1:A:689:C:P	11:K:46:GLY:HA3	2.51	0.51
12:L:92:ASP:O	12:L:94:PRO:HD3	2.11	0.51
16:P:8:ARG:HH11	16:P:8:ARG:HG2	1.76	0.51
2:B:48:MET:O	2:B:51:LEU:HB2	2.10	0.50
7:G:6:ARG:O	7:G:6:ARG:HG2	2.10	0.50
13:M:13:LYS:HA	13:M:44:ARG:NE	2.26	0.50
20:T:74:LYS:HZ3	20:T:74:LYS:CA	2.18	0.50
1:A:112:G:H5'	1:A:389:A:H4'	1.93	0.50
1:A:255:G:O6	1:A:266:G:O6	2.30	0.50
1:A:383:A:H2'	1:A:384:G:H5'	1.94	0.50
2:B:114:ARG:C	2:B:117:GLU:HB3	2.32	0.50
11:K:15:ALA:CA	11:K:77:MET:HA	2.41	0.50
17:Q:104:LYS:HD3	17:Q:105:ALA:N	2.26	0.50
1:A:521:G:OP1	12:L:73:GLU:O	2.29	0.50
3:C:154:SER:O	3:C:165:THR:HA	2.10	0.50
4:D:70:ILE:HG22	4:D:75:PHE:HB2	1.93	0.50
5:E:81:GLU:CG	5:E:88:LYS:HE2	2.42	0.50
7:G:15:ASP:HB3	7:G:20:ASP:H	1.77	0.50
10:J:42:THR:HG23	10:J:67:THR:O	2.10	0.50
18:R:59:SER:O	18:R:60:GLY:C	2.49	0.50
1:A:1223:C:P	19:S:78:ARG:NH1	2.85	0.50
1:A:1133:G:H2'	1:A:1134:G:C8	2.41	0.50
1:A:1143:G:H2'	1:A:1144:G:C8	2.46	0.50
1:A:1262:C:O2'	1:A:1263:C:H5'	2.11	0.50
1:A:26:A:H61	1:A:558:G:H1'	1.76	0.50
1:A:370:C:O2'	1:A:371:G:H5'	2.11	0.50
1:A:501:C:H2'	1:A:502:G:H8	1.75	0.50
1:A:538:G:H2'	1:A:539:A:C8	2.47	0.50
1:A:594:G:H2'	1:A:595:G:H5'	1.92	0.50
6:F:83:ASP:C	6:F:85:VAL:H	2.13	0.50
7:G:143:ARG:O	7:G:147:ALA:HB2	2.12	0.50
16:P:67:THR:CG2	16:P:68:ASP:N	2.74	0.50
17:Q:68:ARG:N	17:Q:70:ARG:HH12	2.08	0.50
1:A:1327:C:OP1	21:U:20:LYS:HB3	2.12	0.50
1:A:1168:A:C6	1:A:1169:A:C6	3.00	0.50
2:B:46:LYS:CA	2:B:46:LYS:HE3	2.37	0.50
5:E:11:ILE:CG2	5:E:105:VAL:HG22	2.41	0.50
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.29	0.50
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.42	0.50
1:A:1346:A:C4	7:G:10:ARG:NH2	2.79	0.50
1:A:384:G:H2'	1:A:385:C:C6	2.47	0.50
1:A:644:G:O2'	1:A:645:C:H5'	2.11	0.50
7:G:52:GLU:O	7:G:53:LYS:HG2	2.12	0.50
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.92	0.50
10:J:39:PRO:HA	10:J:70:ARG:HH11	1.77	0.50
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.74	0.50
10:J:71:LEU:O	10:J:72:VAL:CB	2.59	0.50
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.92	0.50
1:A:1149:C:H2'	1:A:1150:U:H6	1.75	0.50
1:A:1288:A:H1'	1:A:1352:C:O2'	2.11	0.50
1:A:1532:U:H2'	1:A:1533:C:H5''	1.87	0.50
1:A:192:U:O4'	20:T:103:GLY:HA2	2.12	0.50
4:D:8:VAL:HB	4:D:21:LEU:CD1	2.41	0.50
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.93	0.50
12:L:113:ARG:HH12	12:L:116:SER:H	1.58	0.50
13:M:19:LEU:HD11	13:M:34:LEU:HD21	1.94	0.50
13:M:73:GLU:O	13:M:76:ALA:HB3	2.12	0.50
1:A:656:C:O2'	15:O:28:GLN:OE1	2.29	0.50
16:P:42:ARG:O	16:P:43:LYS:C	2.50	0.50
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.12	0.50
1:A:1182:G:O2'	1:A:1183:A:P	2.70	0.50
1:A:397:A:N3	1:A:397:A:H3'	2.26	0.50
1:A:818:G:C3'	1:A:819:A:C5'	2.90	0.50
6:F:40:VAL:HG22	6:F:41:GLU:N	2.27	0.50
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.77	0.50
20:T:14:LYS:O	20:T:18:GLN:HG3	2.11	0.50
5:E:76:ILE:HG13	5:E:142:LEU:HD11	1.92	0.50
1:A:1060:C:H5''	10:J:51:ARG:HB3	1.94	0.49
1:A:900:A:H2'	1:A:901:A:C8	2.47	0.49
2:B:87:ARG:NH1	2:B:233:SER:HA	2.26	0.49
6:F:15:ASP:OD1	6:F:17:SER:HB2	2.12	0.49
1:A:939:G:H5''	7:G:102:ARG:NH2	2.26	0.49
9:I:83:ARG:O	9:I:86:VAL:HB	2.11	0.49
13:M:37:THR:CG2	13:M:55:ARG:HD2	2.38	0.49
10:J:63:PHE:CE1	14:N:45:ARG:HG3	2.46	0.49
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.12	0.49
18:R:86:VAL:O	18:R:87:ARG:CB	2.60	0.49
1:A:580:U:H2'	1:A:581:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:U:O2'	1:A:660:G:H5'	2.12	0.49
1:A:911:U:H2'	1:A:912:C:C6	2.47	0.49
2:B:83:MET:O	2:B:86:GLU:N	2.45	0.49
3:C:63:ASN:HA	3:C:99:VAL:HG12	1.94	0.49
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.94	0.49
20:T:8:ARG:N	20:T:8:ARG:HD2	2.26	0.49
1:A:1006:C:H2'	1:A:1007:C:C6	2.48	0.49
1:A:1230:C:O2'	1:A:1231:G:H5'	2.13	0.49
1:A:1359:C:OP2	14:N:35:ARG:HD2	2.13	0.49
1:A:1509:C:H2'	1:A:1510:U:O4'	2.12	0.49
1:A:945:G:C2	1:A:946:A:C8	3.00	0.49
4:D:61:LYS:NZ	4:D:62:GLN:NE2	2.60	0.49
6:F:19:LEU:O	6:F:23:LYS:HG3	2.11	0.49
8:H:112:LEU:CD2	8:H:112:LEU:N	2.75	0.49
10:J:6:ILE:HG23	10:J:98:ILE:CD1	2.42	0.49
1:A:1525:G:P	11:K:120:ARG:HH22	2.35	0.49
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.11	0.49
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.93	0.49
19:S:43:GLU:CD	19:S:43:GLU:H	2.15	0.49
1:A:1004:A:P	1:A:1025:U:H3	2.35	0.49
1:A:1179:A:C6	1:A:1180:A:C2	3.00	0.49
1:A:1296:C:H4'	1:A:1302:U:C5	2.46	0.49
1:A:390:C:O3'	16:P:28:ARG:NH2	2.45	0.49
1:A:426:G:O2'	1:A:427:U:H5'	2.13	0.49
2:B:162:ILE:HG13	2:B:162:ILE:O	2.12	0.49
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.94	0.49
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.43	0.49
5:E:20:GLN:NE2	5:E:21:ALA:O	2.45	0.49
7:G:12:LEU:H	7:G:12:LEU:HD12	1.78	0.49
13:M:37:THR:O	13:M:39:ILE:HG13	2.12	0.49
13:M:40:ASN:HD22	13:M:40:ASN:C	2.15	0.49
15:O:87:ILE:O	15:O:88:ARG:HB2	2.12	0.49
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.46	0.49
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.44	0.49
1:A:528:C:H5'	1:A:535:A:C6	2.48	0.49
1:A:882:C:O2'	1:A:883:C:H5'	2.11	0.49
2:B:25:ASN:C	2:B:25:ASN:HD22	2.15	0.49
2:B:55:PHE:HD2	2:B:221:LEU:HG	1.77	0.49
3:C:206:GLU:O	3:C:208:ILE:N	2.44	0.49
6:F:100:ASN:HD22	18:R:23:LYS:CG	2.24	0.49
6:F:19:LEU:O	6:F:19:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:PRO:O	10:J:40:LEU:CB	2.60	0.49
10:J:94:VAL:CG1	10:J:95:GLU:N	2.75	0.49
12:L:40:VAL:O	12:L:40:VAL:HG12	2.12	0.49
13:M:4:ILE:O	13:M:5:ALA:O	2.29	0.49
20:T:99:LEU:C	20:T:101:GLY:H	2.16	0.49
1:A:48:C:H5''	1:A:365:U:O4	2.13	0.49
3:C:34:LEU:HD23	3:C:34:LEU:C	2.32	0.49
7:G:120:ILE:N	7:G:120:ILE:HD12	2.28	0.49
1:A:1006:C:H2'	1:A:1007:C:H6	1.77	0.49
2:B:111:ARG:CB	2:B:149:LEU:HD11	2.38	0.49
4:D:150:GLU:N	4:D:150:GLU:CD	2.61	0.49
14:N:4:LYS:C	14:N:6:LEU:H	2.15	0.49
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.90	0.49
1:A:1192:C:O3'	1:A:1193:G:OP2	0.71	0.49
1:A:1499:A:H1'	1:A:1520:G:H5'	1.95	0.49
3:C:11:ARG:NH1	3:C:177:THR:O	2.46	0.49
4:D:19:LEU:HD22	4:D:67:ILE:CG1	2.43	0.49
8:H:54:ASP:CG	8:H:55:GLY:H	2.16	0.49
16:P:11:SER:OG	16:P:14:ASN:HB3	2.13	0.49
1:A:1127:G:N2	1:A:1146:A:N6	2.51	0.49
1:A:1443:G:H5''	1:A:1443:G:N3	2.28	0.49
1:A:513:C:H2'	1:A:514:C:C6	2.48	0.49
2:B:194:PRO:O	2:B:197:VAL:N	2.35	0.49
2:B:96:ARG:O	2:B:98:LEU:HD23	2.13	0.49
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.43	0.49
5:E:75:THR:HG23	5:E:76:ILE:O	2.12	0.49
8:H:104:ARG:O	8:H:105:ARG:C	2.52	0.49
13:M:81:LEU:HD13	13:M:88:ARG:HD3	1.93	0.49
15:O:39:LEU:O	15:O:39:LEU:HD23	2.13	0.49
1:A:1314:C:OP2	19:S:6:LYS:HG3	2.12	0.49
1:A:1052:U:H2'	1:A:1055:A:OP1	2.13	0.49
1:A:1350:A:C6	1:A:1351:U:N3	2.81	0.49
1:A:1474:G:O2'	1:A:1475:G:H5'	2.13	0.49
5:E:144:THR:CG2	5:E:145:LYS:N	2.75	0.49
7:G:16:LEU:H	7:G:16:LEU:HD22	1.78	0.49
14:N:25:VAL:HG12	14:N:38:GLY:O	2.13	0.49
17:Q:67:LYS:C	17:Q:70:ARG:NH1	2.66	0.49
1:A:157:G:O2'	1:A:158:G:H5'	2.13	0.48
1:A:432:A:H2'	1:A:433:C:O4'	2.13	0.48
1:A:438:G:C4'	1:A:439:A:OP1	2.59	0.48
2:B:132:LYS:HD2	2:B:135:GLN:CB	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLU:HA	2:B:48:MET:SD	2.52	0.48
3:C:128:PHE:CD2	3:C:129:ALA:N	2.79	0.48
3:C:155:GLY:O	3:C:196:LEU:HD13	2.13	0.48
4:D:24:GLU:C	4:D:26:CYS:H	2.16	0.48
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.48	0.48
8:H:56:LYS:N	8:H:56:LYS:HD2	2.28	0.48
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.48	0.48
11:K:117:ASN:HD22	11:K:117:ASN:N	2.11	0.48
1:A:706:A:C4'	11:K:29:ILE:HD11	2.43	0.48
1:A:1347:G:O2'	1:A:1348:U:C6	2.66	0.48
1:A:457:C:H2'	1:A:458:C:C6	2.47	0.48
1:A:56:U:H2'	1:A:57:G:C8	2.48	0.48
1:A:792:A:C4	1:A:794:A:C6	3.01	0.48
3:C:14:ILE:O	3:C:15:THR:C	2.50	0.48
4:D:145:GLU:OE2	4:D:182:LYS:HD2	2.13	0.48
4:D:50:ARG:HD2	4:D:51:PRO:O	2.13	0.48
8:H:103:VAL:HG21	8:H:109:ILE:C	2.33	0.48
8:H:59:LEU:O	8:H:61:VAL:HG23	2.13	0.48
10:J:30:SER:HB3	10:J:84:GLN:NE2	2.26	0.48
20:T:99:LEU:O	20:T:101:GLY:N	2.47	0.48
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.25	0.48
3:C:155:GLY:CA	3:C:164:ARG:H	2.26	0.48
4:D:28:SER:O	4:D:30:LYS:N	2.46	0.48
6:F:23:LYS:O	6:F:27:GLN:HG2	2.12	0.48
6:F:45:LEU:HA	6:F:59:TYR:HA	1.95	0.48
7:G:112:PRO:O	7:G:113:GLU:C	2.50	0.48
9:I:37:PHE:O	9:I:38:GLN:O	2.32	0.48
1:A:706:A:O4'	11:K:29:ILE:HD11	2.13	0.48
16:P:45:THR:HB	16:P:46:PRO:HD2	1.94	0.48
1:A:474:G:H5''	16:P:81:ARG:NH1	2.28	0.48
18:R:25:THR:O	18:R:26:LEU:HB2	2.14	0.48
1:A:1249:C:H4'	9:I:36:TYR:OH	2.13	0.48
1:A:1425:U:H3	1:A:1475:G:H1	1.60	0.48
2:B:170:GLU:OE2	2:B:170:GLU:HA	2.13	0.48
2:B:74:LYS:HD3	2:B:205:ASP:O	2.12	0.48
3:C:3:ASN:O	3:C:4:LYS:CB	2.61	0.48
4:D:57:ARG:NH2	5:E:107:ARG:HE	2.11	0.48
6:F:27:GLN:C	6:F:29:ALA:H	2.16	0.48
11:K:124:LYS:HZ2	11:K:125:PHE:HZ	1.58	0.48
19:S:15:LEU:HD12	19:S:16:LEU:N	2.28	0.48
19:S:20:LEU:HD12	19:S:21:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:37:SER:O	20:T:41:VAL:HG23	2.13	0.48
1:A:1125:U:H5'	1:A:1126:U:C5	2.47	0.48
1:A:1232:U:OP1	9:I:124:GLN:NE2	2.46	0.48
1:A:1284:C:H3'	1:A:1285:A:H8	1.77	0.48
1:A:135:C:O2	16:P:1:MET:N	2.42	0.48
1:A:814:A:H2'	1:A:816:A:C5'	2.43	0.48
2:B:60:ASP:OD2	2:B:64:ARG:HD2	2.13	0.48
3:C:148:GLY:HA3	3:C:172:ARG:O	2.13	0.48
3:C:11:ARG:O	3:C:14:ILE:N	2.47	0.48
7:G:141:VAL:O	7:G:144:MET:HB2	2.13	0.48
9:I:114:TYR:C	9:I:116:LYS:H	2.17	0.48
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.46	0.48
12:L:111:LYS:HA	12:L:111:LYS:CE	2.37	0.48
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.48	0.48
17:Q:67:LYS:HG2	17:Q:68:ARG:N	2.28	0.48
1:A:1109:C:OP2	3:C:176:HIS:CD2	2.66	0.48
1:A:1124:G:H2'	1:A:1145:C:H5	1.79	0.48
1:A:1194:U:O2'	1:A:1195:C:H5'	2.13	0.48
1:A:1277:C:H2'	1:A:1278:U:H5'	1.94	0.48
1:A:477:G:O2'	1:A:478:A:H5'	2.13	0.48
2:B:122:PHE:O	2:B:123:ALA:HB2	2.13	0.48
2:B:159:PRO:HB2	2:B:161:ALA:O	2.13	0.48
3:C:47:LEU:N	3:C:47:LEU:HD12	2.29	0.48
6:F:8:ILE:HG22	6:F:10:LEU:CD1	2.44	0.48
10:J:16:LEU:HD21	10:J:94:VAL:HG13	1.96	0.48
12:L:18:VAL:O	12:L:18:VAL:HG23	2.13	0.48
13:M:94:ARG:HD2	13:M:94:ARG:N	2.29	0.48
19:S:15:LEU:HD12	19:S:16:LEU:H	1.78	0.48
1:A:1156:G:H21	1:A:1179:A:H61	1.61	0.48
1:A:1347:G:N7	9:I:107:ARG:NH1	2.60	0.48
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.95	0.48
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.95	0.48
11:K:48:ILE:HG22	11:K:49:GLY:H	1.79	0.48
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.48
1:A:1505:G:H3'	1:A:1505:G:C8	2.49	0.48
3:C:70:VAL:C	3:C:106:VAL:HG23	2.34	0.48
5:E:144:THR:H	5:E:147:ASP:HB2	1.79	0.48
9:I:55:ALA:O	9:I:56:LEU:CB	2.61	0.48
12:L:27:LEU:C	12:L:29:GLY:N	2.66	0.48
13:M:96:LEU:O	13:M:97:PRO:C	2.52	0.48
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:27:GLU:CD	19:S:27:GLU:N	2.67	0.48
1:A:1278:U:H5''	1:A:1279:A:O4'	2.14	0.48
1:A:627:G:H2'	1:A:628:G:C8	2.49	0.48
1:A:839:U:C2'	1:A:839:U:O2	2.62	0.48
1:A:838:G:N2	1:A:849:C:C2	2.81	0.48
1:A:945:G:H2'	1:A:945:G:N3	2.29	0.48
5:E:81:GLU:HG2	5:E:88:LYS:HE2	1.96	0.48
7:G:136:LYS:HE2	7:G:136:LYS:CA	2.38	0.48
10:J:3:LYS:O	10:J:101:VAL:N	2.47	0.48
1:A:1241:G:H2'	1:A:1242:C:H6	1.77	0.48
1:A:1370:G:C2	1:A:1371:G:C8	3.02	0.48
1:A:1465:C:H2'	1:A:1466:C:O4'	2.14	0.48
1:A:930:C:C2'	1:A:931:C:H5'	2.44	0.48
11:K:101:SER:O	11:K:103:LEU:N	2.40	0.48
11:K:14:VAL:O	11:K:15:ALA:HB3	2.14	0.48
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.95	0.48
13:M:102:ARG:NH1	13:M:102:ARG:HB2	2.29	0.48
13:M:14:ARG:N	13:M:44:ARG:HD2	2.28	0.48
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.44	0.47
1:A:1054:C:O2'	1:A:1055:A:H5''	2.13	0.47
1:A:1178:G:N2	1:A:1180:A:H3'	2.29	0.47
1:A:411:A:O2'	1:A:413:G:H5'	2.14	0.47
4:D:92:VAL:O	4:D:96:LEU:HD13	2.14	0.47
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.37	0.47
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.97	0.47
14:N:4:LYS:C	14:N:6:LEU:N	2.67	0.47
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.95	0.47
1:A:1156:G:H3'	1:A:1157:A:OP2	2.12	0.47
1:A:1191:A:HO3'	1:A:1192:C:C5'	2.15	0.47
1:A:1402:C:H2'	1:A:1403:C:O4'	2.14	0.47
1:A:404:U:H2'	1:A:405:U:C6	2.49	0.47
1:A:457:C:O2'	1:A:458:C:H5'	2.14	0.47
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.49	0.47
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.14	0.47
14:N:8:GLU:O	14:N:9:LYS:C	2.52	0.47
1:A:101:A:O2'	1:A:102:G:H5'	2.14	0.47
1:A:200:G:H2'	1:A:201:C:O4'	2.15	0.47
1:A:640:A:C2'	1:A:641:U:H5'	2.44	0.47
1:A:861:G:O2'	1:A:862:C:H5'	2.14	0.47
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.96	0.47
6:F:10:LEU:HD12	6:F:10:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:MET:CE	6:F:75:LEU:HD12	2.43	0.47
6:F:86:ARG:O	6:F:87:ARG:HG2	2.13	0.47
1:A:1091:U:O2	1:A:1093:A:H8	1.98	0.47
1:A:1161:C:H2'	1:A:1162:C:H6	1.79	0.47
1:A:129(A):G:O2'	1:A:130:A:OP2	2.33	0.47
1:A:179:A:O2'	1:A:180:U:H5'	2.15	0.47
2:B:118:LEU:HB2	2:B:142:LEU:CD2	2.37	0.47
2:B:96:ARG:HG3	2:B:96:ARG:O	2.13	0.47
3:C:25:GLY:O	3:C:27:LYS:N	2.47	0.47
4:D:166:LYS:HG3	4:D:178:VAL:HG11	1.96	0.47
5:E:90:VAL:O	5:E:120:THR:HA	2.13	0.47
1:A:1128:C:H4'	9:I:16:ARG:NH1	2.29	0.47
10:J:12:ASP:HB3	10:J:15:THR:HB	1.96	0.47
11:K:27:ASN:OD1	11:K:28:THR:N	2.47	0.47
1:A:1066:C:C2'	1:A:1067:A:H5'	2.45	0.47
1:A:1128:C:H4'	9:I:16:ARG:HH12	1.78	0.47
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.47
1:A:757:U:H2'	1:A:758:G:O4'	2.14	0.47
1:A:953:G:H1'	13:M:125:ARG:HA	1.96	0.47
2:B:73:THR:HG23	2:B:95:GLN:O	2.15	0.47
3:C:155:GLY:O	3:C:156:ARG:CB	2.61	0.47
1:A:1112:C:O2	3:C:179:ARG:HG2	2.14	0.47
4:D:31:CYS:C	4:D:33:MET:H	2.18	0.47
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.32	0.47
11:K:110:ASP:HB2	18:R:88:LYS:CD	2.43	0.47
15:O:5:LYS:HD2	15:O:5:LYS:H	1.80	0.47
18:R:37:VAL:O	18:R:41:LYS:HB2	2.14	0.47
1:A:1339:A:H2'	1:A:1340:A:O4'	2.13	0.47
1:A:175:C:H2'	1:A:176:C:H6	1.80	0.47
1:A:487:A:H2'	1:A:488:C:O4'	2.14	0.47
1:A:490:G:H2'	1:A:491:G:H8	1.80	0.47
1:A:522:C:OP2	12:L:69:TYR:OH	2.24	0.47
1:A:730:G:N2	1:A:765:G:H5''	2.29	0.47
3:C:127:ARG:HG2	3:C:127:ARG:NH1	2.29	0.47
1:A:1112:C:N3	3:C:178:LEU:HD23	2.29	0.47
4:D:19:LEU:HD22	4:D:67:ILE:HG12	1.96	0.47
5:E:12:LEU:C	5:E:12:LEU:HD22	2.35	0.47
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.45	0.47
7:G:51:GLN:O	7:G:52:GLU:C	2.53	0.47
8:H:53:VAL:O	8:H:54:ASP:HB3	2.15	0.47
12:L:57:LYS:HD3	12:L:67:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:91:ARG:CB	13:M:98:VAL:HG22	2.44	0.47
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.47
1:A:1474:G:H2'	1:A:1475:G:H8	1.80	0.47
1:A:459:G:C6	1:A:461:C:H5''	2.49	0.47
3:C:27:LYS:H	3:C:27:LYS:HD3	1.80	0.47
3:C:87:LEU:C	3:C:89:GLU:H	2.18	0.47
7:G:75:VAL:HG11	7:G:144:MET:CE	2.44	0.47
9:I:126:SER:O	9:I:127:LYS:CB	2.62	0.47
10:J:6:ILE:HD12	10:J:72:VAL:CG1	2.44	0.47
13:M:65:LYS:CG	13:M:69:GLU:HB3	2.45	0.47
13:M:8:GLU:C	13:M:9:ILE:HD12	2.35	0.47
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.95	0.47
19:S:80:TYR:OH	19:S:81:ARG:HD3	2.14	0.47
1:A:1201:A:O2'	1:A:1202:G:OP2	2.29	0.47
1:A:1234:C:O2'	1:A:1235:U:H5'	2.15	0.47
1:A:1305:G:H22	1:A:1331:G:H2'	1.77	0.47
1:A:783:C:O2'	1:A:784:C:H5'	2.14	0.47
1:A:989:C:O2'	1:A:990:C:H5'	2.14	0.47
3:C:123:GLN:O	3:C:128:PHE:HB2	2.15	0.47
3:C:70:VAL:HG12	3:C:71:ALA:H	1.76	0.47
4:D:153:ARG:HG2	4:D:181:MET:SD	2.55	0.47
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.49	0.47
13:M:4:ILE:CG2	13:M:5:ALA:N	2.65	0.47
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.27	0.47
1:A:325:A:OP2	20:T:70:SER:HB3	2.15	0.47
1:A:1002:G:H2'	1:A:1003:G:C8	2.50	0.47
1:A:1065:U:H1'	1:A:1066:C:OP2	2.15	0.47
1:A:1175:G:O2'	1:A:1176:A:O5'	2.32	0.47
1:A:1422:G:O2'	1:A:1423:G:H5'	2.14	0.47
1:A:1451:A:O2'	1:A:1452:C:OP1	2.31	0.47
1:A:147:G:O2'	1:A:148:G:H5'	2.15	0.47
1:A:409:G:H1	1:A:433:C:N4	2.11	0.47
3:C:23:TYR:C	3:C:23:TYR:CD2	2.88	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.50	0.47
11:K:11:LYS:HD2	11:K:11:LYS:O	2.14	0.47
17:Q:78:GLU:HG3	17:Q:78:GLU:O	2.14	0.47
20:T:10:LEU:HG	20:T:12:ALA:CB	2.44	0.47
20:T:74:LYS:NZ	20:T:74:LYS:HA	2.24	0.47
1:A:1399:C:C2	1:A:1502:A:N6	2.82	0.47
1:A:417:C:H2'	1:A:418:C:H6	1.79	0.47
1:A:421:U:O2	1:A:421:U:O4'	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:C8	2.50	0.47
1:A:620:C:H2'	1:A:621:A:O4'	2.15	0.47
1:A:818:G:H3'	1:A:819:A:H5''	1.97	0.47
3:C:195:VAL:O	3:C:196:LEU:HD22	2.15	0.47
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.50	0.47
5:E:20:GLN:O	5:E:21:ALA:C	2.53	0.47
8:H:102:ARG:NE	8:H:102:ARG:H	2.13	0.47
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.45	0.47
12:L:55:VAL:CG1	12:L:56:ALA:H	2.22	0.47
14:N:9:LYS:HD2	14:N:9:LYS:O	2.15	0.47
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.97	0.47
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.14	0.47
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.15	0.47
17:Q:6:LEU:O	17:Q:59:ILE:N	2.48	0.47
1:A:1003(A):G:H2'	1:A:1004:A:O4'	2.14	0.47
2:B:115:LEU:HD21	2:B:153:ARG:HE	1.79	0.47
2:B:62:ALA:C	2:B:64:ARG:H	2.18	0.47
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.96	0.47
4:D:31:CYS:O	4:D:33:MET:N	2.43	0.47
7:G:49:ILE:HG22	7:G:49:ILE:O	2.15	0.47
8:H:46:LYS:HG3	8:H:64:LYS:HB2	1.96	0.47
12:L:26:ALA:O	12:L:27:LEU:O	2.33	0.47
13:M:108:ARG:HH21	13:M:111:LYS:HB2	1.80	0.47
15:O:36:ILE:CG1	15:O:59:MET:HE3	2.43	0.47
1:A:1117:G:H5'	1:A:1117:G:H8	1.80	0.46
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.46
1:A:1256:A:H5'	1:A:1258:G:C1'	2.44	0.46
1:A:1355:G:O2'	1:A:1356:G:H5'	2.14	0.46
1:A:1394:A:C5	1:A:1501:C:H4'	2.50	0.46
1:A:414:A:H2'	1:A:415:A:H8	1.80	0.46
1:A:915:A:C2'	1:A:916:G:H5'	2.45	0.46
2:B:102:LEU:HD12	2:B:102:LEU:N	2.30	0.46
9:I:32:ASP:O	9:I:35:GLU:HB3	2.15	0.46
13:M:21:TYR:N	13:M:21:TYR:CD1	2.82	0.46
1:A:442:C:H42	1:A:492:G:H1	1.62	0.46
1:A:960:U:O2	1:A:960:U:H2'	2.14	0.46
2:B:69:LEU:CD1	2:B:155:LEU:HD11	2.45	0.46
2:B:69:LEU:HD23	2:B:70:PHE:N	2.31	0.46
3:C:36:ASP:O	3:C:39:ILE:HB	2.15	0.46
3:C:6:HIS:HD2	3:C:8:ILE:N	2.00	0.46
3:C:84:ILE:HD11	3:C:88:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:ALA:HB2	18:R:28:GLU:OE1	2.15	0.46
10:J:96:ILE:HG22	10:J:98:ILE:HG13	1.97	0.46
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.50	0.46
1:A:950:U:H5	13:M:102:ARG:HE	1.62	0.46
14:N:18:VAL:HG23	14:N:19:ARG:N	2.30	0.46
1:A:1129:C:O2'	1:A:1130:A:P	2.74	0.46
1:A:1461:G:O2'	1:A:1462:G:H5'	2.15	0.46
