



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:02 PM GMT

PDB ID : 4B3M  
Title : Crystal structure of the 30S ribosome in complex with compound 1  
Authors : Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.  
Deposited on : 2012-07-25  
Resolution : 2.90 Å(reported)

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

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

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

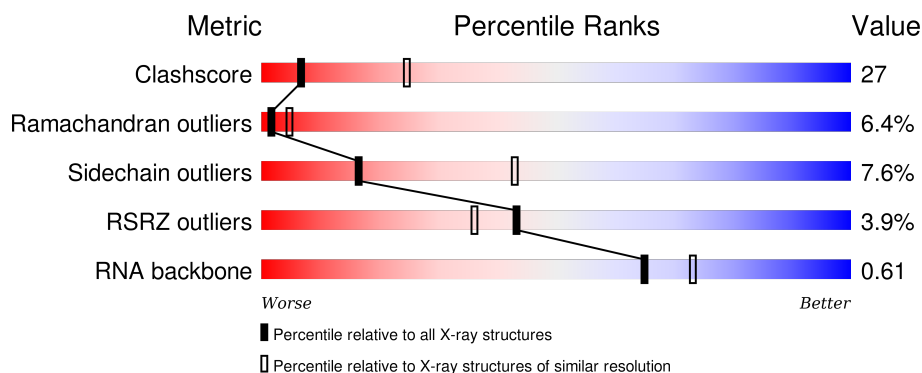
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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




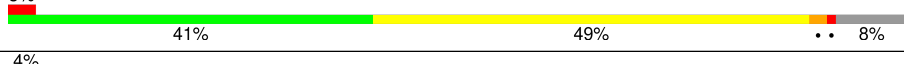
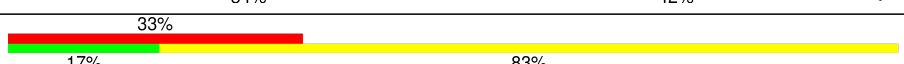
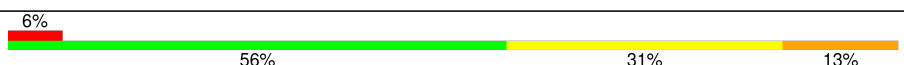
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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	1521	<div> <div>8%</div> <div>41%</div> <div>45%</div> <div>12%</div> <div>••</div> </div>
2	B	256	<div> <div>8%</div> <div>24%</div> <div>53%</div> <div>12%</div> <div>•</div> <div>8%</div> </div>
3	C	239	<div> <div>3%</div> <div>32%</div> <div>41%</div> <div>13%</div> <div>13%</div> </div>
4	D	208	<div> <div>5%</div> <div>53%</div> <div>38%</div> <div>8%</div> </div>
5	E	161	<div> <div>45%</div> <div>42%</div> <div>6%</div> <div>•</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	132	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	W	6	
23	Z	16	

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	2555	-	-	-	X
24	MG	A	2560	-	-	-	X
24	MG	A	2562	-	-	-	X
24	MG	A	2569	-	-	-	X
24	MG	A	2571	-	-	-	X
24	MG	A	2572	-	-	-	X
24	MG	A	2577	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2584	-	-	-	X
24	MG	A	2586	-	-	-	X
24	MG	A	2587	-	-	-	X
24	MG	A	2588	-	-	-	X
24	MG	A	2591	-	-	-	X
24	MG	A	2594	-	-	-	X
24	MG	A	2599	-	-	-	X
24	MG	A	2601	-	-	-	X
24	MG	A	2604	-	-	-	X
24	MG	A	2609	-	-	-	X
24	MG	A	2611	-	-	-	X
24	MG	A	2612	-	-	-	X
24	MG	A	2615	-	-	-	X
24	MG	A	2616	-	-	-	X
24	MG	A	2619	-	-	-	X
24	MG	A	2628	-	-	-	X
24	MG	A	2632	-	-	-	X
24	MG	A	2639	-	-	-	X
24	MG	A	2641	-	-	-	X
24	MG	A	2647	-	-	-	X
24	MG	A	2657	-	-	-	X
24	MG	A	2659	-	-	-	X
24	MG	A	2661	-	-	-	X
24	MG	A	2662	-	-	-	X
24	MG	A	2684	-	-	-	X
24	MG	A	2696	-	-	-	X
24	MG	A	2697	-	-	-	X
24	MG	A	2706	-	-	-	X
24	MG	A	2713	-	-	-	X
24	MG	A	2716	-	-	-	X
24	MG	A	2718	-	-	-	X
24	MG	A	2733	-	-	-	X
24	MG	A	2735	-	-	-	X
24	MG	A	2738	-	-	-	X
24	MG	A	2740	-	-	-	X
24	MG	A	2742	-	-	-	X
24	MG	A	2747	-	-	-	X
24	MG	A	2749	-	-	-	X
24	MG	A	2766	-	-	-	X
24	MG	A	2770	-	-	-	X
24	MG	E	1151	-	-	-	X
24	MG	E	1152	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	H	1139	-	-	-	X
24	MG	H	1140	-	-	-	X
24	MG	I	1128	-	-	-	X
24	MG	N	1062	-	-	-	X
24	MG	T	1100	-	-	-	X
25	K	A	2672	-	-	-	X
25	K	A	2673	-	-	-	X
25	K	A	2675	-	-	-	X
26	ON0	A	2759	-	-	-	X

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 52505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32486	14462	6011	10503	1510			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	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				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	57	ARG	HIS	CONFLICT	UNP P80374

- 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
			795	499	157	138	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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	CONFLICT	UNP Q5SHP7

- 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				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	CONFLICT	UNP Q5SLQ0



- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	CONFLICT	UNP P80380

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	16	Total	C	N	O	P	0	0	0
			342	154	65	108	15			

- 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		

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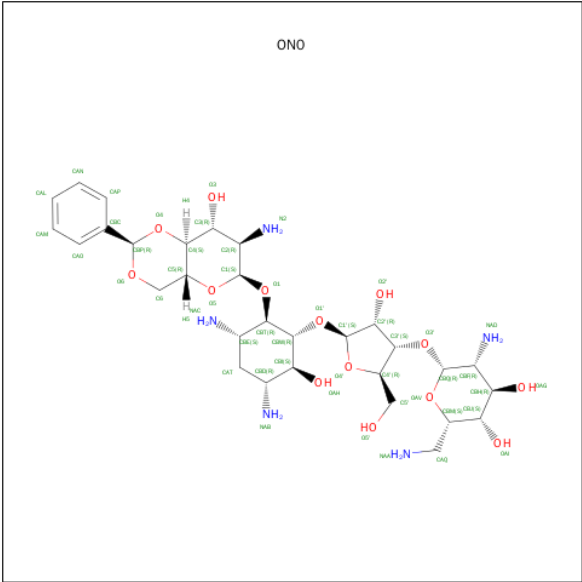
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	K	1	Total 1	Mg 1	0	0
24	E	3	Total 3	Mg 3	0	0
24	H	4	Total 4	Mg 4	0	0
24	B	1	Total 1	Mg 1	0	0
24	I	1	Total 1	Mg 1	0	0
24	Z	1	Total 1	Mg 1	0	0
24	A	223	Total 223	Mg 223	0	0
24	T	1	Total 1	Mg 1	0	0
24	N	1	Total 1	Mg 1	0	0
24	L	1	Total 1	Mg 1	0	0
24	M	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	17	Total 17	K 17	0	0

- Molecule 26 is (1R,2R,3S,4R,6S)-4,6-DIAMINO-2-{{[3-O-(2,6-DIAMINO-2,6-DIDEOXY-BETA-L-IDOPYRANOSYL)-BETA-D-RIBOFURANOSYL]OXY}-3-HYDROXYCYCLOHEXYL 2-AMINO-4,6-O-BENZYLIDENE-2-DEOXY-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: ON0) (formula: C<sub>30</sub>H<sub>49</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			49	30	5	14		

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

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

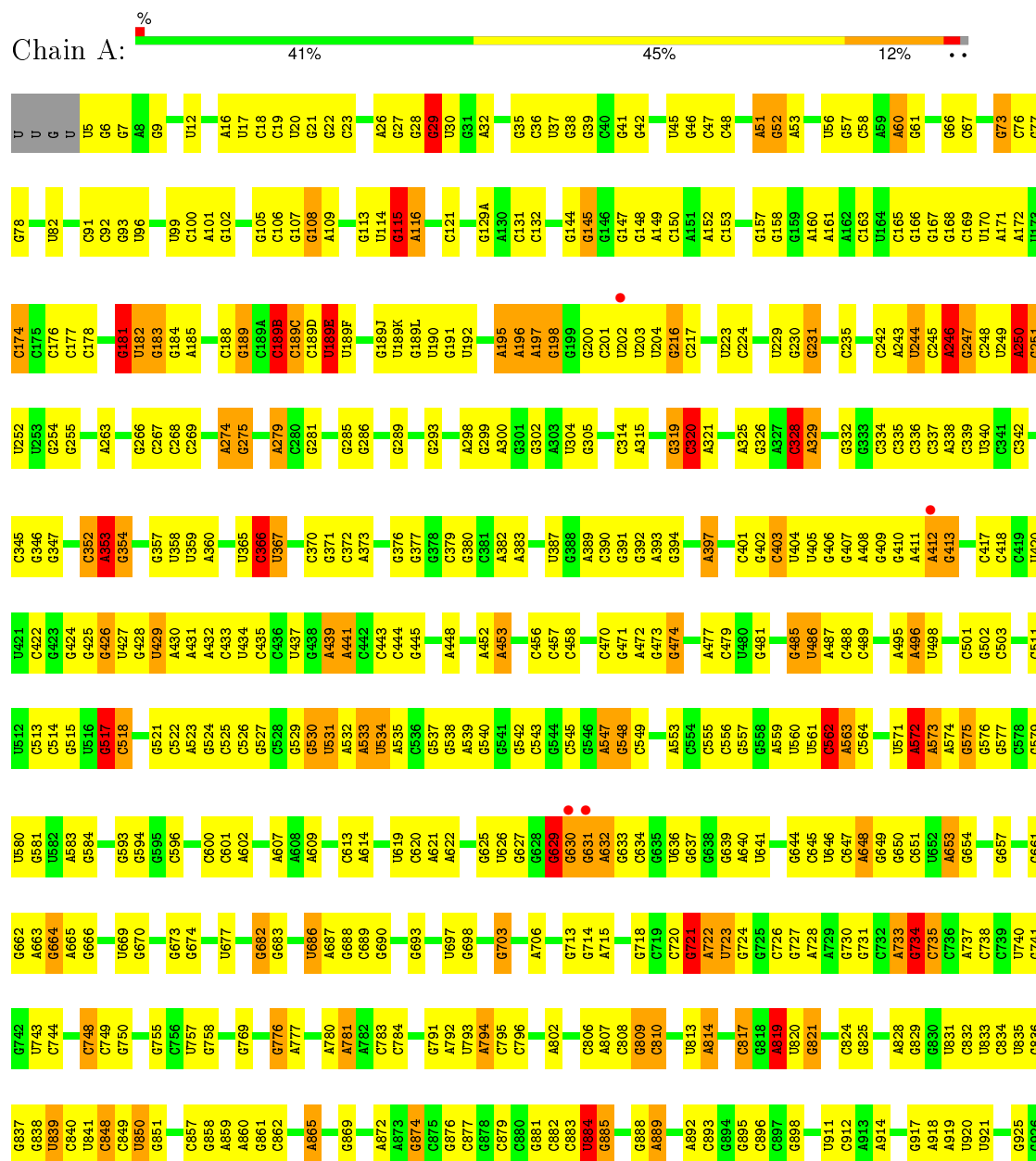
- Molecule 28 is water.

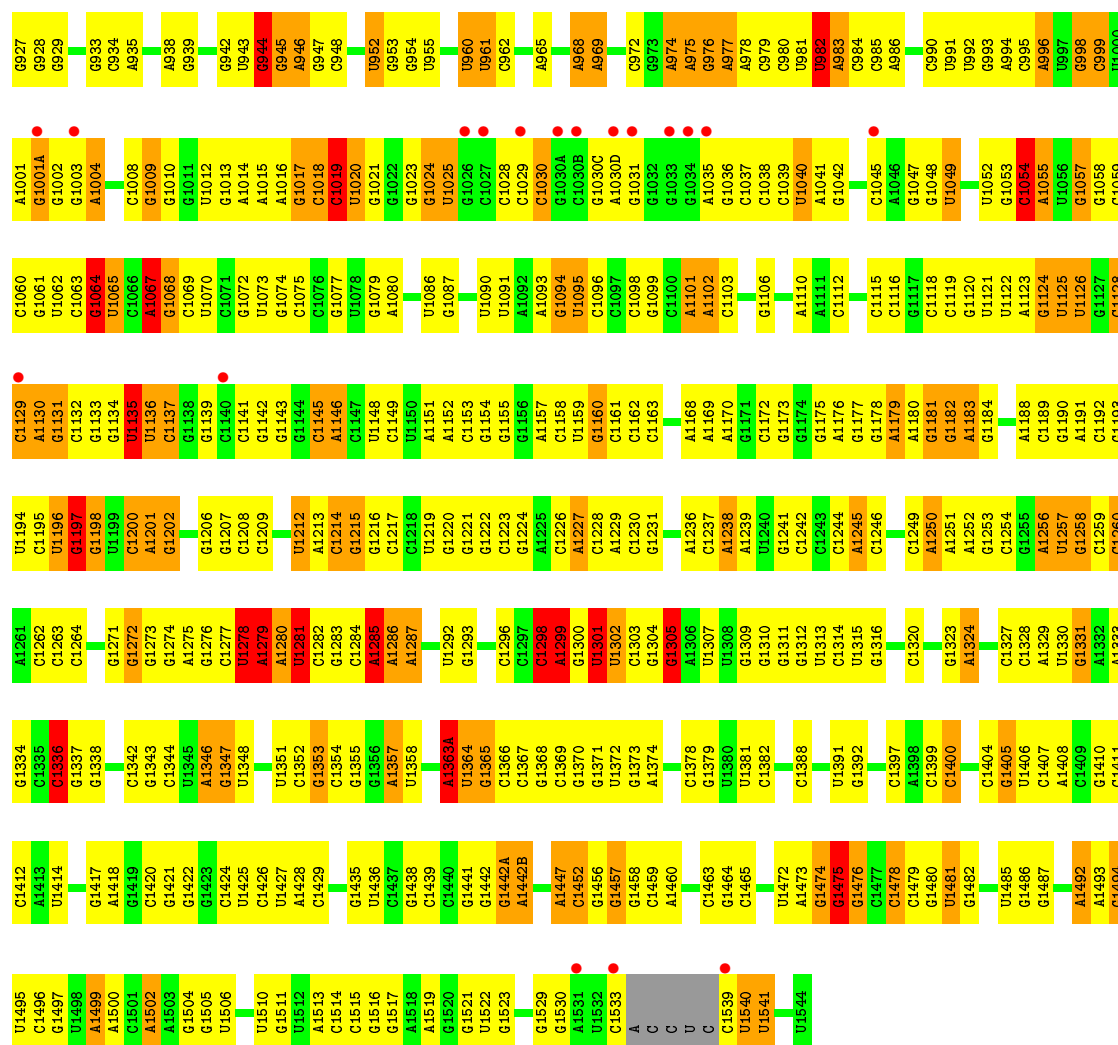
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	7	Total	O	0	0
			7	7		

### 3 Residue-property plots

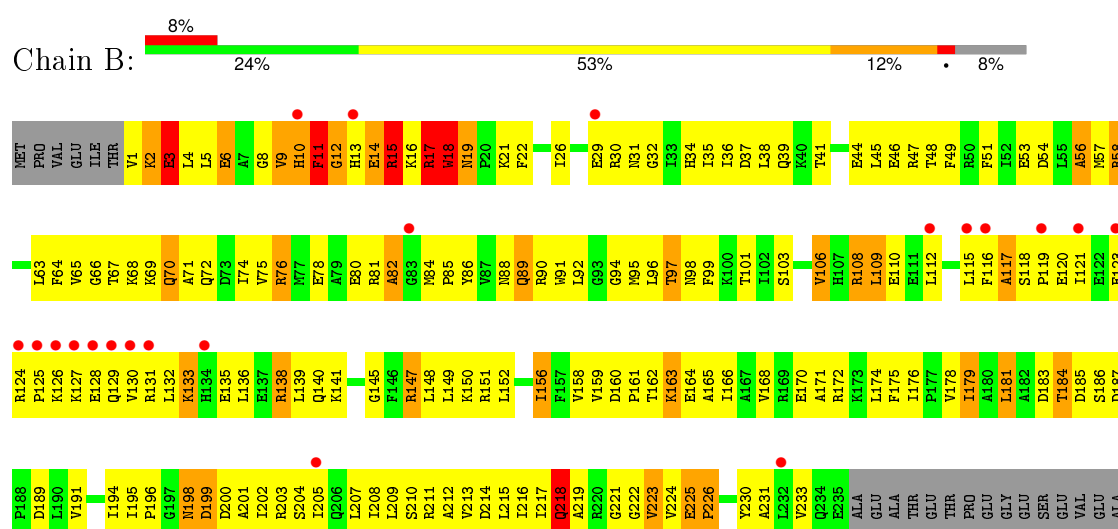
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16S RIBOSOMAL RNA