1:A:411:A:C2'	1:A:412:A:H5'	2.45	0.46
1:A:824:C:H2'	1:A:825:G:C8	2.50	0.46
5:E:89:ILE:HD13	5:E:90:VAL:H	1.80	0.46
7:G:85:TYR:O	7:G:87:VAL:HG23	2.14	0.46
7:G:8:GLU:OE1	7:G:8:GLU:O	2.33	0.46
10:J:80:LYS:HZ3	10:J:80:LYS:HB2	1.79	0.46
13:M:106:ASN:O	13:M:107:ALA:HB3	2.16	0.46
16:P:3:LYS:O	16:P:21:VAL:HA	2.16	0.46
1:A:1160:G:N2	1:A:1161:C:H1'	2.31	0.46
1:A:1238:A:H5'	1:A:1336:C:H41	1.80	0.46
1:A:1305:G:OP2	1:A:1305:G:C8	2.69	0.46
1:A:1406:U:O2'	1:A:1407:C:H5'	2.16	0.46
1:A:513:C:O2'	1:A:514:C:H5'	2.15	0.46
1:A:778:G:O2'	1:A:779:C:H5'	2.15	0.46
2:B:100:GLY:O	2:B:104:ASN:N	2.43	0.46
2:B:61:LEU:HD12	2:B:68:ILE:HD11	1.96	0.46
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.45	0.46
5:E:107:ARG:HH11	5:E:107:ARG:CB	2.26	0.46
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.48	0.46
1:A:448:A:H2'	1:A:449:C:C6	2.51	0.46
1:A:604:G:O2'	1:A:605:U:H5'	2.16	0.46
2:B:102:LEU:CD1	2:B:102:LEU:N	2.79	0.46
2:B:137:ARG:HB3	2:B:137:ARG:HH11	1.80	0.46
2:B:50:GLU:HB3	2:B:200:ILE:O	2.15	0.46
6:F:25:ILE:CD1	6:F:82:ARG:HD2	2.46	0.46
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.81	0.46
13:M:37:THR:CG2	13:M:37:THR:O	2.62	0.46
1:A:1019:C:O2'	1:A:1020:U:H5'	2.16	0.46
1:A:1095:U:H2'	1:A:1096:C:H6	1.72	0.46
1:A:1343:G:H2'	1:A:1344:C:H6	1.81	0.46
1:A:556:C:C2'	1:A:557:G:H5'	2.45	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.14	0.46
1:A:947:G:H2'	1:A:948:C:O4'	2.16	0.46
2:B:128:GLU:O	2:B:129:GLU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:ASN:ND2	3:C:111:LEU:HG	2.31	0.46
4:D:57:ARG:NE	4:D:205:GLU:OE2	2.48	0.46
5:E:147:ASP:O	5:E:151:LEU:HG	2.16	0.46
8:H:101:PRO:HG2	8:H:133:LEU:HD11	1.97	0.46
13:M:13:LYS:O	13:M:14:ARG:C	2.53	0.46
17:Q:45:HIS:CD2	17:Q:47:PRO:HD3	2.51	0.46
1:A:1157:A:C6	1:A:1180:A:N6	2.84	0.46
1:A:1229:A:H2'	1:A:1230:C:H6	1.81	0.46
1:A:954:G:H2'	1:A:955:U:H6	1.81	0.46
2:B:59:GLU:O	2:B:63:MET:HG2	2.16	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
3:C:95:THR:O	3:C:95:THR:OG1	2.33	0.46
1:A:408:A:H4'	4:D:112:VAL:HG11	1.97	0.46
4:D:90:GLY:N	4:D:204:ILE:HD11	2.31	0.46
5:E:143:ARG:HA	5:E:143:ARG:HD3	1.55	0.46
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.97	0.46
12:L:50:SER:O	12:L:51:ALA:HB2	2.15	0.46
18:R:20:ALA:O	18:R:21:LYS:C	2.53	0.46
20:T:53:LEU:HD13	20:T:102:GLY:H	1.81	0.46
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.48	0.46
1:A:1124:G:H2'	1:A:1145:C:C5	2.51	0.46
1:A:1154:G:O2'	1:A:1155:G:H5'	2.16	0.46
1:A:1256:A:H5'	1:A:1258:G:H1'	1.98	0.46
1:A:1299:A:C5	1:A:1301:U:O2	2.69	0.46
1:A:1354:C:H2'	1:A:1355:G:H8	1.79	0.46
1:A:180:U:H2'	1:A:181:G:H5'	1.96	0.46
1:A:509:A:H5''	4:D:55:ALA:HB2	1.98	0.46
5:E:18:ARG:NH1	5:E:25:ARG:HB2	2.31	0.46
8:H:6:ILE:O	8:H:10:LEU:HG	2.14	0.46
12:L:86:ARG:HG3	12:L:86:ARG:HH11	1.80	0.46
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.46	0.46
1:A:1024:G:H2'	1:A:1025:U:H5''	1.97	0.46
1:A:1130:A:OP2	1:A:1130:A:H3'	2.16	0.46
1:A:1169:A:H2'	1:A:1171:G:O4'	2.16	0.46
1:A:1428:A:H2'	1:A:1429:C:C6	2.50	0.46
1:A:497:A:H1'	1:A:498:U:OP1	2.16	0.46
3:C:11:ARG:O	3:C:12:LEU:C	2.54	0.46
7:G:46:ALA:O	7:G:50:ILE:HG12	2.16	0.46
10:J:25:GLU:C	10:J:27:ALA:H	2.19	0.46
13:M:60:VAL:CG1	13:M:66:LEU:HD11	2.46	0.46
16:P:20:VAL:CG1	16:P:21:VAL:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:A:H5'	9:I:68:GLY:O	2.16	0.46
1:A:979:C:H2'	1:A:980:C:H5'	1.97	0.46
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.98	0.46
5:E:91:LEU:HD23	5:E:120:THR:HG22	1.98	0.46
7:G:18:TYR:OH	7:G:58:PRO:CG	2.64	0.46
9:I:108:VAL:CG1	9:I:109:VAL:N	2.78	0.46
9:I:118:LYS:O	9:I:119:ALA:CB	2.58	0.46
13:M:13:LYS:HD3	13:M:17:VAL:CG1	2.45	0.46
19:S:36:ARG:NH2	19:S:75:ALA:HB3	2.31	0.46
1:A:114:U:O2'	1:A:115:G:H5'	2.16	0.45
1:A:1279:A:H61	3:C:26:LYS:NZ	2.14	0.45
1:A:1289:A:H2'	1:A:1290:G:H5'	1.98	0.45
1:A:131:C:H2'	1:A:132:C:H6	1.81	0.45
1:A:285:G:O2'	1:A:286:G:H5'	2.15	0.45
2:B:97:TRP:HZ3	2:B:100:GLY:H	1.64	0.45
3:C:11:ARG:O	3:C:13:GLY:N	2.49	0.45
3:C:95:THR:O	3:C:97:LYS:N	2.49	0.45
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.81	0.45
7:G:77:SER:O	7:G:78:ARG:HB2	2.16	0.45
12:L:113:ARG:NH1	12:L:116:SER:N	2.63	0.45
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.98	0.45
21:U:6:ARG:HD2	21:U:15:ARG:HH12	1.81	0.45
1:A:1054:C:H42	23:Y:34:TM2:C1'	2.28	0.45
1:A:1152:A:H2'	1:A:1153:C:C6	2.50	0.45
1:A:1191:A:H3'	1:A:1192:C:P	2.45	0.45
1:A:149:A:H2'	1:A:150:C:C6	2.51	0.45
1:A:1533:C:H2'	1:A:1534:A:C5'	2.42	0.45
1:A:393:A:O2'	1:A:394:G:H5'	2.16	0.45
1:A:721:G:H4'	1:A:722:A:O4'	2.17	0.45
3:C:107:GLN:O	3:C:108:ASN:CB	2.64	0.45
7:G:51:GLN:HB2	7:G:52:GLU:OE1	2.16	0.45
13:M:44:ARG:O	13:M:45:VAL:C	2.53	0.45
18:R:16:PRO:O	18:R:54:ARG:NH1	2.49	0.45
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.45
1:A:928:G:O2'	1:A:1533:C:OP1	2.34	0.45
1:A:633:G:H2'	1:A:634:C:C6	2.52	0.45
2:B:80:ILE:O	2:B:84:GLU:HB2	2.16	0.45
5:E:11:ILE:HD11	5:E:33:VAL:CG2	2.46	0.45
11:K:13:GLN:HA	11:K:75:TYR:O	2.16	0.45
13:M:60:VAL:HG12	13:M:66:LEU:HD11	1.99	0.45
13:M:65:LYS:HG3	13:M:69:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:ILE:HG12	15:O:38:ARG:NH1	2.31	0.45
1:A:377:G:OP1	16:P:3:LYS:HD3	2.17	0.45
19:S:12:ASP:O	19:S:15:LEU:HD12	2.16	0.45
1:A:1141:C:O2'	1:A:1142:G:H5'	2.16	0.45
1:A:1347:G:C8	9:I:107:ARG:NH1	2.84	0.45
1:A:1347:G:O2'	1:A:1348:U:H6	1.99	0.45
1:A:151:A:H2'	1:A:152:A:O4'	2.16	0.45
1:A:184:G:H2'	1:A:185:A:H8	1.80	0.45
1:A:280:C:O2	17:Q:38:ARG:HG3	2.17	0.45
1:A:781:A:C5	1:A:802:A:C2	3.05	0.45
2:B:10:LEU:C	2:B:12:GLU:H	2.19	0.45
3:C:44:GLU:HA	3:C:52:LEU:HD11	1.97	0.45
3:C:73:PRO:O	3:C:75:VAL:N	2.49	0.45
7:G:62:PHE:HA	7:G:124:LEU:HD12	1.98	0.45
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.34	0.45
9:I:53:VAL:HG13	9:I:96:LEU:HD11	1.99	0.45
1:A:1080:A:H4'	5:E:16:THR:HG21	1.99	0.45
1:A:1207:G:H2'	1:A:1208:C:H6	1.82	0.45
2:B:118:LEU:C	2:B:120:ALA:N	2.69	0.45
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.98	0.45
7:G:82:GLY:O	7:G:83:ALA:HB2	2.16	0.45
9:I:12:GLU:O	9:I:12:GLU:HG2	2.16	0.45
13:M:11:ARG:CD	13:M:12:ASN:H	2.28	0.45
1:A:742:G:P	15:O:35:ARG:HH22	2.39	0.45
1:A:163:C:H2'	1:A:164:U:H6	1.80	0.45
1:A:245:C:O2	1:A:283:C:N3	2.49	0.45
1:A:922:G:H4'	5:E:20:GLN:HA	1.98	0.45
1:A:961:U:H2'	1:A:962:C:C5'	2.47	0.45
4:D:128:VAL:O	4:D:129:ASN:HB2	2.17	0.45
9:I:102:LEU:HD12	9:I:102:LEU:N	2.30	0.45
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.98	0.45
10:J:46:ARG:HH12	10:J:64:GLU:HB3	1.81	0.45
11:K:78:GLN:O	11:K:103:LEU:HD23	2.16	0.45
1:A:1229:A:H2'	1:A:1230:C:C6	2.52	0.45
2:B:178:ARG:NH1	8:H:71:GLY:O	2.50	0.45
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.82	0.45
4:D:81:GLU:O	4:D:85:LYS:HG3	2.16	0.45
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.16	0.45
6:F:10:LEU:HA	6:F:84:ASN:O	2.17	0.45
7:G:72:ARG:O	7:G:73:MET:HG2	2.17	0.45
8:H:82:HIS:HB3	8:H:138:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.51	0.45
1:A:1127:G:N2	1:A:1147:C:N4	2.64	0.45
1:A:978:A:O2'	1:A:1322:C:N3	2.47	0.45
1:A:1386:G:O2'	1:A:1387:G:H5'	2.17	0.45
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.45
2:B:101:MET:O	2:B:105:PHE:HA	2.16	0.45
2:B:204:ASN:C	2:B:204:ASN:ND2	2.70	0.45
2:B:51:LEU:O	2:B:55:PHE:HD1	2.00	0.45
3:C:108:ASN:C	3:C:110:ASN:H	2.19	0.45
3:C:40:ARG:HG2	3:C:55:VAL:HG11	1.98	0.45
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.16	0.45
1:A:262:A:H5'	20:T:74:LYS:HG3	1.99	0.45
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.16	0.45
1:A:433:C:C5'	1:A:433:C:C6	2.98	0.45
1:A:538:G:OP2	12:L:115:LYS:CG	2.65	0.45
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.99	0.45
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.52	0.45
3:C:112:SER:C	3:C:114:PRO:HD2	2.37	0.45
6:F:8:ILE:HG22	6:F:10:LEU:HD12	1.99	0.45
8:H:84:ARG:O	8:H:135:CYS:HB2	2.17	0.45
9:I:37:PHE:HD1	9:I:43:ALA:HB1	1.82	0.45
15:O:2:PRO:HB2	15:O:3:ILE:H	1.63	0.45
18:R:88:LYS:CG	18:R:88:LYS:OXT	2.64	0.45
20:T:105:SER:O	20:T:106:ALA:C	2.55	0.45
1:A:662:G:H2'	1:A:663:A:C8	2.52	0.45
1:A:81:U:H2'	1:A:83:U:OP2	2.17	0.45
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.82	0.45
3:C:5:ILE:N	3:C:5:ILE:HD12	2.32	0.45
4:D:117:ALA:O	4:D:121:VAL:HG23	2.16	0.45
7:G:15:ASP:OD2	7:G:16:LEU:N	2.50	0.45
13:M:108:ARG:HH21	13:M:111:LYS:CB	2.29	0.45
13:M:14:ARG:H	13:M:44:ARG:HE	1.64	0.45
1:A:974:A:OP2	14:N:41:ARG:NH1	2.50	0.45
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.38	0.45
17:Q:101:ARG:NE	17:Q:101:ARG:HA	2.31	0.45
18:R:45:SER:O	18:R:47:THR:O	2.34	0.45
1:A:165:C:O2'	1:A:166:G:H5'	2.16	0.44
1:A:290:C:O2'	1:A:291:C:H5'	2.17	0.44
1:A:513:C:H2'	1:A:514:C:H6	1.81	0.44
1:A:67:C:H2'	1:A:68:G:C8	2.52	0.44
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:48:LYS:CG	7:G:49:ILE:N	2.79	0.44
10:J:31:GLY:HA3	10:J:78:ASN:ND2	2.32	0.44
10:J:60:ARG:HD3	10:J:60:ARG:HA	1.90	0.44
10:J:39:PRO:O	10:J:69:ASN:O	2.35	0.44
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.98	0.44
1:A:1054:C:H2'	1:A:1055:A:H5''	2.00	0.44
1:A:1057:G:O2'	1:A:1058:G:H5'	2.17	0.44
1:A:1129:C:O2'	1:A:1130:A:OP2	2.34	0.44
1:A:1257:U:H5''	1:A:1258:G:O5'	2.17	0.44
1:A:1312:G:O2'	1:A:1313:U:H5'	2.17	0.44
1:A:500:G:H2'	1:A:501:C:C6	2.52	0.44
1:A:674:G:O2'	1:A:675:A:H5'	2.17	0.44
1:A:723:U:O2	1:A:723:U:H2'	2.16	0.44
1:A:940:C:H2'	1:A:941:G:H8	1.82	0.44
1:A:977:A:C2'	1:A:978:A:H5'	2.47	0.44
2:B:153:ARG:HG3	2:B:153:ARG:HH11	1.82	0.44
2:B:73:THR:O	2:B:75:LYS:N	2.50	0.44
6:F:67:MET:HE1	6:F:75:LEU:HD12	2.00	0.44
12:L:75:HIS:CD2	12:L:77:LEU:H	2.34	0.44
13:M:37:THR:HG23	13:M:55:ARG:CD	2.38	0.44
13:M:40:ASN:ND2	13:M:40:ASN:C	2.71	0.44
14:N:11:LYS:C	14:N:13:THR:N	2.70	0.44
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.16	0.44
18:R:87:ARG:HH21	18:R:87:ARG:HG3	1.82	0.44
19:S:39:THR:HG22	19:S:40:ILE:N	2.32	0.44
1:A:1242:C:O2'	1:A:1243:C:H5'	2.17	0.44
1:A:1238:A:C8	1:A:1303:C:H1'	2.52	0.44
1:A:831:U:O2'	1:A:832:C:H5'	2.17	0.44
2:B:64:ARG:HH11	2:B:64:ARG:CB	2.28	0.44
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.82	0.44
3:C:70:VAL:CG1	3:C:71:ALA:N	2.79	0.44
4:D:103:ASN:O	4:D:106:TYR:HB3	2.17	0.44
4:D:126:ILE:CG2	4:D:127:THR:N	2.80	0.44
4:D:31:CYS:O	4:D:32:ALA:HB3	2.16	0.44
11:K:32:ILE:HG21	11:K:77:MET:CE	2.47	0.44
18:R:43:PHE:C	18:R:51:LEU:HD12	2.37	0.44
23:Y:34:TM2:O3S	23:Y:36:A:N6	2.50	0.44
1:A:1229:A:C2	1:A:1230:C:C4	3.05	0.44
1:A:1307:U:H2'	1:A:1308:U:C6	2.53	0.44
1:A:1318:A:O2'	19:S:37:ARG:HD2	2.17	0.44
1:A:1329:A:OP1	13:M:26:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:G:O2'	1:A:146:G:H5'	2.17	0.44
2:B:30:ARG:C	2:B:32:ILE:H	2.20	0.44
2:B:95:GLN:OE1	2:B:95:GLN:HA	2.16	0.44
3:C:126:ARG:O	3:C:127:ARG:HB2	2.18	0.44
3:C:167:TRP:O	3:C:168:ALA:CB	2.66	0.44
6:F:33:TYR:C	6:F:71:ARG:NH2	2.71	0.44
7:G:149:ARG:CZ	7:G:149:ARG:HB3	2.46	0.44
17:Q:67:LYS:C	17:Q:70:ARG:HH12	2.19	0.44
20:T:12:ALA:C	20:T:14:LYS:N	2.70	0.44
1:A:1329:A:N7	21:U:7:ARG:NH2	2.65	0.44
1:A:542:G:H5'	4:D:41:GLY:HA3	1.99	0.44
1:A:697:U:H2'	1:A:698:G:H5'	1.98	0.44
1:A:892:A:C2	1:A:907:A:C4	3.06	0.44
1:A:994:A:H2'	1:A:994:A:N3	2.32	0.44
2:B:124:SER:CB	2:B:125:PRO:HD2	2.43	0.44
2:B:130:ARG:NH2	3:C:207:VAL:HG11	2.33	0.44
2:B:213:LEU:O	2:B:217:ARG:HG2	2.17	0.44
2:B:223:ILE:C	2:B:225:ALA:H	2.20	0.44
6:F:36:ARG:NH1	6:F:38:GLU:HG2	2.32	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.21	0.44
8:H:55:GLY:C	8:H:56:LYS:HD2	2.37	0.44
2:B:178:ARG:O	8:H:71:GLY:HA2	2.17	0.44
13:M:108:ARG:CA	13:M:108:ARG:HE	2.14	0.44
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.99	0.44
13:M:61:GLU:C	13:M:62:ASN:HD22	2.20	0.44
20:T:74:LYS:NZ	20:T:74:LYS:CA	2.81	0.44
1:A:1353:G:H2'	1:A:1354:C:C6	2.52	0.44
1:A:1495:U:H2'	1:A:1496:C:C6	2.52	0.44
1:A:123:C:OP1	1:A:312:C:H5'	2.17	0.44
1:A:339:C:H2'	1:A:340:U:C6	2.53	0.44
1:A:975:A:C5'	1:A:975:A:C8	2.95	0.44
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.00	0.44
4:D:61:LYS:NZ	4:D:62:GLN:HE21	2.15	0.44
5:E:150:ARG:CG	5:E:150:ARG:NH1	2.77	0.44
5:E:83:GLU:HG3	5:E:88:LYS:HG3	1.99	0.44
9:I:113:LYS:H	9:I:119:ALA:HA	1.81	0.44
10:J:15:THR:O	10:J:15:THR:HG22	2.18	0.44
12:L:77:LEU:HD21	12:L:107:ALA:CB	2.48	0.44
1:A:1423:G:O2'	1:A:1424:C:H5'	2.17	0.44
1:A:1505:G:H4'	1:A:1506:U:O5'	2.17	0.44
1:A:338:A:H2	1:A:351:G:H22	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H2'	1:A:738:C:C6	2.52	0.44
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.53	0.44
5:E:129:ILE:H	5:E:129:ILE:HD12	1.82	0.44
5:E:76:ILE:HG13	5:E:142:LEU:HD13	1.99	0.44
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.18	0.44
8:H:104:ARG:O	8:H:106:GLY:N	2.51	0.44
9:I:31:GLN:HB3	9:I:35:GLU:CG	2.47	0.44
10:J:80:LYS:NZ	10:J:80:LYS:HB2	2.33	0.44
1:A:1228:C:OP1	13:M:115:LYS:HE3	2.18	0.44
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.18	0.44
1:A:1441:G:H4'	1:A:1442:G:C5	2.52	0.44
1:A:625:G:H2'	1:A:626:U:H6	1.83	0.44
2:B:92:TYR:C	2:B:92:TYR:CD1	2.90	0.44
3:C:18:TRP:HE3	3:C:18:TRP:H	1.65	0.44
3:C:113:ALA:HB1	3:C:200:ALA:HB3	2.00	0.44
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.98	0.44
7:G:136:LYS:HZ2	7:G:143:ARG:HH12	1.64	0.44
10:J:22:LYS:HB2	10:J:22:LYS:NZ	2.33	0.44
13:M:62:ASN:O	13:M:63:THR:CB	2.66	0.44
15:O:5:LYS:N	15:O:5:LYS:HD2	2.32	0.44
15:O:74:ASP:O	15:O:76:GLU:N	2.51	0.44
19:S:18:LYS:HD3	19:S:18:LYS:C	2.39	0.44
1:A:1320:C:O2	19:S:36:ARG:NH1	2.50	0.44
1:A:1305:G:N2	1:A:1331:G:C2'	2.81	0.44
1:A:1360:A:O2'	1:A:1361:G:H5'	2.18	0.44
1:A:782:A:H2'	1:A:783:C:O4'	2.18	0.44
2:B:22:LYS:O	2:B:24:TRP:N	2.50	0.44
3:C:79:ARG:CG	3:C:82:GLU:HG2	2.45	0.44
6:F:15:ASP:O	6:F:17:SER:N	2.51	0.44
7:G:108:ALA:O	7:G:119:ARG:HG2	2.18	0.44
10:J:14:LYS:O	10:J:18:ALA:HB3	2.18	0.44
12:L:117:ARG:NH2	12:L:124:LYS:HA	2.33	0.44
14:N:22:THR:HG23	14:N:33:VAL:HG21	2.00	0.44
18:R:37:VAL:HG22	18:R:78:LEU:HB3	2.00	0.44
1:A:1267:C:O2	21:U:20:LYS:HD2	2.18	0.44
1:A:999:C:H2'	1:A:1000:U:C6	2.53	0.43
1:A:630:G:H5'	1:A:631:G:OP2	2.17	0.43
2:B:192:SER:O	2:B:194:PRO:HD3	2.18	0.43
1:A:405:U:O4	4:D:2:GLY:HA2	2.18	0.43
8:H:38:ILE:N	8:H:38:ILE:HD12	2.33	0.43
1:A:1343:G:C1'	9:I:121:ARG:HH12	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:ILE:O	10:J:76:ASN:HB2	2.18	0.43
12:L:82:VAL:HG23	12:L:106:ASP:OD1	2.18	0.43
13:M:44:ARG:O	13:M:46:LYS:N	2.51	0.43
15:O:87:ILE:O	15:O:88:ARG:CB	2.66	0.43
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.18	0.43
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.18	0.43
1:A:1157:A:C6	1:A:1180:A:C5	3.06	0.43
1:A:1178:G:C2	1:A:1180:A:C8	3.06	0.43
1:A:1192:C:H2'	1:A:1193:G:O5'	2.19	0.43
26:A:1854:PAR:H43	26:A:1854:PAR:H642	2.00	0.43
1:A:967:C:OP1	1:A:969:A:H5'	2.19	0.43
3:C:127:ARG:HD2	3:C:127:ARG:N	2.33	0.43
3:C:155:GLY:HA3	3:C:164:ARG:H	1.83	0.43
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.49	0.43
3:C:52:LEU:N	3:C:52:LEU:CD2	2.81	0.43
8:H:13:ILE:O	8:H:17:THR:HG23	2.19	0.43
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.53	0.43
8:H:63:LEU:HD22	8:H:63:LEU:H	1.82	0.43
9:I:53:VAL:O	9:I:54:ASP:CB	2.66	0.43
16:P:1:MET:O	16:P:24:ALA:HB2	2.17	0.43
1:A:1010:G:O2'	1:A:1011:G:H5'	2.18	0.43
1:A:1054:C:C2'	1:A:1055:A:H5''	2.48	0.43
1:A:1206:G:H4'	3:C:192:THR:O	2.19	0.43
1:A:344:A:O2'	1:A:345:C:OP1	2.32	0.43
1:A:677:U:H3	1:A:713:G:H22	1.66	0.43
1:A:920:U:H2'	1:A:921:U:C6	2.53	0.43
4:D:36:ARG:H	4:D:37:PRO:HD3	1.82	0.43
4:D:36:ARG:N	4:D:37:PRO:CD	2.81	0.43
7:G:145:ALA:O	7:G:146:GLU:CB	2.63	0.43
7:G:145:ALA:O	7:G:146:GLU:HB3	2.18	0.43
10:J:16:LEU:CD2	10:J:94:VAL:HG13	2.48	0.43
1:A:761:G:H1'	17:Q:105:ALA:CB	2.47	0.43
17:Q:68:ARG:CG	17:Q:68:ARG:NH1	2.81	0.43
20:T:59:ALA:O	20:T:63:ILE:HG13	2.18	0.43
20:T:8:ARG:HH11	20:T:8:ARG:CB	2.21	0.43
1:A:1097:C:H2'	1:A:1098:C:C6	2.53	0.43
1:A:397:A:H5'	1:A:398:C:P	2.59	0.43
1:A:407:G:H2'	1:A:408:A:C8	2.52	0.43
1:A:415:A:H2'	1:A:416:G:C8	2.53	0.43
1:A:6:G:H4'	1:A:298:A:H4'	2.00	0.43
1:A:951:G:O2'	1:A:952:U:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASN:HD21	2:B:206:ASP:CB	2.30	0.43
7:G:75:VAL:HG11	7:G:144:MET:HE3	1.99	0.43
8:H:77:GLU:CG	8:H:78:GLN:N	2.81	0.43
11:K:84:VAL:CG2	11:K:95:ILE:HD11	2.49	0.43
9:I:128:ARG:HA	13:M:126:LYS:HD2	2.00	0.43
15:O:45:VAL:HG12	15:O:46:HIS:H	1.83	0.43
15:O:55:GLY:O	15:O:59:MET:HG3	2.18	0.43
20:T:93:GLU:O	20:T:94:ALA:HB2	2.18	0.43
1:A:994:A:N7	1:A:1216:G:H4'	2.34	0.43
1:A:1402:C:O2	1:A:1500:A:N1	2.51	0.43
1:A:1532:U:O2	1:A:1534:A:P	2.70	0.43
1:A:186:C:H2'	1:A:187:C:C6	2.53	0.43
1:A:644:G:C5	1:A:645:C:C5	3.06	0.43
1:A:687:A:H2	1:A:700:G:N3	2.16	0.43
2:B:27:LYS:O	2:B:194:PRO:HG2	2.19	0.43
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.33	0.43
3:C:35:GLU:HG3	3:C:95:THR:HG22	2.00	0.43
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.35	0.43
12:L:10:LEU:HD22	12:L:15:ARG:HD3	2.00	0.43
13:M:40:ASN:ND2	13:M:41:PRO:HD2	2.31	0.43
21:U:6:ARG:CG	21:U:15:ARG:NH1	2.80	0.43
1:A:1288:A:N1	1:A:1371:G:H1'	2.33	0.43
1:A:279:A:H5''	1:A:281:G:O4'	2.18	0.43
1:A:590:C:O2'	1:A:591:U:H5'	2.18	0.43
5:E:106:PRO:O	5:E:110:LEU:HG	2.19	0.43
1:A:1346:A:C5	7:G:10:ARG:NH2	2.86	0.43
9:I:23:ASN:HD22	9:I:23:ASN:C	2.21	0.43
9:I:32:ASP:OD1	9:I:33:PHE:N	2.52	0.43
1:A:1193:G:HO2'	1:A:1194:U:H5'	1.80	0.43
1:A:265:G:H2'	1:A:267:C:H5	1.82	0.43
1:A:627:G:O2'	1:A:628:G:H5'	2.18	0.43
1:A:757:U:O2'	1:A:879:C:H1'	2.19	0.43
2:B:97:TRP:HZ3	2:B:100:GLY:N	2.17	0.43
6:F:40:VAL:HG22	6:F:41:GLU:H	1.83	0.43
8:H:61:VAL:O	8:H:63:LEU:HD22	2.17	0.43
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.18	0.43
11:K:24:SER:C	11:K:26:ASN:H	2.20	0.43
12:L:111:LYS:HE2	12:L:112:ASP:H	1.75	0.43
16:P:38:TYR:HE2	16:P:50:LYS:CE	2.31	0.43
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.01	0.43
19:S:13:ASP:N	19:S:13:ASP:OD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:C:H6	1:A:1018:C:O5'	2.02	0.43
1:A:122:G:OP1	1:A:122:G:H8	2.02	0.43
1:A:1347:G:H2'	1:A:1348:U:OP2	2.18	0.43
1:A:1427:U:H2'	1:A:1428:A:H8	1.82	0.43
1:A:254:G:O2'	1:A:255:G:H5'	2.18	0.43
1:A:959:A:H3'	1:A:960:U:H5''	2.00	0.43
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.00	0.43
7:G:21:VAL:HG23	7:G:22:LEU:N	2.33	0.43
10:J:23:ILE:CD1	10:J:23:ILE:N	2.81	0.43
14:N:11:LYS:C	14:N:13:THR:H	2.22	0.43
15:O:42:HIS:O	15:O:45:VAL:O	2.37	0.43
15:O:25:THR:CG2	15:O:70:LEU:HG	2.46	0.43
17:Q:101:ARG:HE	17:Q:101:ARG:HA	1.84	0.43
20:T:44:ALA:HB2	20:T:88:VAL:HG13	2.01	0.43
1:A:58:C:O2'	1:A:59:A:H5'	2.19	0.43
2:B:140:HIS:O	2:B:143:GLU:HB3	2.19	0.43
1:A:1190:G:P	3:C:5:ILE:HG13	2.58	0.43
3:C:65:ALA:O	3:C:66:VAL:HB	2.17	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG23	2.01	0.43
3:C:47:LEU:HG	3:C:76:VAL:HG12	2.01	0.43
4:D:76:ARG:O	4:D:80:GLU:HG2	2.18	0.43
7:G:15:ASP:C	7:G:17:VAL:H	2.22	0.43
9:I:17:VAL:HG21	9:I:80:GLY:HA3	2.01	0.43
11:K:45:GLY:O	11:K:50:TYR:HB2	2.18	0.43
15:O:5:LYS:CD	15:O:5:LYS:H	2.32	0.43
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.87	0.43
1:A:1058:G:C6	1:A:1059:C:N3	2.87	0.43
1:A:1138:G:N1	1:A:1140:C:C2	2.87	0.43
1:A:692:U:H2'	1:A:694:A:OP2	2.19	0.43
2:B:128:GLU:O	2:B:129:GLU:C	2.57	0.43
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.72	0.43
3:C:180:ALA:O	3:C:181:ASN:CB	2.65	0.43
5:E:142:LEU:O	5:E:143:ARG:NE	2.50	0.43
10:J:22:LYS:HD3	10:J:88:LEU:O	2.18	0.43
11:K:48:ILE:HG22	11:K:49:GLY:N	2.34	0.43
21:U:6:ARG:HG3	21:U:15:ARG:HH11	1.81	0.43
1:A:1223:C:OP2	1:A:1224:G:H2'	2.19	0.42
1:A:1305:G:N2	1:A:1331:G:HO2'	2.15	0.42
1:A:186:C:H2'	1:A:187:C:H6	1.84	0.42
1:A:628:G:O2'	1:A:629:G:H5'	2.19	0.42
2:B:22:LYS:C	2:B:24:TRP:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:O	2:B:75:LYS:HB2	2.18	0.42
5:E:51:VAL:O	5:E:55:VAL:HG23	2.19	0.42
10:J:6:ILE:HB	10:J:71:LEU:O	2.19	0.42
13:M:67:GLU:O	13:M:68:GLY:C	2.58	0.42
19:S:51:VAL:HG21	19:S:71:LEU:HB3	2.00	0.42
1:A:1225:A:N3	1:A:1225:A:H2'	2.33	0.42
1:A:1279:A:O2'	1:A:1282:C:N4	2.52	0.42
1:A:1312:G:N7	19:S:3:ARG:O	2.52	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.19	0.42
1:A:1505:G:H8	1:A:1505:G:H3'	1.84	0.42
1:A:490:G:O2'	1:A:491:G:H5'	2.18	0.42
2:B:114:ARG:O	2:B:117:GLU:HB3	2.18	0.42
3:C:178:LEU:C	3:C:180:ALA:H	2.21	0.42
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.48	0.42
5:E:51:VAL:O	5:E:54:ALA:HB3	2.19	0.42
7:G:51:GLN:C	7:G:53:LYS:N	2.70	0.42
7:G:62:PHE:HA	7:G:124:LEU:CD1	2.49	0.42
7:G:9:VAL:HG11	7:G:94:ARG:NH1	2.34	0.42
9:I:11:LYS:O	9:I:11:LYS:HG2	2.19	0.42
9:I:34:ASN:O	9:I:38:GLN:HB2	2.19	0.42
9:I:57:GLY:O	9:I:58:ARG:HB2	2.20	0.42
10:J:22:LYS:CD	10:J:89:ASP:HA	2.50	0.42
13:M:13:LYS:HD3	13:M:17:VAL:HG11	2.00	0.42
1:A:1161:C:O2	1:A:1162:C:C5	2.72	0.42
1:A:1495:U:H2'	1:A:1496:C:H6	1.83	0.42
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.54	0.42
1:A:268:C:H2'	1:A:269:C:C6	2.51	0.42
1:A:434:U:H2'	1:A:435:C:H6	1.81	0.42
1:A:651:C:O2'	1:A:652:U:H5'	2.19	0.42
1:A:880:C:O2'	1:A:881:G:H5'	2.19	0.42
10:J:29:ARG:O	10:J:30:SER:HB3	2.19	0.42
14:N:33:VAL:HA	14:N:40:CYS:HA	2.01	0.42
16:P:26:ARG:HD2	16:P:31:LYS:O	2.19	0.42
1:A:1284:C:H3'	1:A:1285:A:C8	2.53	0.42
1:A:1376:U:H2'	1:A:1377:A:C8	2.54	0.42
1:A:216:G:O2'	1:A:217:C:O5'	2.38	0.42
1:A:414:A:H2'	1:A:415:A:C8	2.54	0.42
1:A:445:G:O2'	1:A:446:G:H5'	2.19	0.42
1:A:624:C:H2'	1:A:625:G:H8	1.83	0.42
1:A:663:A:O2'	1:A:664:G:H5'	2.20	0.42
2:B:47:THR:HA	2:B:202:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ILE:CG2	3:C:15:THR:N	2.66	0.42
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.83	0.42
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.48	0.42
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.84	0.42
1:A:1251:A:H5'	9:I:12:GLU:OE1	2.20	0.42
13:M:91:ARG:HB2	13:M:98:VAL:HG22	2.01	0.42
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.02	0.42
1:A:1047:G:O2'	1:A:1048:G:H5'	2.19	0.42
1:A:1442:G:O2'	1:A:1443:G:H5'	2.20	0.42
1:A:807:A:H2'	1:A:808:C:H6	1.85	0.42
1:A:962:C:H2'	1:A:963:G:O4'	2.19	0.42
4:D:17:VAL:CG1	4:D:18:LYS:H	2.32	0.42
7:G:31:MET:SD	7:G:34:GLY:HA2	2.59	0.42
7:G:38:LEU:HD12	7:G:38:LEU:C	2.38	0.42
9:I:17:VAL:HG11	9:I:81:ILE:N	2.34	0.42
13:M:23:TYR:HE2	13:M:70:LEU:HB3	1.84	0.42
20:T:50:GLU:HB2	20:T:99:LEU:CD1	2.47	0.42
1:A:1159:U:C4	1:A:1182:G:C5	3.08	0.42
1:A:1300:G:O2'	1:A:1301:U:C6	2.60	0.42
1:A:1519:A:C3'	1:A:1520:G:H5'	2.49	0.42
1:A:1532:U:H2'	1:A:1533:C:H3'	2.01	0.42
1:A:16:A:O2'	1:A:17:U:H5'	2.19	0.42
1:A:502:G:H2'	1:A:503:C:O4'	2.19	0.42
1:A:622:A:C8	1:A:623:C:C6	3.08	0.42
1:A:867:G:C2	1:A:868:C:C6	3.07	0.42
2:B:61:LEU:HD13	2:B:61:LEU:C	2.40	0.42
7:G:149:ARG:CB	7:G:149:ARG:HH21	2.32	0.42
8:H:97:VAL:CG1	8:H:98:LYS:N	2.81	0.42
9:I:40:LEU:O	9:I:42:ARG:N	2.52	0.42
1:A:1157:A:C8	1:A:1181:G:N1	2.65	0.42
1:A:1256:A:C2'	1:A:1257:U:OP2	2.67	0.42
1:A:1298:C:N4	7:G:114:ARG:HG2	2.35	0.42
1:A:1337:G:H5''	1:A:1338:G:OP1	2.19	0.42
1:A:866:C:H2'	1:A:867:G:O4'	2.19	0.42
4:D:2:GLY:O	4:D:4:TYR:N	2.53	0.42
5:E:91:LEU:CD2	5:E:120:THR:HG22	2.49	0.42
5:E:18:ARG:HH12	5:E:25:ARG:HD2	1.85	0.42
6:F:83:ASP:C	6:F:85:VAL:N	2.73	0.42
8:H:102:ARG:N	8:H:102:ARG:NE	2.67	0.42
10:J:9:ARG:HH11	10:J:9:ARG:CB	2.33	0.42
14:N:41:ARG:HG3	14:N:42:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:LYS:HD3	14:N:4:LYS:HA	1.82	0.42
20:T:48:LYS:HB3	20:T:51:GLU:HB3	2.01	0.42
20:T:72:LEU:O	20:T:73:HIS:C	2.58	0.42
1:A:1120:G:O2'	1:A:1121:U:H5'	2.19	0.42
1:A:1260:C:H4'	1:A:1283:G:O2'	2.19	0.42
1:A:609:A:C2'	1:A:610:G:H5'	2.50	0.42
1:A:767:A:H2'	1:A:768:A:C8	2.54	0.42
1:A:925:G:C2	1:A:927:G:C8	3.08	0.42
2:B:212:GLN:NE2	2:B:216:SER:HB3	2.35	0.42
3:C:54:ARG:HG2	3:C:55:VAL:H	1.84	0.42
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.55	0.42
6:F:33:TYR:HA	6:F:71:ARG:NH1	2.34	0.42
1:A:939:G:H5''	7:G:102:ARG:CZ	2.50	0.42
7:G:40:ALA:O	7:G:41:ARG:C	2.58	0.42
9:I:53:VAL:HG12	9:I:96:LEU:HD11	2.01	0.42
12:L:27:LEU:C	12:L:29:GLY:H	2.22	0.42
17:Q:79:SER:O	17:Q:80:GLY:O	2.37	0.42
1:A:1020:U:H2'	1:A:1021:G:C8	2.55	0.42
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.42
1:A:1178:G:C2	1:A:1180:A:H8	2.38	0.42
1:A:1286:A:H2'	1:A:1287:A:C4'	2.45	0.42
1:A:1333:A:H2'	1:A:1334:G:O4'	2.20	0.42
1:A:1355:G:H2'	1:A:1356:G:C8	2.55	0.42
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.53	0.42
1:A:960:U:O2	1:A:960:U:H5'	2.19	0.42
2:B:16:HIS:O	2:B:41:ILE:HG23	2.20	0.42
2:B:50:GLU:O	2:B:51:LEU:C	2.58	0.42
3:C:31:HIS:C	3:C:33:LEU:H	2.23	0.42
3:C:79:ARG:C	3:C:81:GLY:H	2.23	0.42
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.35	0.42
4:D:8:VAL:HB	4:D:21:LEU:HD12	2.00	0.42
6:F:22:GLU:O	6:F:26:ILE:HG13	2.19	0.42
13:M:3:ARG:NH1	13:M:7:VAL:HG12	2.35	0.42
13:M:93:ARG:HB3	13:M:94:ARG:HD2	2.01	0.42
20:T:56:MET:CE	20:T:88:VAL:HG11	2.48	0.42
1:A:1054:C:H42	23:Y:34:TM2:C6	2.32	0.42
23:Y:34:TM2:H4'	23:Y:35:A:OP1	2.20	0.42
1:A:1518:A:H2'	1:A:1519:A:C8	2.54	0.42
1:A:242:C:H2'	1:A:243:A:H5'	2.02	0.42
1:A:613:C:O2'	1:A:614:A:H5'	2.20	0.42
1:A:749:C:H2'	1:A:750:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:C:H2'	1:A:931:C:H5'	2.02	0.42
2:B:71:VAL:O	2:B:165:VAL:HG23	2.19	0.42
3:C:167:TRP:HB3	3:C:168:ALA:H	1.44	0.42
3:C:189:ALA:O	3:C:191:THR:HG23	2.20	0.42
3:C:39:ILE:O	3:C:43:LEU:HB2	2.20	0.42
3:C:86:VAL:O	3:C:89:GLU:HB3	2.20	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.42
9:I:27:THR:HG22	9:I:28:VAL:N	2.34	0.42
14:N:36:PHE:O	14:N:36:PHE:CD1	2.72	0.42
16:P:82:GLN:O	16:P:84:ALA:N	2.53	0.42
16:P:82:GLN:O	16:P:83:GLU:C	2.59	0.42
17:Q:82:MET:O	17:Q:86:GLU:HG2	2.20	0.42
20:T:89:ARG:O	20:T:93:GLU:HG3	2.20	0.42
1:A:1094:G:O5'	1:A:1095:U:H5	2.02	0.41
1:A:1253:G:H2'	1:A:1254:C:H6	1.85	0.41
1:A:432:A:C3'	1:A:433:C:H5''	2.39	0.41
1:A:444:C:H2'	1:A:444:C:O2	2.19	0.41
1:A:573:A:C2	1:A:574:A:C2	3.08	0.41
1:A:930:C:O2'	1:A:931:C:H5'	2.19	0.41
2:B:19:HIS:O	2:B:39:ILE:HG23	2.19	0.41
6:F:34:GLY:N	6:F:71:ARG:NH2	2.68	0.41
7:G:149:ARG:CB	7:G:149:ARG:NH2	2.80	0.41
9:I:14:VAL:HG23	9:I:66:ARG:O	2.20	0.41
10:J:89:ASP:CB	10:J:91:PRO:HD2	2.49	0.41
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.41
11:K:51:LYS:O	11:K:55:LYS:HE2	2.19	0.41
13:M:62:ASN:N	13:M:62:ASN:HD22	2.17	0.41
16:P:59:TRP:HA	16:P:62:VAL:CG2	2.50	0.41
17:Q:17:LYS:N	17:Q:49:GLU:OE2	2.33	0.41
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.54	0.41
19:S:35:SER:C	19:S:37:ARG:H	2.23	0.41
1:A:1041:A:H2'	1:A:1042:G:H8	1.85	0.41
1:A:1053:G:C3'	1:A:1054:C:C5'	2.96	0.41
1:A:16:A:C2'	1:A:17:U:H5'	2.49	0.41
1:A:41:G:H2'	1:A:42:G:H8	1.85	0.41
1:A:448:A:C4	1:A:487:A:C2	3.08	0.41
1:A:463:A:H4'	16:P:80:PHE:O	2.20	0.41
1:A:538:G:H2'	1:A:539:A:H8	1.84	0.41
1:A:582:U:OP1	15:O:64:ARG:NH2	2.45	0.41
1:A:933:G:OP2	7:G:3:ARG:HB3	2.19	0.41
1:A:959:A:H2'	1:A:960:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.55	0.41
4:D:151:LYS:H	4:D:151:LYS:HD2	1.85	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.88	0.41
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.85	0.41
6:F:69:GLU:C	6:F:71:ARG:H	2.23	0.41
10:J:9:ARG:NH1	10:J:9:ARG:CB	2.82	0.41
12:L:34:ARG:HG3	12:L:105:TYR:CE1	2.55	0.41
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.20	0.41
18:R:36:ASN:O	18:R:39:VAL:HG12	2.21	0.41
1:A:1051:C:O2'	1:A:1052:U:H5'	2.19	0.41
1:A:256:U:O2'	1:A:257:G:H5'	2.20	0.41
1:A:948:C:O2'	1:A:949:A:H5'	2.20	0.41
3:C:134:ILE:O	3:C:138:VAL:HG23	2.20	0.41
9:I:97:LYS:HB3	9:I:98:PRO:CD	2.41	0.41
10:J:39:PRO:HA	10:J:70:ARG:NH1	2.35	0.41
10:J:89:ASP:OD2	10:J:91:PRO:HD2	2.20	0.41
1:A:881:G:P	12:L:12:ARG:HH22	2.43	0.41
14:N:41:ARG:HH11	14:N:41:ARG:HG2	1.85	0.41
15:O:36:ILE:HA	15:O:59:MET:CE	2.51	0.41
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.02	0.41
1:A:191:G:N2	20:T:103:GLY:O	2.44	0.41
1:A:1157:A:C5	1:A:1180:A:C6	3.09	0.41
1:A:1157:A:H2	1:A:1181:G:C1'	2.33	0.41
1:A:1193:G:C2'	1:A:1194:U:H5'	2.50	0.41
1:A:730:G:H21	1:A:765:G:H5''	1.86	0.41
1:A:780:A:C2	1:A:801:U:C5	3.09	0.41
3:C:28:GLN:O	3:C:31:HIS:HB2	2.21	0.41
5:E:99:GLY:O	5:E:117:ASP:HA	2.20	0.41
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.55	0.41
7:G:51:GLN:HA	7:G:54:THR:O	2.21	0.41
11:K:82:VAL:HG23	11:K:105:VAL:HG13	2.02	0.41
12:L:27:LEU:O	12:L:28:LYS:C	2.59	0.41
17:Q:33:GLY:O	17:Q:34:LYS:C	2.59	0.41
1:A:1499:A:H1'	1:A:1520:G:C5'	2.51	0.41
1:A:602:A:O2'	1:A:603:U:H5'	2.20	0.41
1:A:960:U:H1'	1:A:1223:C:H5'	2.03	0.41
2:B:159:PRO:HG2	2:B:182:ILE:HD13	2.02	0.41
2:B:90:MET:HE3	2:B:222:ILE:HD13	2.02	0.41
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.73	0.41
2:B:97:TRP:HZ3	2:B:99:GLY:HA2	1.86	0.41
7:G:116:ALA:O	7:G:120:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:126:LYS:C	8:H:128:GLY:H	2.24	0.41
9:I:17:VAL:HG11	9:I:81:ILE:HG12	2.02	0.41
10:J:23:ILE:O	10:J:23:ILE:CG2	2.64	0.41
13:M:44:ARG:HH11	13:M:44:ARG:HG2	1.86	0.41
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.35	0.41
1:A:1353:G:H2'	1:A:1354:C:H6	1.85	0.41
1:A:415:A:H2'	1:A:416:G:H8	1.86	0.41
1:A:52:G:O2'	1:A:53:A:H5'	2.20	0.41
4:D:199:ASN:C	4:D:199:ASN:HD22	2.23	0.41
8:H:100:ILE:HB	8:H:125:ARG:HH12	1.86	0.41
9:I:9:ARG:HD3	9:I:14:VAL:CG1	2.51	0.41
10:J:82:ILE:O	10:J:82:ILE:HG22	2.20	0.41
11:K:12:ARG:O	11:K:13:GLN:HB2	2.20	0.41
13:M:102:ARG:HG3	13:M:102:ARG:O	2.19	0.41
13:M:108:ARG:O	13:M:112:GLY:N	2.48	0.41
13:M:22:ILE:HG21	13:M:25:ILE:HD12	2.03	0.41
15:O:3:ILE:HG13	15:O:38:ARG:HD2	2.02	0.41
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.34	0.41
19:S:44:MET:O	19:S:47:HIS:HB2	2.21	0.41
1:A:109:A:C6	1:A:326:G:C6	3.09	0.41
1:A:1172:C:O2'	1:A:1173:G:H5'	2.20	0.41
1:A:1157:A:C6	1:A:1180:A:N7	2.89	0.41
1:A:1305:G:O2'	1:A:1331:G:N2	2.54	0.41
1:A:46:G:O2'	1:A:365:U:H1'	2.20	0.41
1:A:743:U:H2'	1:A:744:C:C6	2.56	0.41
1:A:993:G:O2'	1:A:994:A:P	2.78	0.41
2:B:235:SER:C	2:B:237:ALA:N	2.73	0.41
2:B:8:LYS:O	2:B:9:GLU:CB	2.67	0.41
3:C:188:LEU:O	3:C:189:ALA:CB	2.67	0.41
9:I:16:ARG:HD2	9:I:64:THR:CB	2.51	0.41
1:A:718:G:H5'	11:K:117:ASN:ND2	2.35	0.41
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.21	0.41
13:M:80:ARG:HB3	13:M:80:ARG:NH1	2.36	0.41
14:N:30:ALA:O	14:N:33:VAL:HG22	2.21	0.41
14:N:4:LYS:HA	14:N:7:ILE:HG12	2.02	0.41
1:A:1147:C:O2	9:I:16:ARG:NH2	2.54	0.41
1:A:248:C:O2'	1:A:249:U:H5'	2.21	0.41
1:A:877:C:O2'	1:A:878:G:H5'	2.20	0.41
1:A:940:C:H2'	1:A:941:G:C8	2.56	0.41
2:B:104:ASN:OD1	2:B:107:THR:HB	2.21	0.41
3:C:108:ASN:HD22	3:C:111:LEU:HG	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:N	3:C:52:LEU:HD23	2.34	0.41
3:C:91:LEU:C	3:C:91:LEU:HD23	2.40	0.41
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.53	0.41
7:G:149:ARG:CA	7:G:149:ARG:HH21	2.33	0.41
9:I:9:ARG:HA	9:I:13:ALA:O	2.20	0.41
17:Q:68:ARG:O	17:Q:68:ARG:HG3	2.21	0.41
2:B:111:ARG:HB3	2:B:149:LEU:CD1	2.44	0.41
2:B:112:VAL:C	2:B:114:ARG:N	2.74	0.41
2:B:228:GLY:O	2:B:229:VAL:C	2.58	0.41
3:C:116:VAL:HG21	3:C:202:ILE:HD11	2.03	0.41
3:C:34:LEU:HD21	3:C:38:ARG:CZ	2.51	0.41
4:D:112:VAL:HG12	4:D:116:GLN:NE2	2.36	0.41
1:A:620:C:C1'	4:D:135:LEU:HD13	2.51	0.41
5:E:24:ARG:HG2	5:E:24:ARG:NH1	2.34	0.41
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.56	0.41
9:I:42:ARG:O	9:I:44:VAL:N	2.53	0.41
9:I:50:LEU:O	9:I:53:VAL:HG22	2.21	0.41
10:J:22:LYS:O	10:J:26:ALA:HB3	2.21	0.41
10:J:72:VAL:HG12	10:J:73:ASP:N	2.35	0.41
17:Q:69:LYS:H	17:Q:70:ARG:HH11	1.69	0.41
18:R:37:VAL:CG2	18:R:78:LEU:HB3	2.51	0.41
21:U:6:ARG:CD	21:U:15:ARG:HH12	2.33	0.41
1:A:1332:A:C2	1:A:1333:A:C4	3.08	0.41
1:A:298:A:H2'	1:A:299:G:O4'	2.21	0.41
1:A:328:C:H1'	1:A:329:A:OP2	2.21	0.41
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.85	0.41
2:B:236:TYR:O	2:B:236:TYR:CD2	2.74	0.41
2:B:69:LEU:HD22	2:B:71:VAL:CG2	2.51	0.41
4:D:36:ARG:HG3	4:D:38:TYR:CE2	2.56	0.41
4:D:42:GLN:O	4:D:42:GLN:CG	2.69	0.41
5:E:43:LEU:HD22	5:E:44:GLY:N	2.36	0.41
5:E:57:LYS:HG2	5:E:61:TYR:HE2	1.83	0.41
6:F:69:GLU:OE1	6:F:69:GLU:N	2.54	0.41
8:H:39:LEU:HD12	8:H:39:LEU:HA	1.80	0.41
9:I:4:TYR:O	9:I:18:PHE:HA	2.20	0.41
10:J:6:ILE:O	10:J:71:LEU:O	2.39	0.41
12:L:69:TYR:HB2	12:L:90:VAL:HG21	2.03	0.41
14:N:25:VAL:HG13	14:N:39:LEU:HD23	2.02	0.41
18:R:68:LYS:O	18:R:72:ARG:HG3	2.20	0.41
20:T:45:GLN:NE2	20:T:45:GLN:O	2.54	0.41
1:A:1043:C:O2'	1:A:1044:A:H5'	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:H2'	1:A:1153:C:H6	1.86	0.41
1:A:1192:C:C2'	1:A:1193:G:O5'	2.69	0.41
1:A:335:C:H2'	1:A:336:C:C6	2.56	0.41
1:A:408:A:O2'	1:A:409:G:H5'	2.20	0.41
2:B:118:LEU:HD11	2:B:141:GLU:OE2	2.21	0.41
3:C:100:ALA:O	3:C:101:LEU:HB2	2.21	0.41
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.86	0.41
9:I:37:PHE:CD1	9:I:43:ALA:HB1	2.56	0.41
9:I:81:ILE:HG22	9:I:81:ILE:O	2.21	0.41
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.56	0.41
13:M:45:VAL:HA	13:M:48:LEU:HG	2.02	0.41
13:M:91:ARG:HB3	13:M:98:VAL:HG22	2.03	0.41
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.57	0.41
19:S:10:PHE:O	19:S:11:VAL:HG23	2.21	0.41
20:T:53:LEU:HB2	20:T:100:ILE:HG22	2.02	0.41
1:A:1498:U:H4'	1:A:1519:A:H2	1.82	0.40
1:A:1513:A:H2'	1:A:1514:C:C6	2.56	0.40
1:A:693:G:O2'	1:A:694:A:H5'	2.21	0.40
1:A:761:G:H1'	17:Q:105:ALA:HB2	2.03	0.40
1:A:84:U:H2'	1:A:88:A:O4'	2.21	0.40
1:A:884:U:H4'	1:A:885:G:H5''	2.03	0.40
3:C:36:ASP:OD2	3:C:36:ASP:N	2.54	0.40
5:E:80:ILE:HD13	5:E:91:LEU:HD12	2.02	0.40
1:A:1377:A:C6	7:G:5:ARG:NH2	2.89	0.40
8:H:123:GLU:O	8:H:127:LEU:HG	2.21	0.40
9:I:128:ARG:HA	13:M:126:LYS:CD	2.51	0.40
14:N:24:CYS:SG	14:N:43:CYS:SG	3.17	0.40
1:A:1033:G:O2'	1:A:1034:G:H5'	2.21	0.40
1:A:1047:G:C2'	1:A:1048:G:H5'	2.50	0.40
1:A:1056:U:O2	1:A:1056:U:H2'	2.20	0.40
1:A:1065:U:H5''	1:A:1190:G:H22	1.77	0.40
1:A:1192:C:H3'	1:A:1193:G:P	2.23	0.40
1:A:1206:G:C6	1:A:1207:G:C5	3.09	0.40
1:A:1217:C:H2'	1:A:1218:C:O4'	2.21	0.40
1:A:1367:C:N3	1:A:1368:G:C8	2.89	0.40
1:A:344:A:H5''	1:A:345:C:H5	1.87	0.40
1:A:420:U:H2'	1:A:422:C:C5	2.56	0.40
1:A:502:G:C2	1:A:503:C:C2	3.09	0.40
1:A:515:G:C5	1:A:516:U:C5	3.09	0.40
1:A:645:C:H2'	1:A:646:U:C6	2.56	0.40
1:A:671:G:H2'	1:A:672:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:O	3:C:64:VAL:HA	2.21	0.40
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.86	0.40
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.36	0.40
8:H:11:THR:O	8:H:12:ARG:C	2.59	0.40
9:I:79:LEU:O	9:I:83:ARG:N	2.48	0.40
11:K:101:SER:C	11:K:103:LEU:H	2.23	0.40
14:N:6:LEU:C	14:N:8:GLU:N	2.73	0.40
1:A:1024:G:C2'	1:A:1025:U:H5''	2.51	0.40
1:A:1070:U:O2'	1:A:1071:C:H5'	2.21	0.40
1:A:1124:G:O5'	10:J:35:SER:O	2.39	0.40
1:A:193:C:H2'	1:A:194:C:H6	1.86	0.40
1:A:232:G:H1'	1:A:262:A:N1	2.37	0.40
1:A:259:G:O2'	1:A:260:G:H5'	2.21	0.40
1:A:357:G:H1'	1:A:368:U:O2	2.22	0.40
2:B:25:ASN:HD22	2:B:27:LYS:N	2.08	0.40
2:B:58:ILE:HG23	2:B:68:ILE:CD1	2.51	0.40
2:B:73:THR:O	2:B:73:THR:HG22	2.21	0.40
1:A:1056:U:H5'	3:C:163:ALA:CB	2.51	0.40
1:A:1279:A:H61	3:C:26:LYS:HZ3	1.70	0.40
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.55	0.40
3:C:95:THR:C	3:C:97:LYS:N	2.74	0.40
5:E:41:VAL:HG21	5:E:113:ALA:HB2	2.03	0.40
10:J:9:ARG:HB3	10:J:9:ARG:CZ	2.51	0.40
13:M:94:ARG:O	13:M:95:GLY:C	2.60	0.40
14:N:10:ALA:O	14:N:11:LYS:HE3	2.20	0.40
14:N:25:VAL:HG12	14:N:38:GLY:C	2.41	0.40
15:O:70:LEU:O	15:O:72:ARG:N	2.54	0.40
16:P:43:LYS:HD2	16:P:43:LYS:N	2.36	0.40
19:S:19:VAL:CG1	19:S:20:LEU:N	2.84	0.40
20:T:57:ARG:HE	20:T:102:GLY:CA	2.34	0.40
20:T:79:ARG:O	20:T:83:ARG:HG3	2.22	0.40
1:A:190(L):U:H3	20:T:105:SER:HG	1.70	0.40
1:A:579:G:H5'	1:A:728:A:C1'	2.43	0.40
1:A:750:G:N3	15:O:23:GLY:HA3	2.37	0.40
3:C:64:VAL:HG12	3:C:66:VAL:CG2	2.50	0.40
4:D:8:VAL:HG11	4:D:115:ARG:CZ	2.51	0.40
4:D:146:ILE:N	4:D:146:ILE:CD1	2.82	0.40
1:A:587:G:OP1	8:H:89:PRO:HB3	2.21	0.40
17:Q:70:ARG:N	17:Q:70:ARG:HD2	2.37	0.40
20:T:57:ARG:NE	20:T:102:GLY:HA3	2.37	0.40
1:A:949:A:C2	1:A:1233:G:N3	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:A:H2'	1:A:1246:C:C6	2.57	0.40
1:A:262:A:C6	1:A:263:A:C6	3.09	0.40
1:A:65:U:C5	1:A:381:C:C4	3.10	0.40
1:A:792:A:H1'	1:A:794:A:N7	2.37	0.40
1:A:662:G:O2'	1:A:836:G:H5'	2.21	0.40
1:A:922:G:C6	1:A:923:A:C6	3.10	0.40
2:B:112:VAL:C	2:B:114:ARG:H	2.23	0.40
2:B:83:MET:C	2:B:86:GLU:H	2.23	0.40
3:C:157:ILE:CD1	3:C:166:GLU:HB2	2.51	0.40
3:C:147:LYS:HE3	3:C:203:PHE:CE2	2.57	0.40
3:C:39:ILE:HG22	3:C:40:ARG:N	2.36	0.40
3:C:47:LEU:HD23	3:C:68:VAL:HG11	2.03	0.40
4:D:174:LEU:O	4:D:186:LEU:HD11	2.22	0.40
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.84	0.40
5:E:76:ILE:CG2	5:E:78:HIS:H	2.35	0.40
7:G:115:ARG:HG3	7:G:118:VAL:HG23	2.02	0.40
9:I:107:ARG:CB	9:I:107:ARG:NH1	2.84	0.40
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.91	0.40
10:J:46:ARG:CG	10:J:46:ARG:NH1	2.78	0.40
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.04	0.40
1:A:254:G:OP1	17:Q:68:ARG:HB3	2.21	0.40
20:T:63:ILE:HG22	20:T:77:ALA:HB1	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:NH1	10:J:79:ARG:NH1[8_665]	2.06	0.14