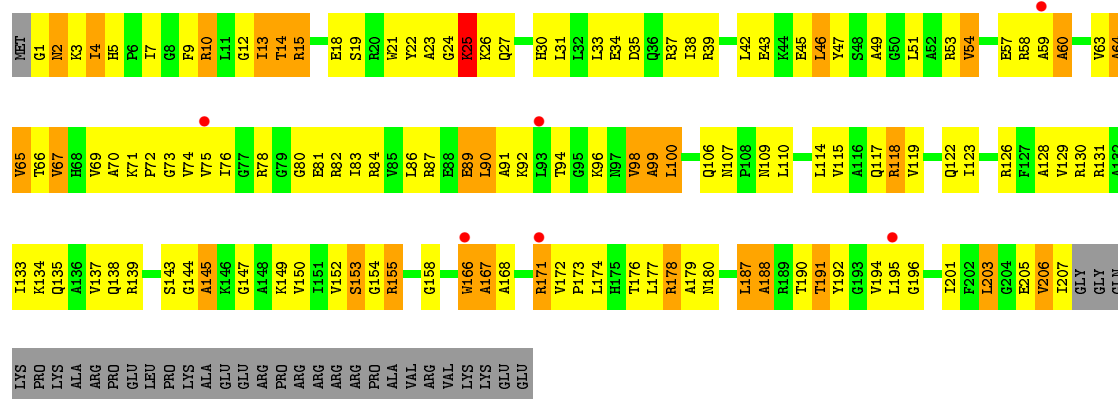


### • Molecule 2: 30S RIBOSOMAL PROBLEM S2

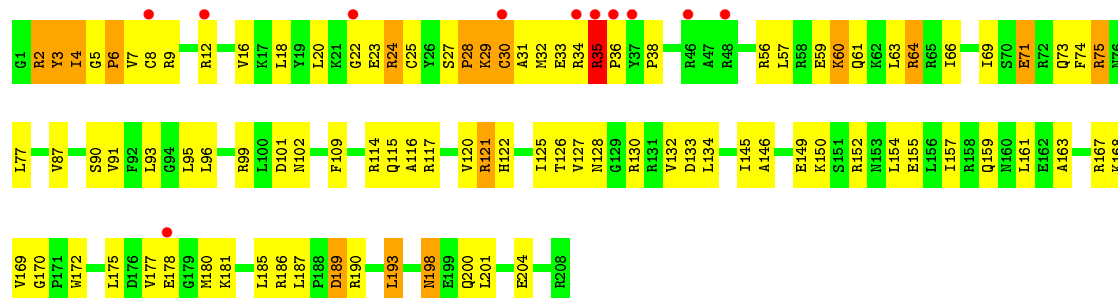


### • Molecule 3: 30S RIBOSOMAL PROBLEM S3

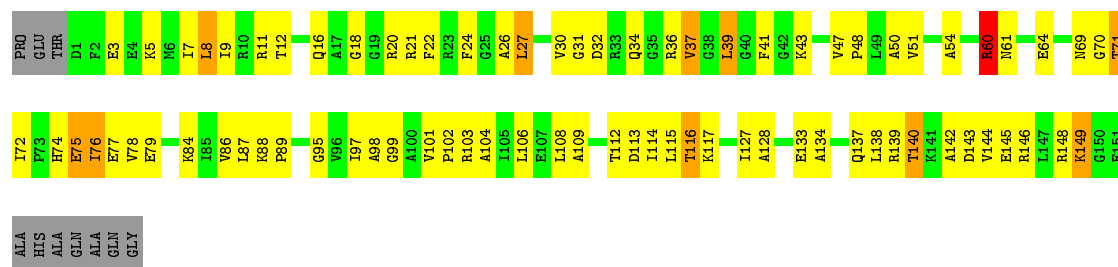




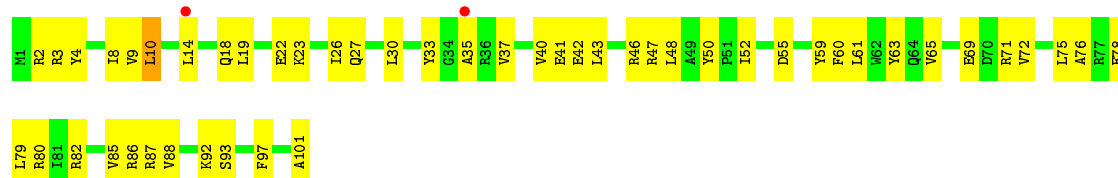
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



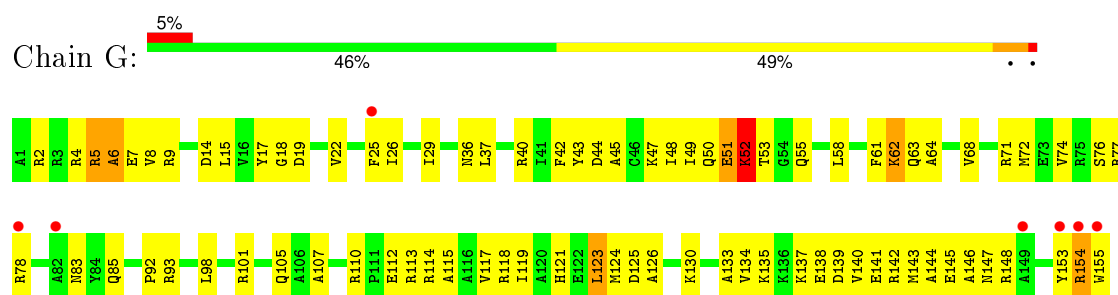
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5



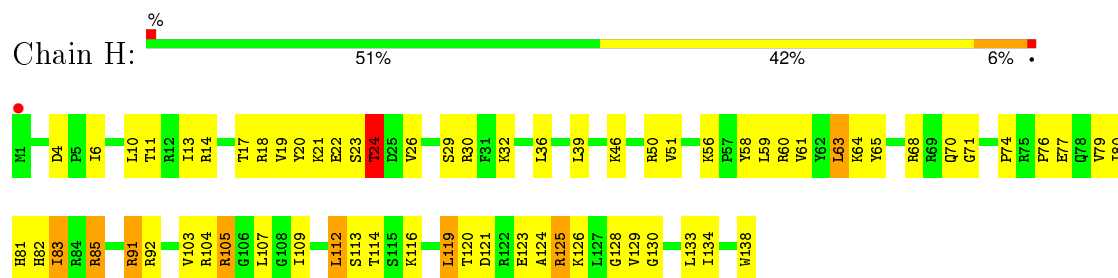
### • Molecule 6: 30S RIBOSOMAL PROTEIN S6



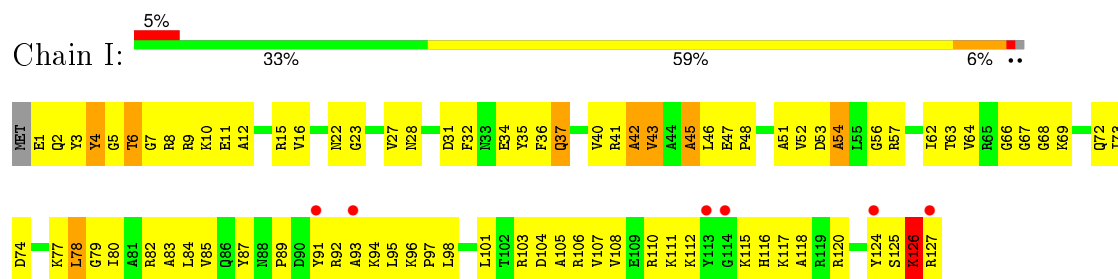
### • Molecule 7: 30S RIBOSOMAL PROTEIN S7



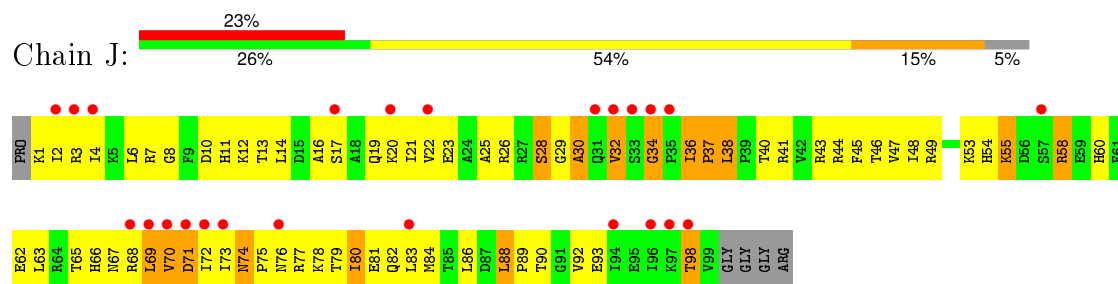
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



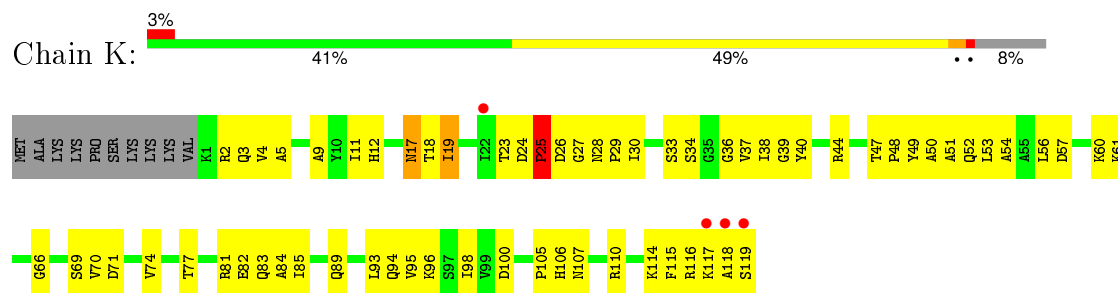
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



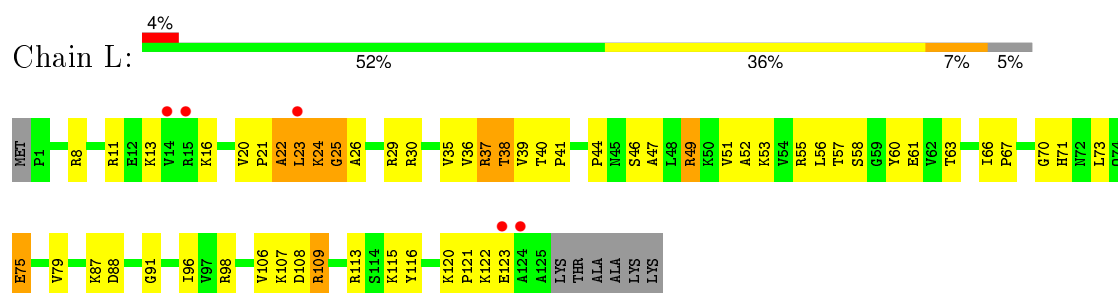
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



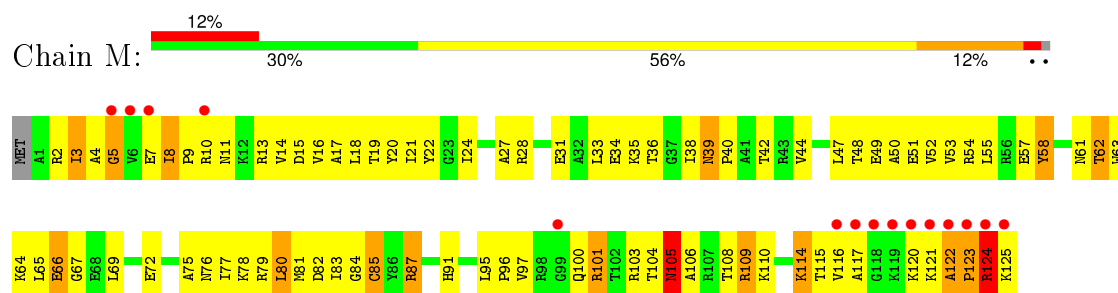
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



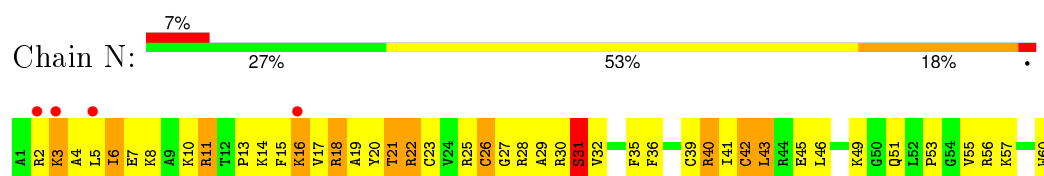
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



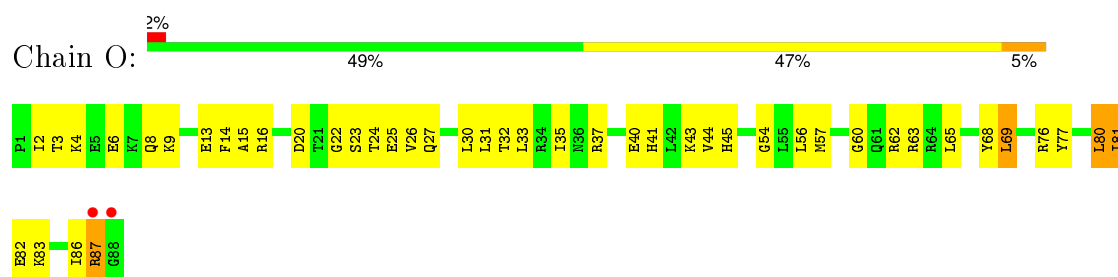
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



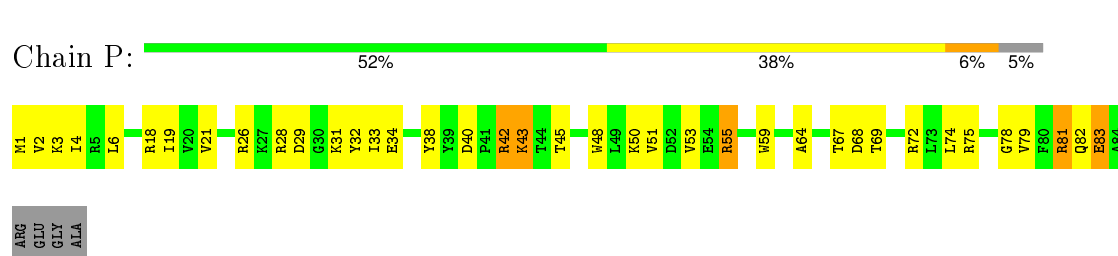
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



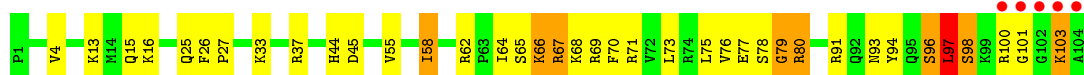
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



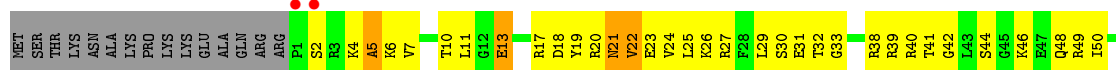
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



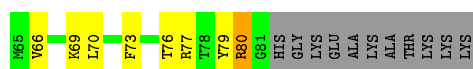
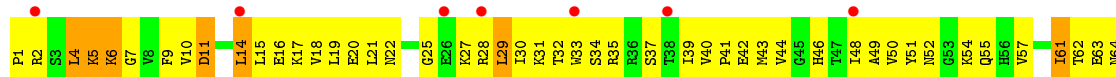




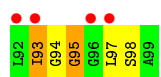
● Molecule 18: 30S RIBOSOMAL PROTEIN S18



● Molecule 19: 30S RIBOSOMAL PROTEIN S19



● Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

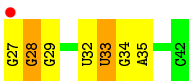


- Molecule 22: 5'-R(\*UP\*UP\*CP\*AP\*AP\*AP)-3'