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	162 (69%)	49 (21%)	23 (10%)	1	0
3	C	205/239 (86%)	139 (68%)	39 (19%)	27 (13%)	0	0
4	D	206/209 (99%)	169 (82%)	29 (14%)	8 (4%)	3	4
5	E	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
6	F	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	5	7
7	G	153/156 (98%)	129 (84%)	14 (9%)	10 (6%)	1	1
8	H	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	25	43
9	I	125/128 (98%)	92 (74%)	23 (18%)	10 (8%)	1	1
10	J	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	0
11	K	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	11	18
12	L	123/135 (91%)	89 (72%)	26 (21%)	8 (6%)	1	1
13	M	123/126 (98%)	94 (76%)	18 (15%)	11 (9%)	1	1
14	N	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	4	5
15	O	86/89 (97%)	71 (83%)	11 (13%)	4 (5%)	3	3
16	P	82/88 (93%)	74 (90%)	6 (7%)	2 (2%)	7	11
17	Q	102/105 (97%)	88 (86%)	10 (10%)	4 (4%)	3	4
18	R	71/88 (81%)	55 (78%)	10 (14%)	6 (8%)	1	1
19	S	79/93 (85%)	58 (73%)	14 (18%)	7 (9%)	1	1
20	T	97/106 (92%)	81 (84%)	10 (10%)	6 (6%)	2	1
21	U	23/27 (85%)	17 (74%)	6 (26%)	0	100	100
All	All	2365/2541 (93%)	1867 (79%)	348 (15%)	150 (6%)	1	1