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.65Å 401.65Å 175.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 39.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.90) 99.6 (39.77-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.218 , 0.251 0.222 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 311372 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	52505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ON0, K, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/36362	0.76	66/56750 (0.1%)
2	B	0.36	0/1936	0.64	0/2611
3	C	0.40	0/1637	0.64	0/2207
4	D	0.38	0/1733	0.60	0/2318
5	E	0.47	0/1163	0.72	1/1566 (0.1%)
6	F	0.36	0/856	0.59	0/1154
7	G	0.37	0/1276	0.59	0/1709
8	H	0.44	0/1136	0.73	0/1527
9	I	0.37	0/1029	0.64	0/1378
10	J	0.38	0/808	0.66	0/1087
11	K	0.39	0/900	0.70	1/1213 (0.1%)
12	L	0.47	0/987	0.78	0/1322
13	M	0.34	0/1008	0.62	0/1347
14	N	0.46	0/501	0.76	0/664
15	O	0.38	0/745	0.61	0/992
16	P	0.43	0/717	0.70	0/965
17	Q	0.47	0/870	0.75	1/1159 (0.1%)
18	R	0.35	0/603	0.62	0/799
19	S	0.48	0/662	0.68	0/892
20	T	0.40	0/764	0.69	0/1006
21	V	0.53	0/213	0.59	0/279
22	W	0.43	0/137	0.65	0/211
23	Z	0.42	0/383	0.68	0/596
All	All	0.44	0/56426	0.73	69/83752 (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	48	44

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	944	G	N9-C1'-C2'	11.13	128.47	114.00
1	A	1064	G	N9-C1'-C2'	10.84	128.09	114.00
1	A	189(B)	C	N1-C1'-C2'	10.52	127.68	114.00
1	A	944	G	C5'-C4'-O4'	10.10	121.22	109.10
1	A	884	U	C2'-C3'-O3'	9.69	130.81	109.50
1	A	562	C	N1-C1'-C2'	9.59	126.47	114.00
1	A	819	A	C5'-C4'-O4'	9.25	120.20	109.10
1	A	517	G	N9-C1'-C2'	9.20	125.96	114.00
1	A	60	A	C2'-C3'-O3'	8.96	129.22	109.50
1	A	115	G	N9-C1'-C2'	8.95	125.64	114.00
1	A	246	A	N9-C1'-C2'	8.80	125.44	114.00
1	A	496	A	C2'-C3'-O3'	8.65	128.54	109.50
1	A	629	G	N9-C1'-C2'	8.57	125.14	114.00
1	A	1067	A	N9-C1'-C2'	8.54	125.10	114.00
1	A	1363(A)	A	N9-C1'-C2'	8.02	124.42	114.00
1	A	944	G	O4'-C1'-N9	-8.00	101.80	108.20
1	A	572	A	C2'-C3'-O3'	7.78	126.61	109.50
1	A	1019	C	N1-C1'-C2'	7.76	124.09	114.00
1	A	1298	C	N1-C1'-C2'	7.65	123.95	114.00
1	A	721	G	N9-C1'-C2'	7.61	123.89	114.00
1	A	366	C	N1-C1'-C2'	7.49	123.74	114.00
1	A	1336	C	C2'-C3'-O3'	7.49	125.98	109.50
1	A	1278	U	N1-C1'-C2'	7.47	123.71	114.00
1	A	1298	C	C2'-C3'-O3'	7.19	125.31	109.50
1	A	196	A	C2'-C3'-O3'	7.16	125.25	109.50
1	A	1299	A	N9-C1'-C2'	7.02	123.13	114.00
1	A	1197	G	C2'-C3'-O3'	6.99	124.88	113.70
1	A	1019	C	C2'-C3'-O3'	6.95	124.82	113.70
1	A	982	U	N1-C1'-C2'	6.78	122.81	114.00
1	A	1502	A	N9-C1'-C2'	6.71	122.73	114.00
1	A	1054	C	C2'-C3'-O3'	6.61	124.27	113.70
1	A	189(B)	C	C5'-C4'-C3'	6.54	126.46	116.00
5	E	60	ARG	N-CA-C	-6.51	93.41	111.00
1	A	1064	G	C5'-C4'-O4'	6.46	116.86	109.10
1	A	721	G	C5'-C4'-O4'	6.43	116.81	109.10
1	A	328	C	N1-C1'-C2'	6.38	122.29	114.00
1	A	944	G	C2'-C3'-O3'	6.35	123.86	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	U	C5'-C4'-C3'	6.31	126.10	116.00
1	A	102	G	C5'-C4'-C3'	-6.29	105.94	116.00
1	A	629	G	C2'-C3'-O3'	6.28	123.75	113.70
1	A	819	A	N9-C1'-C2'	6.22	122.08	114.00
1	A	1278	U	C5'-C4'-O4'	6.15	116.47	109.10
1	A	563	A	C5'-C4'-C3'	-6.14	106.18	116.00
1	A	1135	U	N1-C1'-C2'	5.98	121.78	114.00
1	A	189(B)	C	O4'-C4'-C3'	-5.90	98.10	104.00
1	A	944	G	O4'-C4'-C3'	-5.88	98.12	104.00
1	A	982	U	C2'-C3'-O3'	5.88	123.11	113.70
1	A	189(E)	U	N1-C1'-C2'	5.84	121.59	114.00
1	A	1301	U	N1-C1'-C2'	5.75	121.48	114.00
1	A	776	G	C2'-C3'-O3'	5.67	122.77	113.70
1	A	189(E)	U	C2'-C3'-O3'	5.62	122.70	113.70
1	A	734	G	C5'-C4'-C3'	-5.62	107.02	116.00
1	A	748	C	C2'-C3'-O3'	5.57	122.61	113.70
1	A	181	G	N9-C1'-C2'	5.56	121.23	114.00
1	A	320	C	C5'-C4'-O4'	-5.55	102.44	109.10
17	Q	66	LYS	N-CA-C	-5.53	96.08	111.00
1	A	353	A	C5'-C4'-O4'	-5.48	102.53	109.10
1	A	1285	A	C2'-C3'-O3'	5.47	122.46	113.70
1	A	1363(A)	A	O4'-C1'-N9	5.37	112.50	108.20
1	A	1278	U	C5'-C4'-C3'	5.28	124.45	116.00
1	A	686	U	N1-C1'-C2'	5.24	120.82	114.00
1	A	602	A	C5'-C4'-C3'	-5.24	107.62	116.00
1	A	29	G	C5'-C4'-O4'	-5.20	102.86	109.10
1	A	517	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	1067	A	C1'-O4'-C4'	-5.16	105.77	109.90
1	A	1135	U	C2'-C3'-O3'	5.16	121.95	113.70
11	K	27	GLY	N-CA-C	5.13	125.92	113.10
1	A	1057	G	C5'-C4'-C3'	-5.11	107.83	116.00
1	A	224	C	C5'-C4'-C3'	-5.09	107.85	116.00

All (48) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C4'
1	A	189(B)	C	C4',C3',C1'
1	A	189(E)	U	C4',C3'
1	A	196	A	C3'
1	A	246	A	C4',C3',C1'
1	A	366	C	C4'

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Mol	Chain	Res	Type	Atom
1	A	517	G	C4',C3',C1'
1	A	562	C	C4'
1	A	629	G	C4',C3',C1'
1	A	721	G	C4',C3',C1'
1	A	776	G	C3'
1	A	819	A	C4',C3',C1'
1	A	884	U	C3'
1	A	944	G	C4',C1'
1	A	982	U	C4'
1	A	1019	C	C4',C3',C1'
1	A	1064	G	C4',C3',C1'
1	A	1067	A	C4'
1	A	1135	U	C4',C3'
1	A	1278	U	C4',C1'
1	A	1298	C	C4',C3'
1	A	1336	C	C4',C3'
1	A	1346	A	C4'
1	A	1363(A)	A	C4',C3',C1'

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	U	Sidechain
1	A	1077	G	Sidechain
1	A	1079	G	Sidechain
1	A	108	G	Sidechain
1	A	12	U	Sidechain
1	A	1279	A	Sidechain
1	A	1281	U	Sidechain
1	A	1299	A	Sidechain
1	A	1301	U	Sidechain
1	A	1305	G	Sidechain
1	A	1331	G	Sidechain
1	A	1405	G	Sidechain
1	A	1414	U	Sidechain
1	A	1457	G	Sidechain
1	A	1475	G	Sidechain
1	A	1492	A	Sidechain
1	A	1519	A	Sidechain
1	A	189(B)	C	Sidechain
1	A	195	A	Sidechain
1	A	246	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	250	A	Sidechain
1	A	274	A	Sidechain
1	A	380	G	Sidechain
1	A	387	U	Sidechain
1	A	481	G	Sidechain
1	A	529	G	Sidechain
1	A	560	U	Sidechain
1	A	562	C	Sidechain
1	A	571	U	Sidechain
1	A	629	G	Sidechain
1	A	641	U	Sidechain
1	A	664	G	Sidechain
1	A	682	G	Sidechain
1	A	721	G	Sidechain
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	73	G	Sidechain
1	A	733	A	Sidechain
1	A	874	G	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	944	G	Sidechain
1	A	946	A	Sidechain
1	A	952	U	Sidechain

## 5.2 Too-close contacts [i](#)

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	32486	0	16403	937	0
2	B	1901	0	1954	226	0
3	C	1613	0	1680	206	0
4	D	1703	0	1767	117	0
5	E	1147	0	1210	90	0
6	F	843	0	857	57	0
7	G	1257	0	1299	85	0
8	H	1116	0	1177	63	0
9	I	1011	0	1045	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	795	0	843	112	0
11	K	885	0	907	62	0
12	L	971	0	1059	71	0
13	M	997	0	1075	105	0
14	N	492	0	534	51	0
15	O	734	0	773	40	0
16	P	701	0	720	34	0
17	Q	857	0	932	38	0
18	R	597	0	670	68	0
19	S	648	0	675	91	0
20	T	762	0	862	43	0
21	V	209	0	221	12	0
22	W	123	0	66	8	0
23	Z	342	0	175	11	0
24	A	223	0	0	0	0
24	B	1	0	0	0	0
24	D	1	0	0	0	0
24	E	3	0	0	0	0
24	H	4	0	0	0	0
24	I	1	0	0	0	0
24	K	1	0	0	0	0
24	L	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
24	T	1	0	0	0	0
24	Z	1	0	0	0	0
25	A	17	0	0	0	0
26	A	49	0	49	2	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	7	0	0	0	0
All	All	52505	0	36953	2412	0