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	88	ALA
2	B	123	ALA
2	B	129	GLU
2	B	229	VAL
3	C	15	THR
3	C	26	LYS
3	C	61	ALA
3	C	65	ALA
3	C	154	SER
3	C	189	ALA
3	C	207	VAL

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Mol	Chain	Res	Type
4	D	3	ARG
4	D	36	ARG
7	G	155	ARG
8	H	105	ARG
9	I	7	THR
9	I	38	GLN
9	I	43	ALA
9	I	55	ALA
9	I	58	ARG
9	I	88	TYR
10	J	30	SER
10	J	39	PRO
10	J	72	VAL
10	J	85	LEU
12	L	27	LEU
12	L	28	LYS
12	L	30	ALA
12	L	47	LYS
12	L	126	LYS
12	L	127	GLU
13	M	5	ALA
13	M	12	ASN
13	M	45	VAL
13	M	63	THR
13	M	67	GLU
14	N	10	ALA
16	P	83	GLU
17	Q	80	GLY
17	Q	81	ARG
18	R	20	ALA
19	S	6	LYS
19	S	81	ARG
20	T	73	HIS
20	T	94	ALA
20	T	99	LEU
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	74	LYS
2	B	80	ILE
2	B	89	GLY
2	B	240	GLN

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Mol	Chain	Res	Type
3	C	16	ARG
3	C	96	GLY
3	C	100	ALA
3	C	156	ARG
6	F	16	GLN
7	G	78	ARG
7	G	81	GLY
9	I	31	GLN
10	J	32	ALA
10	J	34	VAL
11	K	12	ARG
13	M	7	VAL
13	M	14	ARG
13	M	23	TYR
13	M	95	GLY
15	O	88	ARG
16	P	10	GLY
17	Q	100	LYS
18	R	87	ARG
19	S	9	VAL
20	T	95	ALA
20	T	100	ILE
20	T	102	GLY
2	B	44	LEU
2	B	131	PRO
3	C	12	LEU
3	C	29	TYR
3	C	81	GLY
3	C	98	ASN
3	C	146	ALA
3	C	168	ALA
4	D	29	PRO
4	D	35	ARG
4	D	39	PRO
7	G	7	ALA
7	G	53	LYS
7	G	83	ALA
9	I	56	LEU
10	J	40	LEU
10	J	60	ARG
14	N	15	LYS
15	O	71	GLN