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

All (2412) 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:1029:C:H2'	1:A:1030:C:H5''	1.24	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:A:H4'	1:A:1102:A:H5'	1.21	1.14
1:A:1023:G:H3'	1:A:1024:G:H5''	1.16	1.14
1:A:1271:G:H2'	1:A:1272:G:H5''	1.31	1.11
10:J:30:ALA:HB2	10:J:74:ASN:HD22	1.16	1.09
1:A:1540:U:H2'	1:A:1541:U:H5''	1.33	1.09
1:A:1008:C:H2'	1:A:1009:G:H5''	1.29	1.09
1:A:402:G:H2'	1:A:403:C:H5''	1.32	1.08
19:S:32:THR:HG22	19:S:34:SER:H	1.18	1.06
1:A:1060:C:C5	3:C:1:GLY:HA3	1.91	1.05
1:A:425:G:H2'	1:A:426:G:H5''	1.35	1.04
1:A:975:A:H4'	1:A:976:G:H5''	1.35	1.04
1:A:1128:C:H3'	1:A:1129:C:H5''	1.40	1.03
2:B:78:GLU:HB3	2:B:213:VAL:HG21	1.38	1.03
11:K:38:ILE:HG22	11:K:39:GLY:H	1.24	1.01
1:A:411:A:H2'	1:A:412:A:H5''	1.42	1.01
21:V:6:ARG:HD2	21:V:15:ARG:HH12	1.24	1.01
1:A:1357:A:H5'	1:A:1358:U:OP2	1.58	1.01
19:S:40:VAL:H	19:S:43:MET:HE3	1.22	1.01
1:A:1130:A:H3'	1:A:1131:G:H5'	1.39	1.01
1:A:144:G:H2'	1:A:145:G:H5''	1.41	0.99
1:A:1480:G:H2'	1:A:1481:U:H5''	1.42	0.99
1:A:1286:A:H2'	1:A:1287:A:H4'	1.45	0.98
1:A:38:G:H22	1:A:397:A:H5'	1.27	0.98
1:A:944:G:H4'	1:A:945:G:O5'	1.62	0.97
1:A:1277:C:HO2'	1:A:1279:A:H8	1.02	0.97
1:A:1281:U:H5'	1:A:1282:C:H5	1.30	0.97
1:A:1475:G:HO2'	1:A:1476:G:H8	0.99	0.97
1:A:1190:G:OP1	3:C:3:LYS:HA	1.65	0.97
1:A:1029:C:C2'	1:A:1030:C:H5''	1.95	0.96
1:A:1060:C:H5	3:C:1:GLY:HA3	1.29	0.95
11:K:44:ARG:O	11:K:47:THR:HG22	1.65	0.95
7:G:74:VAL:HG21	7:G:85:GLN:HB3	1.44	0.95
1:A:411:A:C2'	1:A:412:A:H5''	1.97	0.95
1:A:1244:C:H2'	1:A:1245:A:H5''	1.46	0.95
1:A:1063:C:H3'	1:A:1064:G:H5''	1.47	0.94
1:A:547:A:H4'	1:A:548:G:H5'	1.49	0.93
1:A:1399:C:H4'	1:A:1400:C:H5''	1.50	0.93
9:I:96:LYS:HB2	9:I:97:PRO:HD3	1.51	0.93
1:A:189(B):C:H6	1:A:189(B):C:H5''	1.34	0.93
10:J:25:ALA:HB2	10:J:83:LEU:HD11	1.50	0.93
1:A:402:G:C2'	1:A:403:C:H5''	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:C:H2'	1:A:648:A:H5''	1.49	0.92
1:A:473:G:C2'	1:A:474:G:H5''	1.99	0.92
1:A:664:G:H22	1:A:741:G:H1	1.18	0.92
13:M:9:PRO:HB2	13:M:17:ALA:HB1	1.48	0.92
1:A:647:C:C2'	1:A:648:A:H5''	2.01	0.91
11:K:17:ASN:HD22	11:K:18:THR:N	1.68	0.91
1:A:1195:C:H3'	1:A:1196:U:C5'	2.00	0.91
11:K:89:GLN:HG2	11:K:95:VAL:HG21	1.51	0.91
5:E:76:ILE:CD1	5:E:87:LEU:HB2	2.01	0.90
1:A:850:U:H6	1:A:850:U:H5'	1.36	0.90
3:C:25:LYS:H	3:C:25:LYS:HD3	1.36	0.90
1:A:998:G:H3'	1:A:999:C:H5''	1.53	0.89
1:A:425:G:C2'	1:A:426:G:H5''	2.02	0.89
3:C:49:ALA:HB1	3:C:69:VAL:HG11	1.53	0.89
1:A:250:A:H4'	1:A:251:G:O5'	1.69	0.89
1:A:51:A:H5''	1:A:52:G:H5''	1.53	0.89
2:B:71:ALA:HB2	2:B:205:ILE:HD13	1.52	0.89
10:J:48:ILE:HD12	10:J:48:ILE:H	1.38	0.89
1:A:1271:G:C2'	1:A:1272:G:H5''	2.02	0.88
20:T:93:ILE:HG22	20:T:95:GLY:H	1.38	0.88
4:D:28:PRO:O	4:D:29:LYS:HG3	1.73	0.87
1:A:1145:C:O2'	1:A:1146:A:H5'	1.73	0.87
10:J:29:GLY:HA2	10:J:76:ASN:HD22	1.40	0.87
3:C:13:ILE:HG22	3:C:14:THR:H	1.38	0.87
1:A:530:G:O6	22:W:3:C:H1'	1.75	0.87
11:K:17:ASN:HD22	11:K:18:THR:H	0.92	0.87
18:R:71:VAL:O	18:R:72:ARG:HG2	1.75	0.87
3:C:12:GLY:HA3	14:N:56:ARG:HH21	1.40	0.87
11:K:17:ASN:ND2	11:K:18:THR:H	1.73	0.87
1:A:1366:C:H2'	1:A:1367:C:H6	1.39	0.86
4:D:149:GLU:HG3	4:D:152:ARG:HH22	1.39	0.86
5:E:76:ILE:HD11	5:E:87:LEU:HB2	1.56	0.86
3:C:5:HIS:HD2	3:C:7:ILE:H	1.20	0.86
17:Q:66:LYS:HA	17:Q:69:ARG:HH12	1.40	0.86
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.57	0.86
1:A:1346:A:H61	1:A:1374:A:H5''	1.38	0.86
1:A:972:C:H4'	10:J:55:LYS:HG2	1.57	0.86
1:A:1130:A:H3'	1:A:1131:G:C5'	2.06	0.85
13:M:2:ARG:HA	13:M:7:GLU:O	1.77	0.85
1:A:1197:G:C2'	1:A:1198:G:H5''	2.06	0.84
1:A:1244:C:C2'	1:A:1245:A:H5''	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:GLU:O	14:N:10:LYS:HB2	1.76	0.84
1:A:838:G:H2'	1:A:839:U:H5''	1.59	0.84
1:A:1281:U:H5'	1:A:1282:C:C5	2.11	0.84
13:M:48:THR:HG22	13:M:50:ALA:H	1.42	0.84
1:A:1367:C:H5'	10:J:58:ARG:HH11	1.41	0.84
1:A:144:G:C2'	1:A:145:G:H5''	2.05	0.83
12:L:23:LEU:HD23	12:L:24:LYS:HB2	1.58	0.83
5:E:88:LYS:HB3	5:E:115:LEU:HB2	1.61	0.83
1:A:1480:G:C2'	1:A:1481:U:H5''	2.07	0.83
15:O:16:ARG:HG3	15:O:16:ARG:HH11	1.43	0.83
4:D:25:CYS:HA	4:D:30:CYS:HB2	1.61	0.83
1:A:1197:G:O2'	1:A:1198:G:H5''	1.76	0.83
15:O:54:GLY:HA2	15:O:57:MET:HE3	1.60	0.83
1:A:473:G:H2'	1:A:474:G:C5'	2.09	0.82
18:R:7:VAL:O	18:R:11:LEU:HD23	1.79	0.82
11:K:9:ALA:HB2	11:K:70:VAL:HG11	1.62	0.82
2:B:89:GLN:O	2:B:90:ARG:HD2	1.79	0.82
4:D:35:ARG:H	4:D:36:PRO:HD3	1.43	0.82
1:A:1502:A:H2	1:A:1505:G:H1	1.23	0.82
1:A:473:G:O2'	1:A:474:G:H5''	1.79	0.82
1:A:320:C:H5'	1:A:320:C:H6	1.42	0.82
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.79	0.82
1:A:473:G:H2'	1:A:474:G:H5''	1.60	0.82
2:B:63:LEU:HD12	2:B:149:LEU:HD11	1.61	0.81
1:A:1123:A:H4'	10:J:34:GLY:HA3	1.60	0.81
1:A:579:G:H5'	1:A:728:A:H1'	1.61	0.81
10:J:30:ALA:HB2	10:J:74:ASN:ND2	1.94	0.81
1:A:1023:G:H3'	1:A:1024:G:C5'	2.05	0.81
3:C:57:GLU:HB3	10:J:90:THR:HG21	1.62	0.81
1:A:1367:C:H5'	10:J:58:ARG:NH1	1.96	0.81
1:A:984:C:H2'	1:A:985:C:H6	1.46	0.81
1:A:522:C:H41	12:L:49:ARG:HH22	1.29	0.81
1:A:1008:C:C2'	1:A:1009:G:H5''	2.08	0.80
2:B:96:LEU:HD21	2:B:156:ILE:HD11	1.62	0.80
3:C:33:LEU:O	3:C:33:LEU:HD23	1.79	0.80
5:E:77:GLU:HG2	5:E:86:VAL:HG22	1.63	0.80
2:B:118:SER:HB2	2:B:119:PRO:HD2	1.64	0.80
1:A:953:G:H1'	13:M:124:ARG:HA	1.64	0.80
2:B:191:VAL:HB	2:B:194:ILE:HG12	1.62	0.80
1:A:1063:C:H3'	1:A:1064:G:C5'	2.12	0.80
3:C:27:GLN:HA	3:C:30:HIS:HD2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:THR:O	3:C:15:ARG:HB2	1.81	0.79
2:B:85:PRO:HG3	2:B:148:LEU:HB2	1.62	0.79
1:A:1086:U:H3	1:A:1099:G:H22	1.29	0.79
21:V:6:ARG:HD2	21:V:15:ARG:NH1	1.97	0.79
15:O:25:GLU:HG3	15:O:80:LEU:HG	1.64	0.79
5:E:32:ASP:OD2	5:E:36:ARG:HB2	1.82	0.79
6:F:33:TYR:HA	6:F:71:ARG:NH2	1.97	0.79
1:A:975:A:H4'	1:A:976:G:C5'	2.12	0.79
12:L:21:PRO:O	12:L:23:LEU:N	2.16	0.79
18:R:38:ARG:NH1	18:R:44:SER:HA	1.98	0.79
1:A:1540:U:C2'	1:A:1541:U:H5''	2.10	0.79
1:A:1063:C:C3'	1:A:1064:G:H5''	2.12	0.79
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.65	0.79
9:I:42:ALA:HA	9:I:73:ILE:HD13	1.65	0.79
1:A:677:U:H3	1:A:713:G:H22	1.27	0.79
13:M:80:LEU:HD13	13:M:87:ARG:NH1	1.98	0.79
1:A:693:G:C5	1:A:1539:C:H1'	2.17	0.78
12:L:55:ARG:HD3	12:L:61:GLU:HG3	1.63	0.78
11:K:38:ILE:HD13	11:K:53:LEU:HB3	1.66	0.78
6:F:80:ARG:NH1	6:F:88:VAL:HB	1.98	0.78
10:J:29:GLY:HA2	10:J:76:ASN:ND2	1.97	0.78
19:S:32:THR:HG22	19:S:34:SER:N	1.96	0.78
1:A:1330:U:H2'	1:A:1331:G:H5'	1.64	0.78
1:A:293:G:H5'	1:A:609:A:H61	1.48	0.78
1:A:1502:A:H2	1:A:1505:G:N1	1.81	0.78
1:A:648:A:H8	1:A:648:A:H5'	1.48	0.78
5:E:47:VAL:HB	5:E:48:PRO:HD3	1.63	0.78
4:D:24:ARG:NH1	4:D:29:LYS:HD3	1.99	0.78
2:B:17:ARG:C	2:B:17:ARG:HH11	1.87	0.78
1:A:342:C:H42	1:A:347:G:H1	1.29	0.78
13:M:80:LEU:H	13:M:80:LEU:HD23	1.46	0.77
1:A:113:G:H1'	1:A:354:G:H5'	1.65	0.77
1:A:1038:C:H2'	1:A:1039:C:H6	1.49	0.77
1:A:839:U:O2	1:A:839:U:H2'	1.84	0.77
1:A:1425:U:H2'	1:A:1426:C:C6	2.18	0.77
2:B:166:ILE:H	2:B:166:ILE:HD12	1.50	0.77
1:A:1284:C:H3'	1:A:1285:A:H5''	1.64	0.77
4:D:35:ARG:H	4:D:36:PRO:CD	1.97	0.77
1:A:420:U:H2'	1:A:422:C:C5	2.19	0.77
12:L:71:HIS:HD2	12:L:73:LEU:H	1.32	0.77
1:A:975:A:H5'	1:A:975:A:H8	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:ARG:HD3	12:L:58:SER:HB3	1.65	0.77
1:A:1369:C:H2'	1:A:1370:G:C8	2.20	0.77
11:K:38:ILE:HG22	11:K:39:GLY:N	1.98	0.77
1:A:849:C:C3'	1:A:850:U:H5''	2.14	0.76
1:A:411:A:H2'	1:A:412:A:C5'	2.13	0.76
1:A:734:G:H5''	1:A:734:G:C8	2.21	0.76
10:J:82:GLN:O	10:J:86:LEU:HD12	1.85	0.76
1:A:1125:U:H5'	1:A:1126:U:H5	1.50	0.76
1:A:275:G:H5''	17:Q:13:LYS:HB3	1.66	0.76
1:A:1343:G:H2'	1:A:1344:C:C6	2.20	0.76
1:A:981:U:H3'	1:A:982:U:O4'	1.85	0.76
17:Q:58:ILE:HG23	17:Q:70:PHE:CD1	2.21	0.76
1:A:188:C:C2'	1:A:189:G:H5''	2.16	0.75
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.68	0.75
19:S:4:LEU:O	19:S:5:LYS:HB2	1.86	0.75
1:A:1057:G:H5'	3:C:153:SER:HB2	1.67	0.75
1:A:1197:G:H2'	1:A:1198:G:C5'	2.16	0.75
18:R:29:LEU:HD11	18:R:64:LEU:HD22	1.69	0.75
1:A:188:C:C3'	1:A:189:G:H5''	2.17	0.74
1:A:1330:U:C2'	1:A:1331:G:H5'	2.18	0.74
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.74
1:A:274:A:H4'	1:A:275:G:OP2	1.86	0.74
7:G:22:VAL:O	7:G:26:ILE:HG13	1.87	0.74
1:A:51:A:H5''	1:A:52:G:C5'	2.18	0.74
3:C:69:VAL:HG12	3:C:71:LYS:H	1.53	0.74
1:A:1223:C:P	19:S:77:ARG:HH12	2.09	0.74
1:A:189:G:H5'	1:A:189:G:H8	1.52	0.74
4:D:149:GLU:HG3	4:D:152:ARG:NH2	2.03	0.74
1:A:1230:C:H1'	13:M:125:LYS:HA	1.69	0.74
3:C:57:GLU:HB2	3:C:64:ALA:HB3	1.70	0.74
20:T:43:GLU:HG3	20:T:93:ILE:HG12	1.69	0.73
1:A:1023:G:C3'	1:A:1024:G:H5''	2.10	0.73
2:B:209:LEU:O	2:B:213:VAL:HG23	1.89	0.73
1:A:1346:A:N6	1:A:1374:A:H5''	2.03	0.73
13:M:48:THR:HB	13:M:51:GLU:HG3	1.69	0.73
1:A:841:U:H3'	1:A:848:C:O4'	1.88	0.73
1:A:647:C:H2'	1:A:648:A:C5'	2.18	0.73
1:A:1366:C:H2'	1:A:1367:C:C6	2.23	0.73
6:F:97:PHE:HB2	18:R:17:ARG:NH2	2.02	0.73
5:E:5:LYS:HG3	5:E:108:LEU:HD11	1.71	0.73
1:A:1197:G:H2'	1:A:1198:G:H5''	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:C:H2'	1:A:1162:C:H6	1.53	0.73
1:A:1231:G:H4'	9:I:125:SER:OG	1.89	0.73
1:A:1195:C:H3'	1:A:1196:U:H5'	1.71	0.73
12:L:41:PRO:HG3	12:L:49:ARG:HD3	1.70	0.73
19:S:4:LEU:HD11	19:S:69:LYS:HZ1	1.53	0.73
1:A:189(B):C:OP2	1:A:189(B):C:H3'	1.88	0.72
1:A:35:G:H2'	1:A:36:C:C6	2.24	0.72
11:K:12:HIS:HB3	11:K:19:ILE:HG23	1.71	0.72
1:A:189(B):C:C5'	1:A:189(B):C:H6	2.02	0.72
1:A:353:A:H8	1:A:353:A:H5'	1.54	0.72
12:L:37:ARG:HH12	12:L:53:LYS:HZ1	1.34	0.72
1:A:946:A:H2'	1:A:947:G:C8	2.25	0.72
1:A:849:C:H2'	1:A:850:U:H5''	1.72	0.72
12:L:37:ARG:HH12	12:L:53:LYS:NZ	1.87	0.72
3:C:65:VAL:HG12	3:C:66:THR:N	2.03	0.72
18:R:21:ASN:ND2	18:R:23:GLU:HG2	2.04	0.72
9:I:47:GLU:N	9:I:48:PRO:HD2	2.05	0.72
19:S:52:ASN:HD21	19:S:55:GLN:HB2	1.53	0.72
5:E:11:ARG:HD3	5:E:22:PHE:CD1	2.24	0.72
1:A:1178:G:N2	1:A:1180:A:H3'	2.05	0.72