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Mol	Chain	Res	Type
19	S	8	GLY
19	S	30	LEU
19	S	43	GLU
2	B	23	ARG
2	B	60	ASP
2	B	63	MET
2	B	190	THR
3	C	4	LYS
3	C	47	LEU
3	C	66	VAL
3	C	79	ARG
3	C	108	ASN
9	I	54	ASP
10	J	27	ALA
10	J	90	LEU
12	L	29	GLY
13	M	38	GLY
13	M	124	PRO
18	R	17	SER
18	R	26	LEU
19	S	27	GLU
2	B	115	LEU
2	B	195	ASP
3	C	74	GLY
3	C	101	LEU
3	C	157	ILE
3	C	188	LEU
4	D	4	TYR
4	D	5	ILE
4	D	175	SER
6	F	39	LYS
6	F	70	ASP
7	G	17	VAL
7	G	42	ILE
7	G	116	ALA
9	I	41	VAL
10	J	61	GLU
10	J	73	ASP
10	J	86	MET
12	L	41	ARG
18	R	21	LYS
2	B	52	GLU

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Mol	Chain	Res	Type
2	B	198	ASP
7	G	41	ARG
10	J	76	ASN
11	K	52	GLY
17	Q	33	GLY
10	J	24	VAL
3	C	55	VAL
15	O	82	ILE
2	B	227	GLY
2	B	228	GLY
18	R	60	GLY
10	J	77	PRO
15	O	75	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/220 (88%)	176 (91%)	18 (9%)	10	20
3	C	160/188 (85%)	152 (95%)	8 (5%)	28	51
4	D	180/181 (99%)	171 (95%)	9 (5%)	28	51
5	E	115/123 (94%)	101 (88%)	14 (12%)	6	10
6	F	90/90 (100%)	88 (98%)	2 (2%)	57	82
7	G	126/127 (99%)	116 (92%)	10 (8%)	14	27
8	H	119/119 (100%)	109 (92%)	10 (8%)	13	24
9	I	98/99 (99%)	91 (93%)	7 (7%)	17	32
10	J	87/92 (95%)	81 (93%)	6 (7%)	18	34
11	K	90/99 (91%)	87 (97%)	3 (3%)	43	70
12	L	104/111 (94%)	96 (92%)	8 (8%)	15	28
13	M	100/101 (99%)	89 (89%)	11 (11%)	7	13
14	N	49/50 (98%)	41 (84%)	8 (16%)	3	5
15	O	79/80 (99%)	71 (90%)	8 (10%)	9	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	72/74 (97%)	69 (96%)	3 (4%)	34	59
17	Q	96/97 (99%)	93 (97%)	3 (3%)	45	73
18	R	64/77 (83%)	63 (98%)	1 (2%)	68	88
19	S	71/80 (89%)	65 (92%)	6 (8%)	12	23
20	T	76/82 (93%)	68 (90%)	8 (10%)	8	15
21	U	19/22 (86%)	18 (95%)	1 (5%)	26	48
All	All	1989/2112 (94%)	1845 (93%)	144 (7%)	17	31

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	TRP
2	B	25	ASN
2	B	44	LEU
2	B	46	LYS
2	B	64	ARG
2	B	82	ARG
2	B	86	GLU
2	B	97	TRP
2	B	113	HIS
2	B	114	ARG
2	B	153	ARG
2	B	157	ARG
2	B	178	ARG
2	B	187	LEU
2	B	204	ASN
2	B	215	LEU
2	B	221	LEU
2	B	236	TYR
3	C	5	ILE
3	C	27	LYS
3	C	52	LEU
3	C	56	ASP
3	C	82	GLU
3	C	127	ARG
3	C	167	TRP
3	C	196	LEU
4	D	3	ARG
4	D	15	GLU
4	D	36	ARG

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Mol	Chain	Res	Type
4	D	57	ARG
4	D	122	ARG
4	D	132	ARG
4	D	170	VAL
4	D	199	ASN
4	D	201	GLN
5	E	12	LEU
5	E	20	GLN
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	73	ASN
5	E	75	THR
5	E	80	ILE
5	E	89	ILE
5	E	107	ARG
5	E	116	THR
5	E	143	ARG
5	E	150	ARG
6	F	43	LEU
6	F	47	ARG
7	G	8	GLU
7	G	11	GLN
7	G	12	LEU
7	G	38	LEU
7	G	47	CYS
7	G	113	GLU
7	G	114	ARG
7	G	136	LYS
7	G	140	ASP
7	G	156	TRP
8	H	21	LYS
8	H	26	VAL
8	H	39	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	97	VAL
8	H	102	ARG
8	H	112	LEU
8	H	133	LEU

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Mol	Chain	Res	Type
9	I	2	GLU
9	I	14	VAL
9	I	23	ASN
9	I	60	ASP
9	I	102	LEU
9	I	107	ARG
9	I	121	ARG
10	J	29	ARG
10	J	57	LYS
10	J	71	LEU
10	J	73	ASP
10	J	80	LYS
10	J	83	GLU
11	K	11	LYS
11	K	92	GLU
11	K	123	LYS
12	L	15	ARG
12	L	19	ARG
12	L	20	LYS
12	L	33	ARG
12	L	111	LYS
12	L	112	ASP
12	L	113	ARG
12	L	127	GLU
13	M	13	LYS
13	M	40	ASN
13	M	44	ARG
13	M	56	LEU
13	M	58	GLU
13	M	94	ARG
13	M	102	ARG
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS
13	M	125	ARG
14	N	6	LEU
14	N	9	LYS
14	N	11	LYS
14	N	12	ARG
14	N	22	THR
14	N	26	ARG
14	N	41	ARG

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Mol	Chain	Res	Type
14	N	44	LEU
15	O	5	LYS
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	57	LEU
15	O	71	GLN
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	53	VAL
17	Q	38	ARG
17	Q	68	ARG
17	Q	74	LEU
18	R	36	ASN
19	S	7	LYS
19	S	15	LEU
19	S	18	LYS
19	S	25	LYS
19	S	27	GLU
19	S	81	ARG
20	T	8	ARG
20	T	42	GLN
20	T	48	LYS
20	T	57	ARG
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	U	9	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	95	GLN
2	B	146	GLN
2	B	204	ASN
2	B	212	GLN
2	B	240	GLN
3	C	3	ASN

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Mol	Chain	Res	Type
3	C	6	HIS
3	C	107	GLN
3	C	110	ASN
3	C	123	GLN
4	D	42	GLN
4	D	62	GLN
4	D	123	HIS
4	D	199	ASN
4	D	201	GLN
5	E	20	GLN
5	E	73	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	73	ASN
6	F	100	ASN
7	G	37	ASN
7	G	96	GLN
7	G	106	GLN
7	G	122	HIS
9	I	23	ASN
9	I	73	GLN
9	I	124	GLN
10	J	33	GLN
10	J	56	HIS
10	J	62	HIS
10	J	76	ASN
10	J	78	ASN
11	K	38	ASN
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
15	O	13	GLN
15	O	37	ASN
16	P	65	GLN
16	P	76	GLN
17	Q	96	GLN

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Mol	Chain	Res	Type
18	R	36	ASN
19	S	23	ASN
19	S	56	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	196 (12%)	72 (4%)
22	X	2/6 (33%)	0	0
23	Y	6/17 (35%)	1 (16%)	0
All	All	1519/1545 (98%)	197 (12%)	72 (4%)

All (197) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
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	144	G
1	A	181	G
1	A	182	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	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	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	429	U
1	A	430	A
1	A	433	C
1	A	434	U
1	A	439	A
1	A	442	C
1	A	452	A
1	A	461	C
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A

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Mol	Chain	Res	Type
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	874	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A

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Mol	Chain	Res	Type
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1005	A
1	A	1026	G
1	A	1027	C
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
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	1152	A
1	A	1159	U
1	A	1161	C

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Mol	Chain	Res	Type
1	A	1176	A
1	A	1180	A
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1338	G
1	A	1348	U
1	A	1362	C
1	A	1394	A
1	A	1398	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1452	C
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G

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Mol	Chain	Res	Type
1	A	1530	G
1	A	1533	C
23	Y	35	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	203	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	281	G
1	A	328	C
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	410	G
1	A	428	G
1	A	429	U
1	A	433	C
1	A	438	G
1	A	484	G
1	A	497	A
1	A	509	A
1	A	532	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U

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Mol	Chain	Res	Type
1	A	812	C
1	A	819	A
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1063	C
1	A	1065	U
1	A	1067	A
1	A	1127	G
1	A	1129	C
1	A	1160	G
1	A	1175	G
1	A	1182	G
1	A	1191	A
1	A	1192	C
1	A	1201	A
1	A	1212	U
1	A	1225	A
1	A	1256	A
1	A	1257	U
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U
1	A	1532	U

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 271 ligands modelled in this entry, 270 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	$\# Z  > 2$
26	PAR	A	1854	-	45,45,45	1.37	8 (17%)	60,67,67	1.29	5 (8%)

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
26	PAR	A	1854	-	-	0/18/94/94	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1854	PAR	O54-C54	2.03	1.49	1.44
26	A	1854	PAR	O51-C51	2.10	1.49	1.44
26	A	1854	PAR	C52-C42	2.14	1.56	1.52
26	A	1854	PAR	C11-C21	2.46	1.57	1.52
26	A	1854	PAR	O51-C11	2.54	1.48	1.41
26	A	1854	PAR	C64-C54	2.55	1.58	1.51
26	A	1854	PAR	C31-C21	2.66	1.56	1.53
26	A	1854	PAR	O54-C14	3.18	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1854	PAR	O52-C13-O43	-2.02	109.24	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1854	PAR	O52-C13-C23	2.83	113.82	107.96
26	A	1854	PAR	O54-C54-C64	3.85	113.30	106.01
26	A	1854	PAR	C14-O54-C54	3.95	121.15	113.72
26	A	1854	PAR	O33-C14-C24	4.40	116.56	108.20

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
26	A	1854	PAR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1064:G	O3'	1065:U	P	1.30
1	A	1144:G	O3'	1145:C	P	1.24
1	A	1192:C	O3'	1193:G	P	1.10
1	A	1179:A	O3'	1180:A	P	1.08
1	A	1175:G	O3'	1176:A	P	0.99
1	A	1191:A	O3'	1192:C	P	0.98
1	A	1156:G	O3'	1157:A	P	0.89
1	A	1532:U	O3'	1533:C	P	0.83
1	A	1160:G	O3'	1161:C	P	0.72
1	A	1063:C	O3'	1064:G	P	0.70
1	A	1127:G	O3'	1128:C	P	0.46