10:J:48:ILE:N	10:J:48:ILE:HD12	2.04	0.72
3:C:9:PHE:CE2	3:C:177:LEU:HD13	2.24	0.72
4:D:7:VAL:HG21	4:D:114:ARG:NH1	2.03	0.72
1:A:1101:A:C4'	1:A:1102:A:H5'	2.11	0.72
19:S:6:LYS:HG2	19:S:6:LYS:O	1.89	0.72
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.71	0.71
19:S:51:TYR:HA	19:S:55:GLN:O	1.89	0.71
1:A:1142:G:H2'	1:A:1143:G:O4'	1.90	0.71
3:C:65:VAL:HG12	3:C:66:THR:H	1.55	0.71
10:J:44:ARG:HG2	10:J:44:ARG:HH11	1.55	0.71
4:D:34:ARG:O	4:D:35:ARG:HB2	1.90	0.71
1:A:1001(A):G:H2'	1:A:1002:G:O4'	1.90	0.71
1:A:1095:U:H2'	1:A:1096:C:C6	2.25	0.71
3:C:128:ALA:HB3	3:C:131:ARG:HD2	1.72	0.71
1:A:29:G:H5'	1:A:29:G:H8	1.55	0.71
13:M:10:ARG:HA	13:M:44:VAL:HG21	1.71	0.71
1:A:1029:C:H2'	1:A:1030:C:C5'	2.14	0.71
19:S:54:LYS:HG2	19:S:55:GLN:HE21	1.56	0.71
4:D:61:GLN:HE22	4:D:64:ARG:HH12	1.38	0.71
1:A:1189:C:P	10:J:49:ARG:HH22	2.14	0.71
14:N:21:THR:HB	14:N:32:VAL:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:G:H8	1:A:474:G:H5'	1.55	0.71
13:M:48:THR:HG22	13:M:50:ALA:N	2.06	0.71
1:A:115:G:H2'	1:A:116:A:N7	2.05	0.71
18:R:38:ARG:HH11	18:R:44:SER:HA	1.55	0.71
5:E:144:VAL:O	5:E:148:ARG:HG2	1.90	0.71
1:A:188:C:H2'	1:A:189:G:H5''	1.71	0.71
2:B:67:THR:HB	2:B:164:GLU:OE2	1.90	0.71
10:J:36:ILE:HG13	10:J:69:LEU:HB3	1.73	0.70
1:A:990:C:H4'	1:A:1018:C:OP1	1.91	0.70
14:N:43:LEU:HD12	14:N:43:LEU:O	1.90	0.70
1:A:1286:A:H2'	1:A:1287:A:C4'	2.20	0.70
13:M:106:ALA:O	13:M:110:LYS:HG3	1.91	0.70
10:J:37:PRO:HA	10:J:68:ARG:HH11	1.56	0.70
1:A:412:A:H61	4:D:34:ARG:HB3	1.55	0.70
1:A:837:G:H1	1:A:849:C:H42	1.39	0.70
3:C:12:GLY:CA	14:N:56:ARG:HH21	2.03	0.70
13:M:3:ILE:HG22	13:M:4:ALA:N	2.06	0.70
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.07	0.70
10:J:3:ARG:HA	10:J:71:ASP:OD1	1.91	0.70
1:A:1052:U:H5'	1:A:1053:G:OP1	1.91	0.70
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.91	0.70
12:L:24:LYS:HD3	12:L:29:ARG:HH22	1.56	0.70
9:I:69:LYS:O	9:I:73:ILE:HG13	1.91	0.70
9:I:117:LYS:O	9:I:118:ALA:HB3	1.90	0.70
3:C:206:VAL:HG12	3:C:207:ILE:N	2.07	0.70
7:G:134:VAL:O	7:G:138:GLU:HG3	1.91	0.70
1:A:849:C:C2'	1:A:850:U:H5''	2.21	0.70
4:D:64:ARG:HD3	4:D:69:ILE:O	1.91	0.70
11:K:114:LYS:HD2	11:K:115:PHE:CE1	2.27	0.70
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.06	0.69
1:A:457:C:H2'	1:A:458:C:H6	1.58	0.69
15:O:86:ILE:HG22	15:O:87:ARG:HG3	1.74	0.69
1:A:1047:G:C2'	1:A:1048:G:H5'	2.21	0.69
1:A:969:A:H61	13:M:125:LYS:HE3	1.56	0.69
1:A:1250:A:H4'	9:I:67:GLY:H	1.57	0.69
19:S:21:LEU:O	19:S:21:LEU:HD23	1.93	0.69
2:B:212:ALA:O	2:B:216:ILE:HG13	1.91	0.69
1:A:838:G:C2'	1:A:839:U:H5''	2.23	0.69
14:N:17:VAL:HG23	14:N:18:ARG:H	1.56	0.69
17:Q:94:TYR:HA	17:Q:97:LEU:HD11	1.75	0.69
1:A:1472:U:H2'	1:A:1473:A:O4'	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:U:O4	10:J:3:ARG:HG3	1.93	0.69
1:A:1130:A:C3'	1:A:1131:G:H5'	2.21	0.69
1:A:189(B):C:C6	1:A:189(B):C:H5''	2.24	0.69
10:J:47:VAL:O	10:J:58:ARG:HA	1.91	0.69
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.75	0.69
15:O:15:ALA:HB1	15:O:20:ASP:HB3	1.75	0.69
15:O:3:THR:OG1	15:O:6:GLU:HB2	1.92	0.69
2:B:71:ALA:HB2	2:B:205:ILE:CD1	2.23	0.69
12:L:30:ARG:O	12:L:57:THR:HG23	1.92	0.69
1:A:1191:A:P	3:C:2:ASN:HD22	2.15	0.68
2:B:78:GLU:OE2	2:B:210:SER:HA	1.93	0.68
1:A:998:G:C3'	1:A:999:C:H5''	2.22	0.68
3:C:63:VAL:HB	3:C:98:VAL:HG11	1.76	0.68
13:M:44:VAL:HA	13:M:47:LEU:HG	1.73	0.68
1:A:1169:A:H2'	1:A:1170:A:C8	2.28	0.68
17:Q:103:LYS:HZ2	17:Q:103:LYS:HA	1.59	0.68
3:C:4:ILE:CD1	3:C:4:ILE:H	2.07	0.68
18:R:10:THR:HG22	18:R:27:ARG:NH1	2.07	0.68
6:F:101:ALA:HA	18:R:13:GLU:HG3	1.75	0.68
7:G:74:VAL:CG2	7:G:85:GLN:HB3	2.20	0.68
1:A:1305:G:N2	1:A:1331:G:H1'	2.09	0.68
1:A:28:G:C3'	1:A:29:G:H5''	2.23	0.68
1:A:817:C:C6	1:A:819:A:H2'	2.28	0.68
3:C:129:VAL:O	3:C:133:ILE:HG12	1.93	0.68
3:C:173:PRO:O	3:C:176:THR:HG22	1.93	0.68
19:S:15:LEU:O	19:S:19:LEU:HG	1.93	0.68
9:I:3:TYR:CD2	9:I:87:TYR:HA	2.27	0.68
1:A:437:U:H5''	4:D:154:LEU:HD22	1.75	0.68
1:A:750:G:N3	15:O:22:GLY:HA3	2.07	0.68
1:A:235:C:H5'	17:Q:69:ARG:HG2	1.75	0.68
11:K:19:ILE:C	11:K:19:ILE:HD13	2.13	0.68
1:A:1067:A:H2'	1:A:1068:G:O4'	1.93	0.68
1:A:888:G:H3'	1:A:889:A:H5''	1.75	0.68
8:H:112:LEU:HD23	8:H:112:LEU:N	2.09	0.68
26:A:2759:ON0:H1	26:A:2759:ON0:O1'	1.94	0.68
1:A:653:A:OP1	8:H:56:LYS:NZ	2.21	0.68
10:J:6:LEU:HB2	10:J:68:ARG:HB2	1.73	0.68
17:Q:93:ASN:O	17:Q:96:SER:HB3	1.93	0.68
5:E:70:GLY:HA3	5:E:112:THR:HG22	1.76	0.68
1:A:984:C:H2'	1:A:985:C:C6	2.27	0.68
23:Z:32:U:H2'	23:Z:33:U:C5'	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ILE:HD13	10:J:98:THR:OG1	1.94	0.68
1:A:1197:G:C2'	1:A:1198:G:C5'	2.71	0.68
3:C:66:THR:HG22	3:C:67:VAL:N	2.08	0.68
1:A:1346:A:C6	7:G:9:ARG:NH1	2.61	0.68
1:A:319:G:H2'	1:A:320:C:H5''	1.75	0.68
19:S:35:ARG:HH11	19:S:35:ARG:HG3	1.59	0.68
4:D:35:ARG:HH11	4:D:35:ARG:HG2	1.59	0.68
18:R:21:ASN:HD22	18:R:23:GLU:HG2	1.59	0.68
1:A:514:C:O2'	1:A:515:G:H5'	1.94	0.68
7:G:44:ASP:O	7:G:48:ILE:HG12	1.93	0.68
2:B:2:LYS:O	2:B:3:GLU:HB2	1.93	0.67
12:L:24:LYS:O	12:L:26:ALA:N	2.27	0.67
19:S:18:VAL:HG13	19:S:19:LEU:H	1.58	0.67
10:J:48:ILE:CD1	10:J:48:ILE:H	2.07	0.67
1:A:353:A:H5'	1:A:353:A:C8	2.30	0.67
16:P:67:THR:HG22	16:P:69:THR:H	1.59	0.67
2:B:10:HIS:CD2	2:B:204:SER:HB3	2.29	0.67
4:D:29:LYS:C	4:D:31:ALA:H	1.95	0.67
12:L:37:ARG:HG2	12:L:38:THR:H	1.59	0.67
4:D:198:ASN:HD21	4:D:200:GLN:HB3	1.59	0.67
1:A:1354:C:O2'	1:A:1355:G:H5'	1.93	0.67
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.77	0.67
3:C:4:ILE:HG12	3:C:9:PHE:HB2	1.77	0.67
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.77	0.67
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.59	0.67
9:I:15:ARG:HB2	9:I:63:THR:HB	1.77	0.67
1:A:613:C:O2'	1:A:614:A:H5'	1.93	0.67
1:A:580:U:H2'	1:A:581:G:O4'	1.94	0.67
19:S:62:THR:HG22	19:S:63:GLU:N	2.10	0.67
13:M:7:GLU:C	13:M:8:ILE:HD13	2.15	0.67
3:C:187:LEU:HD13	3:C:194:VAL:HG13	1.76	0.67
1:A:600:C:O2'	1:A:601:C:H5'	1.94	0.67
1:A:537:G:OP1	12:L:109:ARG:NH2	2.28	0.67
3:C:147:GLY:HA3	3:C:171:ARG:O	1.94	0.67
3:C:203:LEU:HD12	3:C:203:LEU:O	1.95	0.67
4:D:61:GLN:NE2	4:D:64:ARG:HH12	1.93	0.67
3:C:25:LYS:N	3:C:25:LYS:HD3	2.08	0.67
1:A:1004:A:H5''	1:A:1025:U:O2	1.94	0.67
3:C:133:ILE:O	3:C:137:VAL:HG23	1.94	0.67
1:A:1064:G:H21	1:A:1190:G:H2'	1.60	0.66
1:A:1480:G:C3'	1:A:1481:U:H5''	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:53:VAL:O	13:M:57:GLU:HG2	1.95	0.66
1:A:982:U:H5'	1:A:983:A:OP1	1.96	0.66
1:A:991:U:H2'	1:A:1212:U:O2	1.95	0.66
6:F:22:GLU:O	6:F:26:ILE:HG12	1.96	0.66
1:A:806:C:O2'	1:A:807:A:H5'	1.95	0.66
1:A:409:G:OP1	4:D:24:ARG:HB2	1.93	0.66
5:E:32:ASP:OD1	5:E:34:GLN:N	2.26	0.66
1:A:944:G:H4'	1:A:945:G:C5'	2.25	0.66
7:G:53:THR:HG22	7:G:55:GLN:H	1.61	0.66
5:E:76:ILE:HD13	5:E:87:LEU:HB2	1.75	0.66
1:A:319:G:C2'	1:A:320:C:H5''	2.25	0.66
1:A:1065:U:C5	1:A:1190:G:H1'	2.31	0.66
1:A:439:A:H2'	1:A:441:A:H5'	1.78	0.66
1:A:477:A:O2'	1:A:479:C:H5'	1.94	0.66
1:A:1327:C:O2'	1:A:1328:C:H5'	1.95	0.66
1:A:38:G:N2	1:A:397:A:H5'	2.06	0.66
1:A:1198:G:H8	1:A:1198:G:H5'	1.61	0.66
2:B:19:ASN:C	2:B:19:ASN:HD22	2.00	0.66
1:A:1391:U:H2'	1:A:1392:G:C8	2.31	0.66
1:A:1196:U:H5''	1:A:1197:G:H5'	1.76	0.66
1:A:1001:A:H3'	1:A:1001(A):G:H5'	1.78	0.66
5:E:75:GLU:HG3	5:E:89:PRO:HD2	1.76	0.66
2:B:69:LYS:HG2	2:B:72:GLN:NE2	2.11	0.66
13:M:10:ARG:HA	13:M:44:VAL:CG2	2.25	0.65
6:F:101:ALA:CB	18:R:13:GLU:HG3	2.26	0.65
5:E:20:ARG:O	5:E:21:ARG:HG2	1.96	0.65
20:T:29:LEU:HD12	20:T:55:LEU:HD12	1.77	0.65
10:J:22:VAL:HG13	10:J:23:GLU:HG3	1.78	0.65
2:B:205:ILE:HG22	2:B:209:LEU:HD12	1.78	0.65
2:B:82:ALA:C	2:B:84:MET:H	1.99	0.65
3:C:138:GLN:NE2	3:C:138:GLN:HA	2.11	0.65
2:B:38:LEU:HA	2:B:41:THR:OG1	1.95	0.65
4:D:145:ILE:N	4:D:145:ILE:HD12	2.11	0.65
7:G:154:ARG:O	7:G:155:TRP:HB3	1.96	0.65
1:A:1161:C:H2'	1:A:1162:C:C6	2.32	0.65
10:J:37:PRO:O	10:J:38:LEU:HB2	1.96	0.65
4:D:200:GLN:NE2	4:D:200:GLN:HA	2.11	0.65
18:R:30:SER:C	18:R:32:THR:H	1.99	0.65
10:J:20:LYS:NZ	10:J:88:LEU:HD12	2.11	0.65
1:A:1038:C:H2'	1:A:1039:C:C6	2.32	0.65
19:S:18:VAL:HG13	19:S:19:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:4:TYR:HE2	9:I:15:ARG:HG2	1.60	0.65
1:A:1305:G:H5'	21:V:4:GLY:HA3	1.79	0.65
5:E:11:ARG:HD3	5:E:22:PHE:HB3	1.79	0.65
16:P:28:ARG:HG2	16:P:29:ASP:OD1	1.96	0.65
3:C:122:GLN:HE22	3:C:139:ARG:HH22	1.44	0.65
5:E:139:ARG:NH1	8:H:77:GLU:OE2	2.30	0.65
1:A:1228:C:H4'	13:M:115:THR:HA	1.79	0.65
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.32	0.65
1:A:403:C:H6	1:A:403:C:H5'	1.62	0.65
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.60	0.65
1:A:817:C:C2	1:A:819:A:O2'	2.48	0.65
4:D:200:GLN:HE21	4:D:200:GLN:HA	1.61	0.65
12:L:71:HIS:CD2	12:L:73:LEU:H	2.15	0.64
9:I:9:ARG:HD2	9:I:10:LYS:N	2.11	0.64
3:C:66:THR:O	3:C:67:VAL:HG23	1.97	0.64
3:C:69:VAL:HG12	3:C:70:ALA:N	2.12	0.64
9:I:45:ALA:HB2	9:I:73:ILE:HG23	1.78	0.64
6:F:97:PHE:HB2	18:R:17:ARG:HH21	1.62	0.64
3:C:109:ASN:O	3:C:110:LEU:HD23	1.97	0.64
1:A:1196:U:N3	22:W:5:A:H2'	2.13	0.64
3:C:133:ILE:HG21	3:C:166:TRP:O	1.98	0.64
1:A:718:G:H5'	11:K:107:ASN:OD1	1.98	0.64
4:D:161:LEU:HD13	4:D:180:MET:CE	2.27	0.64
2:B:9:VAL:HG12	2:B:204:SER:OG	1.98	0.64
1:A:998:G:H3'	1:A:999:C:C5'	2.25	0.64
3:C:190:THR:HG21	3:C:192:TYR:CZ	2.33	0.64
1:A:473:G:C2'	1:A:474:G:C5'	2.71	0.64
1:A:1367:C:C5'	10:J:58:ARG:HH11	2.10	0.64
5:E:89:PRO:HG2	8:H:105:ARG:NH2	2.13	0.64
1:A:45:U:H2'	1:A:46:G:C8	2.33	0.64
10:J:10:ASP:O	10:J:13:THR:HG22	1.96	0.64
3:C:59:ALA:O	3:C:60:ALA:HB2	1.97	0.64
1:A:501:C:O2'	1:A:502:G:H5'	1.98	0.64
1:A:1141:C:O2'	1:A:1142:G:H5'	1.98	0.64
3:C:22:TYR:CD1	3:C:23:ALA:N	2.65	0.64
14:N:8:LYS:HG3	14:N:20:TYR:O	1.97	0.64
1:A:1272:G:H8	1:A:1272:G:H5'	1.62	0.64
1:A:29:G:C8	1:A:29:G:H5'	2.32	0.64
1:A:190:U:O2	20:T:98:SER:HB2	1.97	0.64
5:E:99:GLY:O	5:E:102:PRO:HD2	1.97	0.64
1:A:1152:A:H4'	10:J:11:HIS:HD2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:ARG:HD2	5:E:60:ARG:H	1.62	0.64
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.79	0.64
1:A:850:U:C6	1:A:850:U:H5'	2.26	0.64
12:L:24:LYS:O	12:L:25:GLY:C	2.36	0.64
18:R:11:LEU:HD21	18:R:27:ARG:HD2	1.80	0.64
1:A:35:G:H2'	1:A:36:C:H6	1.61	0.64
2:B:63:LEU:HD23	2:B:64:PHE:N	2.13	0.64
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.32	0.64
18:R:2:SER:HB2	18:R:39:ARG:NH2	2.13	0.64
8:H:103:VAL:HG21	8:H:109:ILE:O	1.97	0.64
4:D:6:PRO:HB2	4:D:9:ARG:HD2	1.78	0.63
10:J:17:SER:OG	10:J:89:PRO:HG2	1.97	0.63
5:E:60:ARG:N	5:E:60:ARG:HD2	2.13	0.63
16:P:38:TYR:CE2	16:P:50:LYS:HD3	2.32	0.63
1:A:650:G:C2'	1:A:651:C:H5'	2.27	0.63
19:S:41:PRO:O	19:S:44:VAL:HG23	1.98	0.63
3:C:25:LYS:CD	3:C:25:LYS:H	1.99	0.63
2:B:225:GLU:HB3	2:B:226:PRO:HD2	1.81	0.63
11:K:38:ILE:CG2	11:K:39:GLY:H	2.06	0.63
1:A:429:U:H2'	4:D:24:ARG:HH21	1.63	0.63
1:A:944:G:C4'	1:A:945:G:O5'	2.42	0.63
14:N:56:ARG:HG2	14:N:57:LYS:H	1.63	0.63
12:L:23:LEU:HB3	12:L:58:SER:HB2	1.79	0.63
1:A:1086:U:H3	1:A:1099:G:N2	1.96	0.63
1:A:631:G:H2'	1:A:632:A:C8	2.34	0.63
2:B:22:PHE:CD2	2:B:184:THR:HA	2.34	0.63
3:C:171:ARG:HH11	3:C:171:ARG:HB3	1.62	0.63
1:A:817:C:C5	1:A:819:A:H2'	2.33	0.63
6:F:19:LEU:O	6:F:23:LYS:HG3	1.99	0.63
9:I:16:VAL:HG22	9:I:62:ILE:HD12	1.79	0.63
13:M:116:VAL:HG12	13:M:117:ALA:N	2.14	0.63
9:I:126:LYS:HG2	13:M:125:LYS:HD3	1.79	0.63
7:G:14:ASP:HB3	7:G:18:GLY:N	2.13	0.63
1:A:1422:G:H1	1:A:1478:C:H42	1.46	0.63
20:T:3:LEU:HD12	20:T:5:ALA:HB3	1.80	0.63
1:A:1125:U:H3	10:J:3:ARG:HH21	1.47	0.63
1:A:342:C:N4	1:A:347:G:H1	1.97	0.63
1:A:1002:G:H2'	1:A:1003:G:H8	1.62	0.63
3:C:153:SER:OG	3:C:154:GLY:N	2.25	0.63
1:A:1222:G:OP1	19:S:76:THR:HG21	1.98	0.63
1:A:1067:A:H4'	1:A:1093:A:O3'	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.81	0.63
5:E:60:ARG:HH11	5:E:60:ARG:HG2	1.64	0.63
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.63
10:J:19:GLN:HA	10:J:22:VAL:HG12	1.80	0.63
1:A:969:A:N6	13:M:125:LYS:HE3	2.14	0.63
3:C:107:ASN:HD21	3:C:143:SER:HB2	1.64	0.63
1:A:189(D):C:H2'	1:A:189(E):U:H1'	1.80	0.63
1:A:411:A:O2'	1:A:413:G:H5'	1.99	0.62
1:A:410:G:OP2	4:D:24:ARG:HG2	1.99	0.62
2:B:136:LEU:HD13	2:B:140:GLN:OE1	1.99	0.62
15:O:77:TYR:CZ	15:O:81:ILE:HD11	2.34	0.62
1:A:1381:U:O2'	1:A:1382:C:H5'	1.99	0.62
2:B:2:LYS:HD2	2:B:2:LYS:C	2.19	0.62
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.06	0.62
3:C:194:VAL:O	3:C:195:LEU:HD22	1.99	0.62
1:A:1499:A:H5'	1:A:1499:A:H8	1.64	0.62
1:A:743:U:H2'	1:A:744:C:C6	2.34	0.62
1:A:1244:C:C3'	1:A:1245:A:H5''	2.29	0.62
5:E:140:THR:HG22	5:E:143:ASP:H	1.62	0.62
1:A:407:G:O2'	4:D:115:GLN:HG3	2.00	0.62
1:A:974:A:OP1	14:N:40:ARG:NH1	2.32	0.62
13:M:39:ASN:HD22	13:M:40:PRO:CD	2.12	0.62
2:B:21:LYS:HD3	2:B:189:ASP:OD2	1.99	0.62
2:B:166:ILE:N	2:B:166:ILE:HD12	2.13	0.62
7:G:14:ASP:HB3	7:G:19:ASP:H	1.64	0.62
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.13	0.62
1:A:814:A:H5'	1:A:814:A:H8	1.62	0.62
12:L:106:VAL:HG23	12:L:116:TYR:HB3	1.82	0.62
3:C:66:THR:HG22	3:C:67:VAL:H	1.64	0.62
19:S:62:THR:HG22	19:S:63:GLU:H	1.64	0.62
3:C:190:THR:HG22	3:C:191:THR:N	2.13	0.62
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.30	0.62
6:F:22:GLU:OE1	6:F:82:ARG:HD3	1.99	0.62
3:C:19:SER:O	14:N:53:PRO:HB3	2.00	0.62
10:J:48:ILE:HD13	14:N:40:ARG:HD3	1.82	0.62
3:C:154:GLY:O	3:C:155:ARG:HB2	1.98	0.62
1:A:1352:C:H2'	1:A:1353:G:C8	2.34	0.62
5:E:8:LEU:CD1	5:E:27:LEU:HB2	2.30	0.62
13:M:77:ILE:HG22	13:M:81:MET:HE3	1.81	0.62
12:L:37:ARG:HH12	12:L:53:LYS:CE	2.12	0.62
13:M:49:GLU:O	13:M:53:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:ILE:O	9:I:84:LEU:HB2	1.99	0.62
2:B:89:GLN:C	2:B:90:ARG:HD2	2.20	0.62
4:D:150:LYS:H	4:D:150:LYS:HD2	1.64	0.62
4:D:150:LYS:N	4:D:150:LYS:HD2	2.15	0.62
11:K:70:VAL:HG21	11:K:93:LEU:HD13	1.81	0.61
19:S:19:LEU:HD12	19:S:20:GLU:N	2.14	0.61
1:A:533:A:O2'	1:A:535:A:OP2	2.09	0.61
1:A:850:U:H6	1:A:850:U:C5'	2.08	0.61
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.33	0.61
12:L:79:VAL:CG2	12:L:96:ILE:HG23	2.31	0.61
4:D:23:GLU:C	4:D:25:CYS:H	2.04	0.61
1:A:1392:G:N2	1:A:1502:A:H8	1.98	0.61
1:A:28:G:H3'	1:A:29:G:H5''	1.81	0.61
1:A:883:C:O2'	1:A:884:U:H5'	2.01	0.61
1:A:629:G:H4'	1:A:630:G:OP1	2.00	0.61
1:A:426:G:H8	1:A:426:G:H5'	1.65	0.61
1:A:189(B):C:H4'	1:A:189(C):C:OP1	2.00	0.61
2:B:17:ARG:HH11	2:B:18:TRP:N	1.98	0.61
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.61
1:A:192:U:O3'	20:T:50:ARG:HD2	1.99	0.61
5:E:101:VAL:HB	5:E:102:PRO:HD3	1.82	0.61
13:M:83:ILE:HG12	19:S:64:ASN:ND2	2.15	0.61
1:A:174:C:H5'	1:A:174:C:H6	1.65	0.61
1:A:1029:C:C3'	1:A:1030:C:H5''	2.30	0.61
3:C:63:VAL:HB	3:C:98:VAL:CG1	2.31	0.61
15:O:9:LYS:NZ	15:O:13:GLU:HB2	2.15	0.61
13:M:58:TYR:O	13:M:62:THR:HG22	2.01	0.61
1:A:393:A:O2'	1:A:394:G:H5'	2.00	0.61
3:C:13:ILE:O	3:C:15:ARG:N	2.34	0.61
1:A:319:G:C3'	1:A:320:C:H5''	2.31	0.61
1:A:1168:A:H2'	1:A:1169:A:C8	2.36	0.61
18:R:2:SER:HA	18:R:4:LYS:NZ	2.15	0.61
1:A:1182:G:H4'	1:A:1183:A:H5'	1.82	0.61
2:B:10:HIS:NE2	2:B:208:ILE:HG12	2.15	0.61
20:T:7:LYS:O	20:T:11:GLN:HG3	2.01	0.61
2:B:207:LEU:C	2:B:207:LEU:HD23	2.21	0.61
1:A:1196:U:C4	22:W:5:A:H2'	2.36	0.61
3:C:13:ILE:HG22	3:C:14:THR:N	2.13	0.61
1:A:29:G:O2'	1:A:30:U:H5'	2.00	0.61
19:S:17:LYS:O	19:S:21:LEU:HB2	2.01	0.61
9:I:7:GLY:CA	9:I:78:LEU:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:46:ARG:HB2	6:F:60:PHE:HE2	1.66	0.61
1:A:1540:U:H2'	1:A:1541:U:C5'	2.20	0.60
1:A:1064:G:N2	1:A:1190:G:H2'	2.16	0.60
2:B:225:GLU:CD	2:B:225:GLU:H	2.02	0.60
1:A:473:G:H2'	1:A:474:G:H5'	1.82	0.60
9:I:125:SER:O	9:I:127:ARG:N	2.34	0.60
14:N:17:VAL:HG23	14:N:18:ARG:N	2.16	0.60
1:A:1292:U:P	7:G:40:ARG:HH22	2.24	0.60
5:E:71:THR:HG23	5:E:72:ILE:N	2.16	0.60
2:B:53:GLU:CG	2:B:215:LEU:HD11	2.31	0.60
1:A:1479:C:H2'	1:A:1480:G:C8	2.35	0.60
15:O:86:ILE:HG22	15:O:87:ARG:N	2.16	0.60
1:A:366:C:O2	1:A:366:C:H2'	2.01	0.60
1:A:189:G:H5'	1:A:189:G:C8	2.36	0.60
17:Q:66:LYS:CA	17:Q:69:ARG:HH12	2.12	0.60
19:S:4:LEU:HD11	19:S:69:LYS:NZ	2.16	0.60
23:Z:32:U:H2'	23:Z:33:U:H5'	1.83	0.60
1:A:328:C:O2	1:A:328:C:H2'	2.01	0.60
1:A:1216:G:O2'	1:A:1217:C:H5'	2.01	0.60
4:D:127:VAL:HG12	4:D:128:ASN:ND2	2.15	0.60
1:A:1054:C:H5'	1:A:1054:C:H6	1.65	0.60
1:A:1365:G:H5'	1:A:1365:G:H8	1.65	0.60
14:N:13:PRO:O	14:N:14:LYS:HB2	2.00	0.60
2:B:41:THR:HA	2:B:196:PRO:HG2	1.82	0.60
17:Q:77:GLU:OE2	17:Q:80:ARG:HD2	2.01	0.60
15:O:16:ARG:HG3	15:O:16:ARG:NH1	2.13	0.60
1:A:320:C:C6	1:A:320:C:H5'	2.32	0.60
3:C:123:ILE:HD12	3:C:129:VAL:HG22	1.83	0.60
6:F:43:LEU:N	6:F:43:LEU:HD22	2.15	0.60
1:A:425:G:H2'	1:A:426:G:C5'	2.23	0.60
1:A:275:G:H5''	17:Q:13:LYS:CB	2.32	0.60
1:A:200:G:H2'	1:A:201:C:O4'	2.02	0.60
1:A:1130:A:H5'	1:A:1131:G:O5'	2.02	0.60
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.37	0.60
1:A:1037:C:H2'	1:A:1038:C:C6	2.36	0.60
1:A:1260:C:O5'	1:A:1284:C:H4'	2.02	0.60
1:A:1257:U:H5'	1:A:1258:G:O5'	2.02	0.60
8:H:29:SER:OG	8:H:32:LYS:HG3	2.02	0.60
1:A:1128:C:H5'	1:A:1129:C:OP2	2.02	0.59
1:A:1230:C:O2'	13:M:125:LYS:HG2	2.01	0.59
7:G:49:ILE:O	7:G:53:THR:HB	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:U:H2'	1:A:115:G:H1'	1.82	0.59
19:S:27:LYS:HG2	19:S:28:ARG:N	2.16	0.59
9:I:5:GLY:N	9:I:83:ALA:HB2	2.17	0.59
23:Z:28:G:H2'	23:Z:29:G:C8	2.37	0.59
19:S:43:MET:HA	19:S:46:HIS:HD2	1.68	0.59
1:A:1014:A:C2	1:A:1219:U:H1'	2.38	0.59
1:A:457:C:H2'	1:A:458:C:C6	2.37	0.59
1:A:1499:A:C8	1:A:1499:A:H5'	2.36	0.59
11:K:116:ARG:O	11:K:117:LYS:HB2	2.02	0.59
10:J:92:VAL:HG12	10:J:93:GLU:N	2.17	0.59
7:G:61:PHE:HA	7:G:123:LEU:CD2	2.32	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.38	0.59
13:M:33:LEU:HD13	13:M:40:PRO:HA	1.84	0.59
1:A:522:C:H41	12:L:49:ARG:NH2	2.00	0.59
1:A:248:C:O2'	1:A:249:U:H5'	2.02	0.59
1:A:168:G:O2'	1:A:169:C:H5'	2.03	0.59
3:C:149:LYS:HG3	3:C:168:ALA:HB2	1.85	0.59
19:S:40:VAL:HG22	19:S:43:MET:CE	2.32	0.59
3:C:94:THR:O	3:C:96:LYS:N	2.33	0.59
11:K:24:ASP:OD2	11:K:28:ASN:HB2	2.02	0.59
2:B:6:GLU:C	2:B:8:GLY:H	2.05	0.59
1:A:144:G:C3'	1:A:145:G:H5''	2.33	0.59
3:C:67:VAL:HG12	3:C:69:VAL:HG23	1.83	0.59
9:I:110:ARG:HG2	9:I:111:LYS:N	2.17	0.59
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.84	0.59
3:C:133:ILE:HG22	3:C:167:ALA:HB3	1.85	0.59
7:G:125:ASP:OD1	7:G:130:LYS:HE3	2.02	0.59
1:A:314:C:O2'	1:A:315:A:H5'	2.03	0.59
10:J:32:VAL:HG13	10:J:72:ILE:HG22	1.83	0.59
4:D:35:ARG:NH1	4:D:35:ARG:HG2	2.16	0.59
1:A:697:U:H2'	1:A:698:G:H5'	1.83	0.59
1:A:1130:A:C3'	1:A:1131:G:C5'	2.79	0.59
1:A:1208:C:H2'	1:A:1209:C:C6	2.37	0.59
12:L:37:ARG:HG2	12:L:38:THR:O	2.03	0.59
7:G:14:ASP:CB	7:G:19:ASP:H	2.15	0.59
19:S:32:THR:HG22	19:S:33:TRP:N	2.17	0.59
1:A:189(B):C:C6	1:A:189(B):C:C5'	2.84	0.59
3:C:21:TRP:CH2	3:C:31:LEU:HB2	2.38	0.59
23:Z:32:U:H2'	23:Z:33:U:H5''	1.85	0.59
4:D:161:LEU:HD13	4:D:180:MET:HE2	1.84	0.59
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLU:CB	2:B:226:PRO:HD2	2.32	0.59
3:C:65:VAL:CG1	3:C:66:THR:H	2.16	0.59
1:A:1095:U:H2'	1:A:1096:C:H6	1.68	0.59
16:P:67:THR:HG22	16:P:69:THR:N	2.17	0.59
17:Q:79:GLY:O	17:Q:80:ARG:HB3	2.02	0.59
1:A:575:G:HO2'	1:A:821:G:H5'	1.67	0.59
1:A:945:G:H2'	1:A:945:G:N3	2.17	0.58
1:A:1475:G:O2'	1:A:1476:G:H5''	2.02	0.58
1:A:1197:G:H2'	1:A:1198:G:H5'	1.84	0.58
12:L:24:LYS:HD3	12:L:29:ARG:NH2	2.17	0.58
2:B:44:GLU:HB3	2:B:194:ILE:O	2.03	0.58
3:C:192:TYR:HE1	3:C:195:LEU:HD21	1.67	0.58
20:T:89:GLY:O	20:T:90:ALA:HB3	2.03	0.58
1:A:620:C:N1	4:D:134:LEU:HD13	2.18	0.58
18:R:19:TYR:HA	18:R:54:THR:HG23	1.84	0.58
2:B:217:ILE:C	2:B:219:ALA:H	2.05	0.58
1:A:1368:G:OP2	9:I:111:LYS:HD2	2.03	0.58
2:B:156:ILE:HG23	2:B:158:VAL:HG23	1.84	0.58
2:B:118:SER:O	2:B:121:ILE:HG13	2.03	0.58
1:A:953:G:C5'	1:A:965:A:H61	2.15	0.58
7:G:138:GLU:O	7:G:142:ARG:HG3	2.03	0.58
10:J:20:LYS:HZ1	10:J:88:LEU:HD12	1.67	0.58
2:B:200:ASP:O	2:B:201:ALA:HB3	2.03	0.58
1:A:197:A:H4'	1:A:198:G:OP1	2.02	0.58
1:A:999:C:H4'	1:A:999:C:OP2	2.02	0.58
3:C:71:LYS:O	3:C:74:VAL:HG23	2.03	0.58