## 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%)	-0.07	32 (2%) 64 66	18, 47, 115, 201	0
2	B	236/256 (92%)	0.73	22 (9%) 9 9	41, 79, 129, 136	0
3	C	207/239 (86%)	0.73	22 (10%) 7 6	48, 74, 118, 125	0
4	D	208/209 (99%)	0.65	20 (9%) 9 8	39, 59, 84, 92	0
5	E	151/162 (93%)	0.28	1 (0%) 87 88	25, 41, 69, 84	0
6	F	101/101 (100%)	0.52	7 (6%) 18 18	49, 77, 92, 96	0
7	G	155/156 (99%)	0.54	11 (7%) 17 17	40, 68, 102, 114	0
8	H	138/138 (100%)	0.23	4 (2%) 52 55	21, 38, 55, 65	0
9	I	127/128 (99%)	1.04	24 (18%) 1 1	39, 82, 103, 112	0
10	J	99/105 (94%)	1.27	24 (24%) 1 0	42, 112, 146, 150	0
11	K	119/129 (92%)	0.55	4 (3%) 46 48	23, 50, 79, 96	0
12	L	125/135 (92%)	0.56	6 (4%) 31 32	17, 52, 74, 109	0
13	M	125/126 (99%)	1.88	20 (16%) 2 2	50, 67, 122, 152	0
14	N	60/61 (98%)	1.06	8 (13%) 4 3	47, 66, 101, 107	0
15	O	88/89 (98%)	0.56	5 (5%) 24 25	36, 54, 82, 109	0
16	P	84/88 (95%)	0.27	2 (2%) 59 61	28, 40, 57, 80	0
17	Q	104/105 (99%)	0.73	7 (6%) 19 19	23, 42, 93, 146	0
18	R	73/88 (82%)	0.56	5 (6%) 18 18	43, 60, 107, 139	0
19	S	81/93 (87%)	1.26	16 (19%) 1 1	56, 90, 123, 134	0
20	T	99/106 (93%)	0.45	6 (6%) 22 22	25, 46, 81, 86	0
21	U	25/27 (92%)	1.15	3 (12%) 5 4	44, 53, 88, 94	0
22	X	3/6 (50%)	0.31	0 100 100	83, 83, 83, 88	0
23	Y	6/17 (35%)	0.84	1 (16%) 2 1	97, 105, 124, 134	0
All	All	3927/4086 (96%)	0.41	250 (6%) 20 21	17, 56, 115, 201	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	121	LYS	30.4
13	M	124	PRO	27.0
13	M	123	ALA	26.7
17	Q	105	ALA	25.4
19	S	3	ARG	24.6
1	A	1129	C	20.7
13	M	120	LYS	18.5
1	A	1534	A	16.2
13	M	125	ARG	15.9
13	M	126	LYS	12.6
13	M	7	VAL	12.2
1	A	1540	U	10.8
17	Q	104	LYS	10.7
14	N	6	LEU	10.3
11	K	129	SER	9.3
11	K	128	ALA	7.9
14	N	3	ARG	7.9
13	M	122	LYS	7.9
21	U	6	ARG	6.7
17	Q	103	GLY	6.6
1	A	1539	C	6.5
4	D	23	GLY	6.4
10	J	24	VAL	6.4
21	U	24	ARG	6.4
1	A	1541	U	6.0
1	A	1004	A	6.0
12	L	47	LYS	6.0
14	N	2	ALA	6.0
2	B	133	LYS	5.9
10	J	36	GLY	5.9
1	A	1144	G	5.8
3	C	76	VAL	5.6
1	A	1003(A)	G	5.6
2	B	136	VAL	5.6
23	Y	33	U	5.6
13	M	8	GLU	5.6
7	G	5	ARG	5.5
9	I	66	ARG	5.4
10	J	10	GLY	5.4
8	H	1	MET	5.3
18	R	16	PRO	5.2
7	G	156	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
10	J	6	ILE	5.0
9	I	19	LEU	4.9
4	D	4	TYR	4.9
1	A	1038	C	4.9
1	A	1533	C	4.9
13	M	102	ARG	4.9
13	M	5	ALA	4.8
3	C	196	LEU	4.8
2	B	211	ILE	4.7
3	C	60	ALA	4.6
2	B	226	ARG	4.6
10	J	72	VAL	4.5
7	G	80	VAL	4.5
17	Q	102	GLY	4.5
10	J	34	VAL	4.3
10	J	90	LEU	4.3
4	D	5	ILE	4.3
19	S	49	ILE	4.2
18	R	17	SER	4.2
4	D	21	LEU	4.2
4	D	209	ARG	4.2
1	A	1034	G	4.1
19	S	2	PRO	4.1
10	J	70	ARG	4.1
10	J	71	LEU	4.0
19	S	34	TRP	4.0
4	D	3	ARG	3.9
1	A	723	U	3.9
2	B	165	VAL	3.9
10	J	98	ILE	3.8
10	J	99	LYS	3.8
2	B	229	VAL	3.6
12	L	28	LYS	3.6
19	S	28	LYS	3.6
4	D	20	TYR	3.6
9	I	65	VAL	3.6
10	J	87	THR	3.6
1	A	1006	C	3.6
1	A	1131	G	3.6
20	T	100	ILE	3.5
3	C	167	TRP	3.5
10	J	54	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
13	M	88	ARG	3.4
9	I	14	VAL	3.4
1	A	1130	A	3.4
3	C	94	LEU	3.4
12	L	18	VAL	3.3
1	A	1033	G	3.3
15	O	89	GLY	3.3
6	F	36	ARG	3.3
19	S	5	LEU	3.3
9	I	101	PHE	3.3
13	M	9	ILE	3.2
7	G	2	ALA	3.2
10	J	5	ARG	3.2
9	I	18	PHE	3.2
10	J	96	ILE	3.2
1	A	1037	C	3.1
13	M	25	ILE	3.1
19	S	31	ILE	3.1
13	M	56	LEU	3.1
2	B	35	GLU	3.1
9	I	70	LYS	3.1
3	C	2	GLY	3.1
10	J	43	ARG	3.1
4	D	49	ARG	3.0
1	A	1143	G	3.0
9	I	119	ALA	3.0
20	T	99	LEU	3.0
2	B	81	VAL	3.0
19	S	10	PHE	2.9
19	S	74	PHE	2.9
8	H	2	LEU	2.9
4	D	2	GLY	2.9
4	D	159	ARG	2.9
1	A	1127	G	2.9
3	C	188	LEU	2.9
2	B	58	ILE	2.9
17	Q	95	TYR	2.9
1	A	202	U	2.9
7	G	4	ARG	2.9
15	O	3	ILE	2.8
10	J	97	GLU	2.8
7	G	85	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	413	G	2.8
3	C	201	TYR	2.8
20	T	53	LEU	2.8
2	B	132	LYS	2.8
9	I	28	VAL	2.8
6	F	98	LEU	2.8
19	S	6	LYS	2.7
3	C	42	LEU	2.7
9	I	99	LEU	2.7
13	M	104	ARG	2.7
12	L	115	LYS	2.7
14	N	21	TYR	2.7
1	A	993	G	2.7
8	H	18	ARG	2.7
3	C	66	VAL	2.6
18	R	54	ARG	2.6
3	C	75	VAL	2.6
6	F	72	VAL	2.6
9	I	26	VAL	2.6
14	N	30	ALA	2.6
3	C	208	ILE	2.6
13	M	96	LEU	2.6
1	A	1027	C	2.6
4	D	25	ARG	2.6
12	L	46	LYS	2.6
9	I	64	THR	2.6
19	S	30	LEU	2.6
20	T	10	LEU	2.6
1	A	1030(A)	G	2.6
10	J	47	PHE	2.5
2	B	76	GLN	2.5
2	B	230	VAL	2.5
7	G	76	ARG	2.5
4	D	208	SER	2.5
3	C	4	LYS	2.5
10	J	17	ASP	2.5
4	D	156	GLU	2.5
9	I	114	TYR	2.5
4	D	36	ARG	2.5
12	L	113	ARG	2.5
2	B	140	HIS	2.4
7	G	120	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	89	MET	2.4
4	D	115	ARG	2.4
1	A	1035	A	2.4
3	C	47	LEU	2.4
19	S	29	ARG	2.4
10	J	8	LEU	2.4
1	A	1036	G	2.4
9	I	128	ARG	2.4
21	U	20	LYS	2.4
4	D	32	ALA	2.4
6	F	14	LEU	2.4
3	C	39	ILE	2.4
6	F	101	ALA	2.4
9	I	15	ALA	2.4
10	J	16	LEU	2.4
4	D	201	GLN	2.3
9	I	47	LEU	2.3
2	B	89	GLY	2.3
1	A	984	C	2.3
3	C	85	ARG	2.3
14	N	28	GLY	2.3
14	N	35	ARG	2.3
17	Q	98	LEU	2.3
3	C	134	ILE	2.3
3	C	194	GLY	2.3
9	I	17	VAL	2.3
2	B	77	ALA	2.3
2	B	206	ASP	2.3
19	S	27	GLU	2.3
15	O	23	GLY	2.2
3	C	128	PHE	2.2
2	B	61	LEU	2.2
19	S	71	LEU	2.2
19	S	61	TYR	2.2
20	T	9	ASN	2.2
7	G	66	VAL	2.2
16	P	19	ILE	2.2
18	R	18	ARG	2.2
1	A	1128	C	2.2
3	C	68	VAL	2.2
6	F	65	VAL	2.2
15	O	12	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1124	G	2.2
4	D	11	LEU	2.2
11	K	51	LYS	2.2
9	I	53	VAL	2.2
9	I	31	GLN	2.2
3	C	3	ASN	2.2
20	T	98	PRO	2.2
2	B	208	ILE	2.2
16	P	12	LYS	2.2
13	M	30	ALA	2.2
7	G	155	ARG	2.2
11	K	30	VAL	2.1
4	D	204	ILE	2.1
9	I	27	THR	2.1
10	J	55	LYS	2.1
2	B	15	VAL	2.1
13	M	11	ARG	2.1
5	E	76	ILE	2.1
14	N	16	PHE	2.1
4	D	35	ARG	2.1
17	Q	101	ARG	2.1
3	C	64	VAL	2.1
2	B	215	LEU	2.1
9	I	51	ARG	2.1
9	I	102	LEU	2.1
10	J	20	ALA	2.1
15	O	11	VAL	2.1
10	J	7	LYS	2.1
8	H	30	ARG	2.0
13	M	117	VAL	2.0
9	I	124	GLN	2.0
2	B	127	ILE	2.0
2	B	156	LYS	2.0
9	I	63	ILE	2.0
1	A	373	A	2.0
18	R	25	THR	2.0
1	A	1257	U	2.0
19	S	60	VAL	2.0
1	A	1200	C	2.0
7	G	26	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
24	MG	A	1641	1/1	0.73	0.49	45.10	77,77,77,77	0
24	MG	A	1739	1/1	0.92	0.45	40.01	69,69,69,69	0
24	MG	A	1722	1/1	0.85	0.55	38.32	83,83,83,83	0
24	MG	A	1637	1/1	0.84	0.42	26.43	71,71,71,71	0
24	MG	A	1626	1/1	0.79	0.44	24.58	79,79,79,79	0
24	MG	A	1636	1/1	0.82	0.50	24.56	70,70,70,70	0
24	MG	A	1664	1/1	0.85	0.36	23.05	107,107,107,107	0
24	MG	A	1740	1/1	0.93	0.42	20.57	49,49,49,49	0
24	MG	A	1731	1/1	0.79	0.43	20.46	73,73,73,73	0
24	MG	A	1667	1/1	0.94	0.32	19.16	40,40,40,40	0
25	K	P	101	1/1	0.85	0.34	16.61	94,94,94,94	0
24	MG	A	1787	1/1	0.94	0.38	15.64	65,65,65,65	0
25	K	N	103	1/1	0.86	0.73	15.18	111,111,111,111	0
24	MG	A	1647	1/1	0.93	0.42	14.69	72,72,72,72	0
24	MG	A	1795	1/1	0.93	0.48	13.74	91,91,91,91	0
24	MG	A	1681	1/1	0.95	0.25	13.74	39,39,39,39	0
24	MG	A	1736	1/1	0.88	0.49	12.36	35,35,35,35	0
24	MG	A	1700	1/1	0.94	0.29	10.75	56,56,56,56	0
24	MG	I	201	1/1	0.89	0.87	9.54	62,62,62,62	0
24	MG	A	1654	1/1	0.98	0.50	9.19	85,85,85,85	0
24	MG	A	1676	1/1	0.32	0.21	8.31	103,103,103,103	0
24	MG	A	1703	1/1	0.93	0.26	7.79	44,44,44,44	0
24	MG	A	1746	1/1	0.97	0.30	7.73	66,66,66,66	0
24	MG	A	1671	1/1	0.88	0.54	7.62	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
27	ZN	D	301	1/1	0.88	0.68	6.80	126,126,126,126	0
24	MG	A	1721	1/1	0.91	0.39	6.57	89,89,89,89	0
24	MG	A	1778	1/1	0.88	0.20	5.95	64,64,64,64	0
26	PAR	A	1854	42/42	0.92	0.23	5.54	34,38,57,61	0
25	K	A	1845	1/1	0.65	0.20	5.44	111,111,111,111	0
24	MG	A	1657	1/1	0.86	0.23	5.30	56,56,56,56	0
24	MG	A	1745	1/1	0.98	0.27	4.97	54,54,54,54	0
24	MG	A	1765	1/1	0.98	0.24	4.83	59,59,59,59	0
24	MG	A	1757	1/1	0.85	0.48	4.37	72,72,72,72	0
24	MG	A	1694	1/1	0.86	0.31	4.15	71,71,71,71	0
24	MG	A	1682	1/1	0.87	0.22	3.96	74,74,74,74	0
24	MG	A	1788	1/1	0.88	0.30	3.93	69,69,69,69	0
24	MG	D	302	1/1	0.82	0.34	3.36	80,80,80,80	0
24	MG	A	1719	1/1	0.91	0.16	2.55	50,50,50,50	0
24	MG	A	1733	1/1	0.90	0.40	2.35	56,56,56,56	0
24	MG	A	1779	1/1	0.72	0.19	2.22	78,78,78,78	0
24	MG	A	1766	1/1	0.78	0.32	1.85	77,77,77,77	0
24	MG	A	1750	1/1	0.98	0.18	1.72	52,52,52,52	0
25	K	A	1818	1/1	0.91	0.20	1.34	107,107,107,107	0
24	MG	A	1767	1/1	0.82	0.19	1.07	69,69,69,69	0
24	MG	A	1769	1/1	0.94	0.18	0.98	60,60,60,60	0
24	MG	A	1651	1/1	0.82	0.16	0.77	72,72,72,72	0
27	ZN	N	101	1/1	0.98	0.24	0.66	73,73,73,73	0
24	MG	A	1761	1/1	0.88	0.23	0.52	81,81,81,81	0
25	K	A	1804	1/1	0.77	0.16	0.36	107,107,107,107	0
25	K	R	101	1/1	0.05	0.20	0.30	144,144,144,144	0
25	K	A	1846	1/1	0.61	0.16	0.19	118,118,118,118	0
24	MG	A	1775	1/1	0.92	0.20	-0.39	85,85,85,85	0
25	K	A	1841	1/1	0.79	0.18	-0.53	144,144,144,144	0
24	MG	Q	201	1/1	0.88	0.16	-0.56	73,73,73,73	0
24	MG	A	1649	1/1	0.98	0.16	-0.58	63,63,63,63	0
24	MG	M	201	1/1	0.97	0.16	-0.82	49,49,49,49	0
24	MG	A	1672	1/1	0.97	0.15	-0.91	55,55,55,55	0
24	MG	A	1692	1/1	0.74	0.16	-0.92	109,109,109,109	0
24	MG	A	1751	1/1	0.94	0.13	-1.47	70,70,70,70	0
24	MG	A	1760	1/1	0.94	0.16	-1.59	57,57,57,57	0
24	MG	A	1616	1/1	0.95	0.11	-1.91	53,53,53,53	0
24	MG	A	1723	1/1	0.95	0.09	-2.07	46,46,46,46	0
24	MG	A	1794	1/1	0.92	0.12	-2.27	46,46,46,46	0
25	K	A	1809	1/1	0.95	0.10	-2.45	118,118,118,118	0
24	MG	A	1734	1/1	0.86	0.15	-2.56	59,59,59,59	0
24	MG	N	102	1/1	0.92	0.08	-2.59	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1754	1/1	0.85	0.14	-3.11	80,80,80,80	0
24	MG	A	1742	1/1	0.99	0.11	-3.33	34,34,34,34	0
25	K	A	1811	1/1	0.93	0.11	-3.63	123,123,123,123	0
24	MG	A	1798	1/1	0.95	0.04	-5.44	70,70,70,70	0
24	MG	A	1720	1/1	0.87	0.08	-7.18	52,52,52,52	0
24	MG	A	1701	1/1	0.96	0.07	-8.76	44,44,44,44	0
24	MG	A	1604	1/1	0.99	0.10	-8.77	57,57,57,57	0
25	K	A	1800	1/1	0.96	0.05	-9.32	64,64,64,64	0
24	MG	A	1613	1/1	0.95	0.05	-20.72	35,35,35,35	0
24	MG	A	1716	1/1	0.73	0.36	-	78,78,78,78	0
25	K	A	1814	1/1	0.82	0.08	-	114,114,114,114	0
24	MG	A	1691	1/1	0.90	0.30	-	68,68,68,68	0
25	K	A	1852	1/1	0.66	0.28	-	120,120,120,120	0
24	MG	A	1617	1/1	0.94	0.06	-	55,55,55,55	0
24	MG	A	1708	1/1	0.93	0.35	-	54,54,54,54	0
24	MG	A	1639	1/1	0.97	0.17	-	65,65,65,65	0
24	MG	A	1735	1/1	0.86	0.21	-	78,78,78,78	0
24	MG	A	1796	1/1	0.86	0.27	-	68,68,68,68	0
24	MG	A	1724	1/1	0.89	0.42	-	78,78,78,78	0
24	MG	A	1797	1/1	0.58	0.18	-	101,101,101,101	0
24	MG	A	1792	1/1	0.94	0.29	-	57,57,57,57	0
25	K	A	1847	1/1	0.81	0.08	-	119,119,119,119	0
24	MG	A	1759	1/1	0.82	0.47	-	128,128,128,128	0
24	MG	B	301	1/1	0.94	0.08	-	38,38,38,38	0
24	MG	A	1620	1/1	0.81	0.20	-	73,73,73,73	0
24	MG	A	1669	1/1	0.91	0.36	-	74,74,74,74	0
25	K	T	201	1/1	0.80	0.19	-	92,92,92,92	0
25	K	A	1843	1/1	0.83	0.73	-	80,80,80,80	0
24	MG	A	1715	1/1	0.78	0.44	-	97,97,97,97	0
24	MG	A	1674	1/1	0.93	0.26	-	85,85,85,85	0
24	MG	A	1644	1/1	0.94	0.29	-	69,69,69,69	0
24	MG	E	201	1/1	0.84	0.53	-	78,78,78,78	0
24	MG	A	1707	1/1	0.85	0.21	-	62,62,62,62	0
25	K	A	1851	1/1	0.77	0.59	-	117,117,117,117	0
24	MG	A	1726	1/1	0.65	0.28	-	102,102,102,102	0
24	MG	A	1621	1/1	0.92	0.14	-	33,33,33,33	0
24	MG	A	1781	1/1	0.95	0.32	-	61,61,61,61	0
24	MG	A	1612	1/1	0.91	0.10	-	47,47,47,47	0
25	K	A	1828	1/1	0.94	0.41	-	82,82,82,82	0
24	MG	A	1699	1/1	0.95	0.37	-	31,31,31,31	0
25	K	A	1849	1/1	0.88	0.26	-	117,117,117,117	0
24	MG	A	1697	1/1	0.59	0.28	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1602	1/1	0.86	0.12	-	106,106,106,106	0
24	MG	A	1652	1/1	0.71	0.17	-	56,56,56,56	0
24	MG	A	1642	1/1	0.98	0.42	-	67,67,67,67	0
24	MG	A	1658	1/1	0.79	0.47	-	85,85,85,85	0
25	K	E	202	1/1	0.94	0.28	-	69,69,69,69	0
24	MG	A	1732	1/1	0.83	0.23	-	80,80,80,80	0
24	MG	A	1718	1/1	0.85	0.33	-	64,64,64,64	0
25	K	A	1813	1/1	0.79	0.25	-	126,126,126,126	0
25	K	E	204	1/1	0.83	0.15	-	129,129,129,129	0
24	MG	A	1695	1/1	0.80	0.31	-	90,90,90,90	0
24	MG	A	1630	1/1	0.93	0.45	-	82,82,82,82	0
24	MG	A	1668	1/1	0.85	0.32	-	85,85,85,85	0
25	K	A	1827	1/1	0.59	0.20	-	122,122,122,122	0
24	MG	A	1709	1/1	0.78	0.49	-	114,114,114,114	0
24	MG	A	1747	1/1	0.97	0.30	-	51,51,51,51	0
24	MG	A	1643	1/1	0.73	0.51	-	88,88,88,88	0
24	MG	A	1614	1/1	0.77	0.36	-	54,54,54,54	0
25	K	A	1853	1/1	0.78	0.20	-	119,119,119,119	0
24	MG	A	1693	1/1	0.97	0.28	-	40,40,40,40	0
24	MG	A	1688	1/1	0.93	0.39	-	76,76,76,76	0
24	MG	A	1650	1/1	0.91	0.26	-	66,66,66,66	0
24	MG	A	1762	1/1	0.91	0.20	-	81,81,81,81	0
25	K	A	1833	1/1	0.91	0.38	-	66,66,66,66	0
24	MG	A	1653	1/1	0.76	0.34	-	69,69,69,69	0
24	MG	A	1728	1/1	0.88	0.17	-	81,81,81,81	0
24	MG	A	1632	1/1	0.04	0.59	-	160,160,160,160	0
25	K	A	1815	1/1	0.57	0.34	-	139,139,139,139	0
25	K	A	1848	1/1	0.84	0.20	-	136,136,136,136	0
25	K	A	1802	1/1	0.98	0.06	-	73,73,73,73	0
24	MG	A	1743	1/1	0.98	0.26	-	57,57,57,57	0
24	MG	A	1782	1/1	0.40	0.18	-	132,132,132,132	0
25	K	A	1834	1/1	0.81	0.28	-	115,115,115,115	0
24	MG	A	1744	1/1	0.91	0.35	-	45,45,45,45	0
24	MG	A	1714	1/1	0.72	0.32	-	88,88,88,88	0
24	MG	A	1670	1/1	0.91	0.06	-	66,66,66,66	0
24	MG	A	1725	1/1	0.87	0.15	-	83,83,83,83	0
24	MG	A	1640	1/1	0.93	0.33	-	83,83,83,83	0
25	K	A	1824	1/1	0.93	0.05	-	95,95,95,95	0
24	MG	A	1635	1/1	0.94	0.45	-	79,79,79,79	0
25	K	A	1832	1/1	0.61	0.13	-	101,101,101,101	0
24	MG	A	1677	1/1	0.76	0.18	-	95,95,95,95	0
24	MG	A	1618	1/1	0.96	0.15	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1629	1/1	0.80	0.15	-	68,68,68,68	0
25	K	A	1826	1/1	0.96	0.12	-	83,83,83,83	0
24	MG	A	1749	1/1	0.88	0.28	-	60,60,60,60	0
25	K	A	1822	1/1	0.64	0.13	-	101,101,101,101	0
24	MG	A	1756	1/1	0.85	0.29	-	87,87,87,87	0
25	K	A	1831	1/1	0.83	0.15	-	127,127,127,127	0
24	MG	A	1752	1/1	0.88	0.46	-	91,91,91,91	0
24	MG	A	1665	1/1	0.79	0.50	-	90,90,90,90	0
24	MG	A	1622	1/1	0.81	0.27	-	66,66,66,66	0
24	MG	A	1704	1/1	0.87	0.17	-	57,57,57,57	0
25	K	A	1807	1/1	0.92	0.10	-	93,93,93,93	0
25	K	A	1842	1/1	0.98	0.42	-	43,43,43,43	0
24	MG	A	1686	1/1	0.97	0.34	-	82,82,82,82	0
25	K	A	1821	1/1	0.60	0.19	-	99,99,99,99	0
24	MG	A	1673	1/1	0.72	0.15	-	83,83,83,83	0
24	MG	A	1706	1/1	0.83	0.25	-	63,63,63,63	0
24	MG	A	1748	1/1	0.95	0.45	-	79,79,79,79	0
25	K	A	1836	1/1	0.46	0.27	-	132,132,132,132	0
25	K	A	1801	1/1	0.96	0.17	-	76,76,76,76	0
24	MG	A	1763	1/1	0.85	0.35	-	93,93,93,93	0
24	MG	A	1624	1/1	0.93	0.31	-	61,61,61,61	0
24	MG	A	1790	1/1	0.94	0.48	-	55,55,55,55	0
24	MG	A	1615	1/1	0.86	0.44	-	107,107,107,107	0
25	K	A	1839	1/1	0.78	0.24	-	131,131,131,131	0
25	K	A	1835	1/1	0.83	0.07	-	99,99,99,99	0
24	MG	A	1799	1/1	0.94	0.23	-	86,86,86,86	0
24	MG	A	1727	1/1	0.92	0.12	-	63,63,63,63	0
24	MG	A	1784	1/1	0.68	0.19	-	93,93,93,93	0
24	MG	A	1730	1/1	0.95	0.24	-	84,84,84,84	0
24	MG	A	1625	1/1	0.85	0.19	-	93,93,93,93	0
24	MG	A	1687	1/1	0.79	0.12	-	56,56,56,56	0
24	MG	A	1696	1/1	0.86	0.31	-	70,70,70,70	0
25	K	I	202	1/1	0.89	0.52	-	59,59,59,59	0
24	MG	A	1737	1/1	0.93	0.09	-	43,43,43,43	0
24	MG	A	1679	1/1	0.98	0.22	-	19,19,19,19	0
25	K	E	203	1/1	0.88	0.36	-	93,93,93,93	0
24	MG	A	1666	1/1	0.94	0.51	-	87,87,87,87	0
25	K	A	1803	1/1	0.95	0.07	-	97,97,97,97	0
24	MG	A	1783	1/1	0.76	0.16	-	91,91,91,91	0
24	MG	A	1690	1/1	0.39	0.30	-	91,91,91,91	0
24	MG	A	1741	1/1	0.96	0.28	-	38,38,38,38	0
24	MG	A	1758	1/1	0.77	0.55	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1774	1/1	0.98	0.14	-	40,40,40,40	0
24	MG	A	1771	1/1	0.82	0.18	-	77,77,77,77	0
24	MG	A	1623	1/1	0.86	0.37	-	92,92,92,92	0
24	MG	A	1662	1/1	0.81	0.20	-	91,91,91,91	0
24	MG	A	1605	1/1	0.97	0.36	-	65,65,65,65	0
25	K	A	1825	1/1	0.59	0.26	-	132,132,132,132	0
24	MG	A	1770	1/1	0.87	0.04	-	105,105,105,105	0
24	MG	A	1680	1/1	0.48	0.27	-	85,85,85,85	0
24	MG	A	1776	1/1	0.96	0.42	-	47,47,47,47	0
24	MG	A	1689	1/1	0.91	0.53	-	93,93,93,93	0
24	MG	A	1631	1/1	0.59	0.28	-	100,100,100,100	0
24	MG	A	1683	1/1	0.83	0.45	-	79,79,79,79	0
24	MG	A	1656	1/1	0.61	0.17	-	89,89,89,89	0
24	MG	A	1628	1/1	0.95	0.12	-	59,59,59,59	0
24	MG	A	1645	1/1	0.95	0.35	-	103,103,103,103	0
24	MG	A	1634	1/1	0.89	0.24	-	68,68,68,68	0
24	MG	A	1789	1/1	0.88	0.19	-	121,121,121,121	0
24	MG	A	1780	1/1	0.84	0.15	-	71,71,71,71	0
24	MG	A	1661	1/1	0.97	0.26	-	57,57,57,57	0
24	MG	A	1773	1/1	0.74	0.43	-	96,96,96,96	0
24	MG	A	1648	1/1	0.88	0.51	-	81,81,81,81	0
24	MG	A	1738	1/1	0.61	0.14	-	81,81,81,81	0
24	MG	A	1603	1/1	0.76	0.44	-	104,104,104,104	0
25	K	A	1840	1/1	0.87	0.25	-	96,96,96,96	0
24	MG	A	1638	1/1	0.89	0.22	-	90,90,90,90	0
24	MG	A	1607	1/1	0.97	0.46	-	70,70,70,70	0
24	MG	A	1684	1/1	0.95	0.11	-	55,55,55,55	0
25	K	A	1844	1/1	0.79	0.28	-	107,107,107,107	0
24	MG	A	1675	1/1	0.79	0.15	-	69,69,69,69	0
25	K	A	1810	1/1	0.82	0.12	-	113,113,113,113	0
24	MG	A	1711	1/1	0.83	0.56	-	104,104,104,104	0
24	MG	A	1606	1/1	0.90	0.16	-	70,70,70,70	0
24	MG	A	1608	1/1	0.97	0.28	-	61,61,61,61	0
24	MG	A	1729	1/1	0.95	0.19	-	53,53,53,53	0
25	K	A	1820	1/1	0.59	0.20	-	102,102,102,102	0
24	MG	A	1601	1/1	0.96	0.12	-	56,56,56,56	0
24	MG	A	1702	1/1	0.87	0.15	-	83,83,83,83	0
25	K	A	1806	1/1	0.63	0.11	-	101,101,101,101	0
25	K	A	1808	1/1	0.84	0.18	-	90,90,90,90	0
25	K	A	1837	1/1	0.88	0.16	-	122,122,122,122	0
24	MG	A	1655	1/1	0.88	0.43	-	89,89,89,89	0
24	MG	A	1791	1/1	0.99	0.08	-	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
24	MG	A	1685	1/1	0.88	0.32	-	98,98,98,98	0
24	MG	A	1646	1/1	0.95	0.47	-	75,75,75,75	0
24	MG	A	1627	1/1	0.39	0.35	-	108,108,108,108	0
25	K	A	1823	1/1	0.79	0.10	-	118,118,118,118	0
24	MG	A	1663	1/1	0.88	0.46	-	73,73,73,73	0
24	MG	A	1785	1/1	0.93	0.06	-	93,93,93,93	0
24	MG	A	1713	1/1	0.79	0.26	-	86,86,86,86	0
25	K	A	1817	1/1	0.69	0.13	-	133,133,133,133	0
24	MG	A	1659	1/1	0.85	0.52	-	84,84,84,84	0
24	MG	A	1705	1/1	0.90	0.35	-	74,74,74,74	0
24	MG	A	1793	1/1	0.96	0.08	-	36,36,36,36	0
25	K	A	1830	1/1	0.90	0.49	-	93,93,93,93	0
24	MG	A	1678	1/1	0.74	0.49	-	97,97,97,97	0
24	MG	A	1633	1/1	0.96	0.42	-	86,86,86,86	0
25	K	A	1812	1/1	0.37	0.19	-	120,120,120,120	0
25	K	A	1805	1/1	0.82	0.15	-	113,113,113,113	0
24	MG	A	1772	1/1	0.67	0.17	-	89,89,89,89	0
24	MG	A	1610	1/1	0.68	0.45	-	110,110,110,110	0
25	K	A	1829	1/1	0.77	0.10	-	103,103,103,103	0
24	MG	A	1753	1/1	0.96	0.14	-	45,45,45,45	0
25	K	A	1850	1/1	0.88	0.46	-	93,93,93,93	0
24	MG	A	1611	1/1	0.73	0.22	-	83,83,83,83	0
24	MG	A	1755	1/1	0.89	0.12	-	52,52,52,52	0
24	MG	A	1712	1/1	0.92	0.07	-	54,54,54,54	0
24	MG	A	1717	1/1	0.92	0.07	-	78,78,78,78	0
24	MG	A	1764	1/1	0.91	0.21	-	50,50,50,50	0
24	MG	A	1768	1/1	0.96	0.23	-	66,66,66,66	0
24	MG	A	1777	1/1	0.86	0.19	-	75,75,75,75	0
25	K	A	1819	1/1	0.77	0.80	-	116,116,116,116	0
24	MG	A	1609	1/1	0.97	0.26	-	33,33,33,33	0
24	MG	A	1660	1/1	0.80	0.46	-	83,83,83,83	0
25	K	A	1816	1/1	0.80	0.16	-	116,116,116,116	0
24	MG	A	1698	1/1	0.76	0.11	-	69,69,69,69	0
24	MG	A	1710	1/1	0.73	0.48	-	93,93,93,93	0
24	MG	A	1786	1/1	0.93	0.39	-	59,59,59,59	0
25	K	A	1838	1/1	0.77	0.19	-	94,94,94,94	0
24	MG	A	1619	1/1	0.75	0.09	-	72,72,72,72	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.