10:J:47:VAL:HG13	14:N:40:ARG:HD2	1.84	0.58
18:R:11:LEU:HD22	18:R:27:ARG:NH1	2.18	0.58
13:M:10:ARG:HG2	13:M:11:ASN:N	2.19	0.58
4:D:63:LEU:HD12	4:D:74:PHE:CE1	2.38	0.58
10:J:40:THR:HG23	10:J:65:THR:O	2.04	0.58
2:B:66:GLY:HA3	2:B:75:VAL:HG21	1.85	0.58
1:A:181:G:O2'	1:A:183:G:N7	2.36	0.58
2:B:65:VAL:O	2:B:159:VAL:HG23	2.04	0.58
14:N:28:ARG:HG2	14:N:28:ARG:HH11	1.68	0.58
1:A:1151:A:HO2'	1:A:1152:A:H8	1.51	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.39	0.58
1:A:881:G:P	12:L:8:ARG:HH22	2.27	0.58
1:A:1047:G:O2'	1:A:1048:G:H5'	2.03	0.58
7:G:14:ASP:O	7:G:18:GLY:HA2	2.03	0.58
3:C:31:LEU:HD22	3:C:58:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:G:H4'	1:A:632:A:OP2	2.04	0.58
2:B:131:ARG:HB3	2:B:131:ARG:HH11	1.69	0.58
16:P:74:LEU:O	16:P:79:VAL:HG23	2.04	0.58
1:A:977:A:H2'	1:A:978:A:H5''	1.86	0.58
3:C:5:HIS:NE2	3:C:7:ILE:HD12	2.19	0.58
1:A:1201:A:H4'	1:A:1202:G:O5'	2.04	0.58
2:B:110:GLU:HB3	2:B:147:ARG:NH2	2.17	0.58
2:B:215:LEU:O	2:B:219:ALA:HB2	2.03	0.57
4:D:27:SER:O	4:D:29:LYS:N	2.37	0.57
17:Q:80:ARG:O	17:Q:80:ARG:HG3	2.04	0.57
2:B:127:LYS:O	2:B:131:ARG:HG3	2.04	0.57
5:E:9:ILE:O	5:E:9:ILE:HD12	2.04	0.57
11:K:81:ARG:NH1	18:R:73:LYS:HD2	2.18	0.57
1:A:1200:C:O2'	1:A:1201:A:OP1	2.19	0.57
1:A:1227:A:H2'	1:A:1228:C:H5'	1.86	0.57
4:D:63:LEU:HD12	4:D:74:PHE:CZ	2.39	0.57
1:A:996:A:H5'	1:A:996:A:H8	1.68	0.57
10:J:37:PRO:HA	10:J:68:ARG:NH1	2.19	0.57
1:A:975:A:H5'	1:A:975:A:C8	2.35	0.57
1:A:1312:G:O2'	1:A:1313:U:H5'	2.03	0.57
7:G:42:PHE:O	7:G:45:ALA:HB3	2.04	0.57
6:F:3:ARG:HG2	6:F:93:SER:OG	2.03	0.57
1:A:19:C:H2'	1:A:20:U:H6	1.68	0.57
7:G:25:PHE:O	7:G:29:ILE:HG13	2.03	0.57
3:C:172:VAL:HG12	3:C:174:LEU:HD21	1.86	0.57
1:A:1128:C:H1'	1:A:1146:A:H61	1.69	0.57
17:Q:66:LYS:O	17:Q:68:LYS:N	2.34	0.57
20:T:93:ILE:CG2	20:T:95:GLY:H	2.15	0.57
1:A:954:G:H2'	1:A:955:U:H6	1.69	0.57
15:O:23:SER:HB2	15:O:26:VAL:HG23	1.86	0.57
9:I:7:GLY:HA3	9:I:78:LEU:HB3	1.84	0.57
1:A:1480:G:H2'	1:A:1481:U:C5'	2.26	0.57
1:A:1228:C:H2'	1:A:1229:A:H8	1.69	0.57
1:A:177:C:O2'	1:A:178:C:H5'	2.04	0.57
17:Q:100:ARG:HA	17:Q:100:ARG:NE	2.20	0.57
10:J:2:ILE:HB	10:J:72:ILE:HG13	1.87	0.57
1:A:1063:C:O5'	1:A:1064:G:H5''	2.05	0.57
4:D:5:GLY:O	4:D:7:VAL:HG23	2.05	0.57
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.70	0.57
20:T:87:ALA:O	20:T:88:ALA:HB3	2.04	0.57
3:C:130:ARG:HG2	3:C:134:LYS:HZ3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:PRO:HB2	10:J:80:ILE:HD11	1.86	0.57
1:A:1064:G:H1'	1:A:1190:G:N2	2.19	0.57
2:B:30:ARG:HD2	2:B:35:ILE:HG13	1.85	0.57
2:B:97:THR:HB	2:B:170:GLU:OE1	2.05	0.57
1:A:953:G:H5'	1:A:965:A:H61	1.69	0.57
8:H:83:ILE:HG23	8:H:83:ILE:O	2.04	0.57
1:A:625:G:H2'	1:A:626:U:C6	2.40	0.57
6:F:86:ARG:O	6:F:87:ARG:HG2	2.05	0.57
7:G:71:ARG:O	7:G:72:MET:HG2	2.05	0.57
1:A:968:A:H8	1:A:968:A:O5'	1.88	0.57
1:A:401:C:H1'	1:A:622:A:H1'	1.86	0.57
5:E:112:THR:HG23	5:E:113:ASP:OD2	2.05	0.57
7:G:71:ARG:HH12	7:G:137:LYS:NZ	2.02	0.57
1:A:149:A:H2'	1:A:150:C:C6	2.40	0.57
1:A:524:G:H2'	1:A:525:C:C6	2.40	0.57
1:A:1404:C:H2'	1:A:1405:G:C8	2.40	0.57
20:T:50:ARG:NH1	20:T:50:ARG:HB2	2.19	0.57
1:A:1200:C:H4'	1:A:1201:A:O5'	2.05	0.57
9:I:6:THR:HG22	9:I:7:GLY:N	2.19	0.57
1:A:1128:C:H3'	1:A:1129:C:C5'	2.27	0.56
2:B:172:ARG:O	8:H:71:GLY:HA2	2.05	0.56
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.18	0.56
3:C:123:ILE:CD1	3:C:129:VAL:HG22	2.35	0.56
2:B:110:GLU:HB3	2:B:147:ARG:CZ	2.35	0.56
1:A:377:G:OP2	16:P:3:LYS:HD3	2.05	0.56
1:A:1347:G:C5	9:I:106:ARG:NH1	2.73	0.56
1:A:849:C:H3'	1:A:850:U:H5''	1.88	0.56
3:C:37:ARG:HH11	3:C:37:ARG:HG3	1.70	0.56
1:A:1001:A:N6	1:A:1040:U:H3	2.02	0.56
1:A:1495:U:H2'	1:A:1496:C:H6	1.68	0.56
14:N:23:CYS:HB3	14:N:27:GLY:H	1.70	0.56
1:A:1208:C:H2'	1:A:1209:C:H6	1.69	0.56
6:F:101:ALA:CA	18:R:13:GLU:HG3	2.34	0.56
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.70	0.56
2:B:51:PHE:O	2:B:54:ASP:HB3	2.05	0.56
1:A:1136:U:H5''	1:A:1137:C:OP1	2.06	0.56
10:J:36:ILE:CG1	10:J:69:LEU:HB3	2.35	0.56
2:B:85:PRO:HB3	2:B:145:GLY:O	2.05	0.56
4:D:198:ASN:ND2	4:D:200:GLN:HB3	2.20	0.56
3:C:135:GLN:O	3:C:138:GLN:HB2	2.04	0.56
7:G:110:ARG:NH2	7:G:125:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:VAL:HG22	6:F:41:GLU:N	2.20	0.56
7:G:17:TYR:CD2	7:G:58:LEU:HB2	2.40	0.56
2:B:53:GLU:HG3	2:B:215:LEU:HD11	1.86	0.56
15:O:25:GLU:OE2	15:O:76:ARG:HD2	2.05	0.56
18:R:29:LEU:CD1	18:R:64:LEU:HD22	2.36	0.56
9:I:46:LEU:C	9:I:48:PRO:HD2	2.25	0.56
1:A:473:G:H5'	16:P:81:ARG:NH1	2.21	0.56
6:F:76:ALA:O	6:F:80:ARG:HG3	2.04	0.56
2:B:74:ILE:HG13	2:B:202:ILE:HG23	1.86	0.56
1:A:556:C:OP2	12:L:16:LYS:HE3	2.06	0.56
1:A:657:G:H4'	15:O:27:GLN:HG2	1.88	0.56
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.41	0.56
3:C:4:ILE:CD1	3:C:4:ILE:N	2.67	0.56
2:B:217:ILE:HG21	2:B:224:VAL:HG23	1.87	0.56
1:A:1130:A:H5'	1:A:1131:G:C5'	2.35	0.56
9:I:92:ARG:HD3	9:I:96:LYS:HE3	1.87	0.56
1:A:1222:G:P	19:S:76:THR:HG21	2.45	0.56
3:C:128:ALA:HB3	3:C:131:ARG:CD	2.36	0.56
3:C:64:ALA:O	3:C:65:VAL:HB	2.06	0.56
1:A:1075:C:H5'	2:B:97:THR:HG21	1.88	0.56
9:I:16:VAL:HG21	9:I:79:GLY:HA3	1.88	0.56
17:Q:64:ILE:HD12	17:Q:64:ILE:N	2.21	0.56
1:A:67:C:O2'	1:A:171:A:H1'	2.06	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.56
3:C:65:VAL:CG1	3:C:66:THR:N	2.69	0.56
1:A:192:U:H4'	20:T:50:ARG:HD2	1.87	0.56
10:J:10:ASP:HB3	10:J:13:THR:CG2	2.36	0.56
1:A:320:C:H2'	1:A:321:A:O4'	2.05	0.56
5:E:20:ARG:HH11	5:E:20:ARG:HG2	1.71	0.56
7:G:107:ALA:O	7:G:110:ARG:HB2	2.06	0.56
1:A:170:U:O2'	1:A:171:A:H5'	2.06	0.56
1:A:1438:G:H2'	1:A:1439:C:C6	2.41	0.56
2:B:175:PHE:HD2	8:H:70:GLN:HB3	1.70	0.56
1:A:404:U:H2'	1:A:405:U:C6	2.41	0.56
3:C:2:ASN:OD1	3:C:2:ASN:N	2.39	0.55
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.88	0.55
13:M:39:ASN:HD22	13:M:40:PRO:HD2	1.71	0.55
1:A:1312:G:N7	19:S:2:ARG:O	2.39	0.55
10:J:44:ARG:CG	10:J:44:ARG:HH11	2.19	0.55
1:A:1047:G:H2'	1:A:1048:G:H5'	1.86	0.55
3:C:118:ARG:CZ	3:C:139:ARG:HH12	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:ARG:O	7:G:105:GLN:HG3	2.06	0.55
4:D:75:ARG:HG3	4:D:75:ARG:HH11	1.71	0.55
1:A:1101:A:H4'	1:A:1102:A:C5'	2.15	0.55
1:A:1427:U:H3	1:A:1473:A:H61	1.52	0.55
18:R:40:ARG:NH1	18:R:40:ARG:HB3	2.21	0.55
1:A:1272:G:C2'	1:A:1273:G:H5'	2.37	0.55
10:J:2:ILE:HB	10:J:72:ILE:CG1	2.37	0.55
2:B:6:GLU:C	2:B:8:GLY:N	2.60	0.55
1:A:714:G:H2'	1:A:715:A:C8	2.41	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.41	0.55
20:T:75:SER:O	20:T:79:ARG:HB2	2.06	0.55
13:M:80:LEU:O	13:M:85:CYS:HB3	2.05	0.55
9:I:9:ARG:HG2	9:I:74:ASP:CB	2.36	0.55
1:A:1249:C:H4'	9:I:35:TYR:OH	2.05	0.55
1:A:1062:U:H2'	1:A:1063:C:C6	2.42	0.55
9:I:117:LYS:O	9:I:118:ALA:CB	2.55	0.55
1:A:977:A:H1'	1:A:982:U:O4	2.07	0.55
13:M:114:LYS:H	13:M:114:LYS:HD3	1.70	0.55
14:N:43:LEU:C	14:N:43:LEU:HD12	2.26	0.55
1:A:255:G:H1'	17:Q:15:GLN:NE2	2.22	0.55
1:A:1442(A):G:C5'	1:A:1442(B):A:H3'	2.36	0.55
8:H:13:ILE:O	8:H:17:THR:HG23	2.07	0.55
2:B:82:ALA:HB1	2:B:84:MET:HG2	1.87	0.55
9:I:96:LYS:HB2	9:I:97:PRO:CD	2.32	0.55
1:A:1003:G:N3	1:A:1003:G:H2'	2.21	0.55
13:M:14:VAL:HG23	13:M:42:THR:O	2.07	0.55
4:D:161:LEU:CD1	4:D:180:MET:HE2	2.37	0.55
1:A:191:G:C4	20:T:98:SER:HB3	2.42	0.55
10:J:40:THR:HG23	10:J:65:THR:C	2.27	0.55
2:B:131:ARG:HB3	2:B:131:ARG:NH1	2.22	0.55
7:G:14:ASP:OD1	7:G:43:TYR:OH	2.25	0.55
1:A:1457:G:H2'	1:A:1458:G:H8	1.72	0.55
3:C:5:HIS:CD2	3:C:7:ILE:H	2.12	0.55
1:A:979:C:H2'	1:A:980:C:H5'	1.88	0.55
6:F:69:GLU:HA	6:F:72:VAL:CG2	2.36	0.55
1:A:650:G:H2'	1:A:651:C:H5'	1.89	0.55
1:A:1372:U:O2'	1:A:1373:G:H5'	2.06	0.55
1:A:404:U:H2'	1:A:405:U:H6	1.72	0.55
2:B:126:LYS:HA	2:B:129:GLN:HB2	1.88	0.55
10:J:79:THR:C	10:J:81:GLU:H	2.10	0.55
3:C:4:ILE:HD12	3:C:4:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:A:H4'	1:A:52:G:OP2	2.06	0.55
3:C:33:LEU:HD21	3:C:37:ARG:CZ	2.37	0.55
9:I:126:LYS:CB	13:M:125:LYS:HZ2	2.20	0.55
7:G:148:ARG:HD2	11:K:49:TYR:CE1	2.41	0.55
19:S:21:LEU:HD21	19:S:27:LYS:HB2	1.89	0.55
3:C:166:TRP:O	3:C:167:ALA:HB3	2.07	0.55
9:I:91:TYR:O	9:I:95:LEU:HD13	2.06	0.55
1:A:556:C:O2'	1:A:557:G:H5'	2.06	0.55
2:B:6:GLU:CD	2:B:207:LEU:HD11	2.28	0.54
2:B:63:LEU:C	2:B:63:LEU:HD23	2.27	0.54
15:O:69:LEU:HD12	15:O:80:LEU:HD12	1.88	0.54
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.35	0.54
12:L:37:ARG:HG2	12:L:38:THR:N	2.22	0.54
1:A:1052:U:H2'	1:A:1055:A:OP2	2.06	0.54
23:Z:32:U:C2'	23:Z:33:U:H5''	2.38	0.54
1:A:109:A:H2'	1:A:326:G:N2	2.21	0.54
10:J:73:ILE:O	10:J:74:ASN:HB2	2.07	0.54
2:B:110:GLU:CB	2:B:147:ARG:HH22	2.20	0.54
2:B:4:LEU:O	2:B:6:GLU:N	2.40	0.54
2:B:81:ARG:O	2:B:82:ALA:HB2	2.08	0.54
20:T:50:ARG:NH2	20:T:93:ILE:HD12	2.21	0.54
9:I:126:LYS:HB3	13:M:125:LYS:HZ2	1.71	0.54
19:S:39:ILE:HD11	19:S:70:LEU:HD23	1.89	0.54
10:J:4:ILE:O	10:J:69:LEU:O	2.25	0.54
13:M:4:ALA:HB3	13:M:7:GLU:HG3	1.88	0.54
1:A:981:U:H3'	1:A:982:U:C4'	2.38	0.54
19:S:14:LEU:HD12	19:S:15:LEU:H	1.72	0.54
1:A:439:A:H2'	1:A:441:A:C5'	2.37	0.54
1:A:689:C:P	11:K:36:GLY:HA3	2.47	0.54
3:C:91:ALA:HA	3:C:94:THR:O	2.08	0.54
20:T:50:ARG:HH22	20:T:93:ILE:HD12	1.72	0.54
14:N:25:ARG:NH1	14:N:46:LEU:HG	2.23	0.54
18:R:22:VAL:HG11	18:R:63:LEU:HB3	1.90	0.54
2:B:156:ILE:O	2:B:179:ILE:HG12	2.07	0.54
13:M:83:ILE:HG12	19:S:64:ASN:HD22	1.72	0.54
2:B:19:ASN:ND2	2:B:21:LYS:H	2.05	0.54
6:F:19:LEU:O	6:F:19:LEU:HD23	2.08	0.54
13:M:61:ASN:O	13:M:62:THR:HB	2.08	0.54
1:A:1275:A:O2'	1:A:1276:G:H5'	2.08	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.90	0.54
18:R:10:THR:O	18:R:10:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:H2'	1:A:955:U:C6	2.41	0.54
1:A:953:G:O2'	1:A:954:G:H5'	2.08	0.54
10:J:44:ARG:NH1	10:J:62:GLU:OE1	2.40	0.54
1:A:1014:A:H2'	1:A:1015:A:C8	2.43	0.54
23:Z:27:G:H2'	23:Z:28:G:C8	2.42	0.54
2:B:198:ASN:HD22	2:B:198:ASN:C	2.09	0.54
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.88	0.54
17:Q:44:HIS:HB3	17:Q:71:ARG:HG2	1.90	0.54
1:A:51:A:C5'	1:A:52:G:H5''	2.33	0.54
9:I:48:PRO:O	9:I:51:ALA:HB3	2.07	0.54
4:D:7:VAL:CG1	4:D:20:LEU:HB2	2.38	0.54
18:R:31:GLU:CD	18:R:31:GLU:H	2.10	0.54
19:S:61:ILE:HD13	19:S:61:ILE:C	2.27	0.54
3:C:43:GLU:HG2	3:C:51:LEU:HD11	1.90	0.54
20:T:50:ARG:HH11	20:T:50:ARG:HB2	1.73	0.54
1:A:983:A:H5''	1:A:984:C:OP1	2.08	0.54
1:A:1424:C:O2'	1:A:1425:U:H5'	2.07	0.54
18:R:32:THR:HA	18:R:68:GLU:HB2	1.90	0.54
1:A:718:G:H5'	11:K:107:ASN:CG	2.28	0.54
12:L:79:VAL:HG21	12:L:96:ILE:CG2	2.38	0.54
1:A:412:A:H62	4:D:34:ARG:HD3	1.72	0.54
9:I:92:ARG:HD3	9:I:96:LYS:NZ	2.23	0.54
1:A:1193:G:O2'	1:A:1194:U:H5'	2.08	0.54
11:K:77:THR:HA	11:K:81:ARG:HH21	1.72	0.54
6:F:33:TYR:CB	6:F:75:LEU:HD23	2.38	0.54
5:E:72:ILE:HG23	5:E:138:LEU:HD13	1.90	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.08	0.54
1:A:860:A:H2'	1:A:861:G:O4'	2.08	0.54
1:A:1281:U:C5'	1:A:1282:C:C5	2.88	0.54
2:B:17:ARG:NH2	2:B:185:ASP:HB2	2.23	0.54
1:A:113:G:C1'	1:A:354:G:H5'	2.35	0.54
4:D:150:LYS:CD	4:D:150:LYS:H	2.21	0.54
2:B:233:VAL:O	2:B:233:VAL:HG12	2.08	0.54
1:A:1522:U:O2'	1:A:1523:G:H5'	2.08	0.54
1:A:434:U:O2'	1:A:435:C:H5'	2.07	0.54
1:A:166:G:O2'	1:A:167:G:H5'	2.07	0.54
4:D:163:ALA:O	4:D:167:ARG:HD3	2.08	0.54
2:B:45:LEU:HD22	2:B:49:PHE:HE1	1.73	0.53
9:I:15:ARG:CB	9:I:63:THR:HB	2.38	0.53
1:A:7:G:H21	5:E:117:LYS:HG2	1.73	0.53
13:M:123:PRO:C	13:M:125:LYS:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H2'	1:A:1130:A:N3	2.23	0.53
1:A:1475:G:O2'	1:A:1476:G:C5'	2.56	0.53
17:Q:78:SER:O	17:Q:79:GLY:O	2.25	0.53
2:B:94:GLY:O	2:B:98:ASN:N	2.36	0.53
1:A:809:G:H3'	1:A:810:C:H5''	1.90	0.53
11:K:23:THR:HG22	11:K:29:PRO:HA	1.89	0.53
10:J:21:ILE:O	10:J:21:ILE:HG22	2.08	0.53
2:B:215:LEU:HD13	2:B:215:LEU:O	2.08	0.53
1:A:1301:U:H3'	1:A:1302:U:H5'	1.90	0.53
12:L:23:LEU:HG	12:L:24:LYS:H	1.74	0.53
1:A:1231:G:H4'	9:I:125:SER:HG	1.72	0.53
5:E:60:ARG:O	5:E:61:ASN:HB3	2.07	0.53
1:A:404:U:H5'	4:D:121:ARG:HD2	1.90	0.53
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.53
1:A:1194:U:H2'	1:A:1195:C:C6	2.43	0.53
3:C:18:GLU:O	3:C:39:ARG:NH2	2.42	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
1:A:539:A:H2'	1:A:540:G:C8	2.43	0.53
2:B:163:LYS:NZ	2:B:163:LYS:HB3	2.23	0.53
12:L:113:ARG:NH2	12:L:120:LYS:HD3	2.24	0.53
1:A:1272:G:H2'	1:A:1273:G:H5'	1.90	0.53
1:A:664:G:OP2	18:R:49:ARG:HD2	2.08	0.53
1:A:1305:G:H22	1:A:1331:G:H1'	1.73	0.53
11:K:34:SER:OG	11:K:37:VAL:HG23	2.09	0.53
10:J:32:VAL:CG1	10:J:72:ILE:HG22	2.39	0.53
16:P:82:GLN:O	16:P:83:GLU:O	2.25	0.53
12:L:49:ARG:N	12:L:49:ARG:HD2	2.23	0.53
12:L:55:ARG:HD3	12:L:61:GLU:CG	2.34	0.53
15:O:87:ARG:HB2	15:O:87:ARG:HH11	1.73	0.53
9:I:74:ASP:O	9:I:77:LYS:HB3	2.09	0.53
19:S:35:ARG:NH1	19:S:35:ARG:HG3	2.24	0.53
1:A:1080:A:H5''	5:E:12:THR:HG21	1.91	0.53
1:A:575:G:O2'	1:A:821:G:H5'	2.08	0.53
1:A:37:U:O2'	1:A:38:G:H5'	2.08	0.53
11:K:47:THR:HG23	11:K:50:ALA:H	1.73	0.53
3:C:34:GLU:HG3	3:C:94:THR:HG21	1.90	0.53
12:L:39:VAL:HG12	12:L:40:THR:N	2.22	0.53
1:A:1251:A:H4'	9:I:11:GLU:OE1	2.08	0.53
1:A:553:A:H5''	12:L:20:VAL:HG21	1.91	0.53
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.73	0.53
1:A:1028:C:H2'	1:A:1029:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:A:N6	4:D:34:ARG:HD3	2.24	0.53
7:G:43:TYR:O	7:G:47:LYS:HG2	2.08	0.53
17:Q:55:VAL:O	17:Q:76:VAL:HB	2.09	0.53
3:C:83:ILE:O	3:C:87:ARG:HB2	2.09	0.53
1:A:636:U:O2'	1:A:637:G:H5'	2.09	0.53
1:A:686:U:HO2'	1:A:687:A:H8	1.56	0.53
12:L:24:LYS:C	12:L:26:ALA:N	2.60	0.53
12:L:29:ARG:CD	12:L:58:SER:HB3	2.36	0.53
19:S:79:TYR:O	19:S:80:ARG:C	2.47	0.53
9:I:52:VAL:O	9:I:53:ASP:HB2	2.08	0.53
10:J:67:ASN:O	10:J:68:ARG:HD3	2.08	0.53
3:C:2:ASN:O	3:C:3:LYS:HB2	2.08	0.53
11:K:38:ILE:HD11	11:K:54:ALA:HA	1.91	0.53
13:M:121:LYS:O	13:M:122:ALA:HB2	2.09	0.53
1:A:947:G:H2'	1:A:948:C:O4'	2.09	0.53
1:A:807:A:H2'	1:A:808:C:C6	2.44	0.53
16:P:26:ARG:HD2	16:P:31:LYS:O	2.09	0.53
13:M:106:ALA:HB3	13:M:110:LYS:HD2	1.91	0.52
1:A:738:C:OP1	6:F:92:LYS:NZ	2.39	0.52
10:J:7:ARG:CB	10:J:7:ARG:NH1	2.72	0.52
1:A:1250:A:H4'	9:I:67:GLY:N	2.23	0.52
17:Q:96:SER:HA	17:Q:101:GLY:HA2	1.91	0.52
1:A:1106:G:OP1	3:C:171:ARG:HD3	2.09	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.52
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.13	0.52
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.90	0.52
1:A:6:G:H4'	1:A:298:A:H4'	1.91	0.52
12:L:122:LYS:H	12:L:122:LYS:HZ2	1.55	0.52
1:A:1245:A:H2'	1:A:1246:C:O4'	2.09	0.52
1:A:547:A:H4'	1:A:548:G:C5'	2.32	0.52
3:C:51:LEU:HD23	3:C:51:LEU:H	1.74	0.52
2:B:178:VAL:HG12	2:B:191:VAL:HG13	1.91	0.52
14:N:11:ARG:O	14:N:11:ARG:HD3	2.08	0.52
1:A:1090:U:H2'	1:A:1091:U:H6	1.74	0.52
7:G:107:ALA:O	7:G:118:ARG:HD2	2.09	0.52
1:A:417:C:H2'	1:A:418:C:H6	1.74	0.52
10:J:2:ILE:O	10:J:71:ASP:HA	2.09	0.52
19:S:40:VAL:HG22	19:S:43:MET:HE3	1.90	0.52
1:A:189(B):C:N4	1:A:189(J):G:C6	2.77	0.52
1:A:1346:A:C5	7:G:9:ARG:NH1	2.71	0.52
1:A:352:C:H4'	1:A:354:G:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:A:H1'	11:K:19:ILE:HD11	1.91	0.52
9:I:47:GLU:N	9:I:48:PRO:CD	2.72	0.52
13:M:14:VAL:HG21	13:M:47:LEU:HD21	1.91	0.52
8:H:63:LEU:H	8:H:63:LEU:HD22	1.75	0.52
5:E:27:LEU:HD22	5:E:39:LEU:CD2	2.40	0.52
1:A:328:C:C2'	1:A:328:C:O2	2.57	0.52
7:G:119:ILE:HD12	7:G:119:ILE:H	1.75	0.52
21:V:5:ASP:O	21:V:11:GLY:HA3	2.09	0.52
1:A:961:U:O2'	1:A:962:C:H5'	2.10	0.52
2:B:6:GLU:OE2	2:B:207:LEU:HD11	2.10	0.52
19:S:61:ILE:HD13	19:S:62:THR:N	2.25	0.52
9:I:92:ARG:HD3	9:I:96:LYS:CE	2.38	0.52
1:A:648:A:C8	1:A:648:A:H5'	2.38	0.52
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.52
5:E:97:ILE:O	5:E:116:THR:HB	2.09	0.52
2:B:168:VAL:O	2:B:172:ARG:HG2	2.09	0.52
2:B:19:ASN:HD22	2:B:21:LYS:H	1.58	0.52
4:D:64:ARG:HH11	4:D:64:ARG:HB3	1.74	0.52
5:E:95:GLY:O	5:E:113:ASP:HA	2.08	0.52
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.23	0.52
6:F:46:ARG:HB2	6:F:60:PHE:CE2	2.44	0.52
1:A:1347:G:N2	1:A:1373:G:H2'	2.23	0.52
4:D:59:GLU:HG2	4:D:201:LEU:HB2	1.91	0.52
21:V:9:ARG:NH1	21:V:22:ARG:HA	2.24	0.52
1:A:1128:C:C3'	1:A:1129:C:H5''	2.27	0.52
1:A:1502:A:C2	1:A:1505:G:N1	2.65	0.52
11:K:17:ASN:ND2	11:K:18:THR:N	2.43	0.52
5:E:76:ILE:N	5:E:76:ILE:HD13	2.25	0.52
1:A:1227:A:O3'	13:M:114:LYS:HE3	2.10	0.52
9:I:16:VAL:CG2	9:I:79:GLY:HA3	2.39	0.52
3:C:107:ASN:ND2	3:C:143:SER:HB2	2.24	0.52
12:L:106:VAL:CG2	12:L:116:TYR:HB3	2.40	0.52
1:A:1495:U:H2'	1:A:1496:C:C6	2.43	0.52
19:S:49:ALA:HA	19:S:57:VAL:O	2.09	0.52
8:H:80:ILE:O	8:H:80:ILE:HG22	2.09	0.52
1:A:1125:U:H5'	1:A:1126:U:C5	2.39	0.52
1:A:1370:G:O2'	1:A:1371:G:H5'	2.09	0.52
13:M:39:ASN:HD22	13:M:40:PRO:N	2.08	0.52
1:A:839:U:C2'	1:A:839:U:O2	2.56	0.52
2:B:115:LEU:O	2:B:121:ILE:HG12	2.09	0.52
2:B:17:ARG:C	2:B:17:ARG:NH1	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:29:LEU:O	19:S:30:ILE:HD13	2.09	0.52
15:O:2:ILE:HD12	15:O:2:ILE:N	2.24	0.52
2:B:10:HIS:O	2:B:11:PHE:O	2.28	0.52
1:A:412:A:H4'	1:A:413:G:O5'	2.09	0.52
2:B:92:LEU:O	2:B:95:MET:HG3	2.10	0.52
2:B:110:GLU:CB	2:B:147:ARG:NH2	2.72	0.52
16:P:43:LYS:HB3	16:P:48:TRP:CG	2.45	0.52
18:R:40:ARG:CZ	18:R:40:ARG:HB3	2.40	0.52
1:A:1237:C:H4'	1:A:1334:G:N2	2.25	0.52
1:A:251:G:H4'	1:A:252:U:O5'	2.09	0.52
1:A:1206:G:H4'	3:C:191:THR:O	2.09	0.52
5:E:75:GLU:CD	5:E:75:GLU:H	2.13	0.52
1:A:390:C:H2'	1:A:391:G:H8	1.73	0.52
1:A:1329:A:P	13:M:27:ALA:HB3	2.49	0.52
2:B:2:LYS:O	2:B:211:ARG:NH1	2.41	0.52
3:C:21:TRP:CZ3	3:C:31:LEU:HB2	2.45	0.52
1:A:1346:A:N6	1:A:1374:A:H3'	2.24	0.52
13:M:21:ILE:HD12	13:M:24:ILE:HD12	1.91	0.52
2:B:69:LYS:HD3	2:B:72:GLN:HB2	1.91	0.52
12:L:79:VAL:HG21	12:L:96:ILE:HG23	1.91	0.52
2:B:181:LEU:HA	2:B:195:ILE:HB	1.92	0.52
19:S:30:ILE:HG13	19:S:48:ILE:HD12	1.92	0.52
4:D:155:GLU:HG2	4:D:159:GLN:HE21	1.74	0.52
9:I:105:ALA:O	9:I:107:VAL:HG23	2.10	0.52
10:J:4:ILE:HB	10:J:70:VAL:HB	1.92	0.52
19:S:44:VAL:HA	19:S:61:ILE:HD12	1.91	0.52
3:C:63:VAL:HB	3:C:98:VAL:CB	2.40	0.52
1:A:1292:U:O2'	1:A:1293:G:H5'	2.10	0.52
7:G:71:ARG:HG2	7:G:141:GLU:OE2	2.10	0.52
19:S:50:VAL:O	19:S:57:VAL:HG22	2.10	0.52
9:I:12:ALA:HA	9:I:66:GLY:O	2.10	0.52
1:A:147:G:O2'	1:A:148:G:H5'	2.09	0.52
12:L:67:PRO:O	12:L:98:ARG:HD2	2.10	0.52
1:A:1190:G:OP1	3:C:4:ILE:HD12	2.10	0.51
3:C:4:ILE:N	3:C:4:ILE:HD13	2.25	0.51
2:B:49:PHE:CE2	2:B:212:ALA:HA	2.45	0.51
1:A:1428:A:H2'	1:A:1429:C:C6	2.45	0.51
1:A:1392:G:H21	1:A:1502:A:H8	1.56	0.51
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.45	0.51
1:A:472:A:H2'	1:A:473:G:O4'	2.10	0.51
3:C:82:ARG:C	3:C:84:ARG:H	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:ASN:HD22	4:D:198:ASN:C	2.12	0.51
7:G:153:TYR:O	7:G:155:TRP:N	2.43	0.51
1:A:108:G:H5'	1:A:109:A:H5''	1.92	0.51
18:R:56:LYS:O	18:R:60:ILE:HG12	2.09	0.51
1:A:57:G:H2'	1:A:58:C:C6	2.45	0.51
5:E:146:ARG:HG3	5:E:146:ARG:HH11	1.75	0.51
1:A:1118:C:H1'	1:A:1179:A:C4	2.45	0.51
1:A:52:G:O2'	1:A:53:A:H5'	2.09	0.51
18:R:38:ARG:HG2	18:R:48:GLN:OE1	2.09	0.51
12:L:51:VAL:HG12	12:L:52:ALA:N	2.25	0.51
13:M:10:ARG:CG	13:M:11:ASN:N	2.73	0.51
19:S:17:LYS:NZ	19:S:17:LYS:HB2	2.26	0.51
1:A:1068:G:OP2	1:A:1094:G:H5'	2.10	0.51
3:C:59:ALA:O	3:C:60:ALA:CB	2.58	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.42	0.51
1:A:1296:C:H5''	13:M:13:ARG:HD2	1.92	0.51
1:A:824:C:H2'	1:A:825:G:H8	1.76	0.51
1:A:427:U:OP2	4:D:12:ARG:NH2	2.43	0.51
13:M:3:ILE:HD11	13:M:55:LEU:HD13	1.91	0.51
7:G:53:THR:HG22	7:G:55:GLN:N	2.25	0.51
2:B:110:GLU:HB3	2:B:147:ARG:NH1	2.26	0.51
2:B:175:PHE:CD2	8:H:70:GLN:HB3	2.45	0.51
19:S:11:ASP:H	19:S:37:SER:HB3	1.75	0.51
10:J:28:SER:OG	10:J:79:THR:HA	2.11	0.51
1:A:1399:C:C2	1:A:1502:A:N6	2.79	0.51
3:C:90:LEU:HD13	3:C:98:VAL:HG22	1.92	0.51
3:C:63:VAL:O	3:C:98:VAL:HB	2.10	0.51
9:I:15:ARG:NH2	9:I:63:THR:HG21	2.25	0.51
3:C:7:ILE:HG23	3:C:15:ARG:HG2	1.91	0.51
15:O:86:ILE:CG2	15:O:87:ARG:N	2.73	0.51
14:N:22:ARG:NH1	14:N:29:ALA:HB2	2.25	0.51
12:L:115:LYS:O	12:L:116:TYR:HB2	2.11	0.51
17:Q:16:LYS:HA	17:Q:45:ASP:O	2.11	0.51
1:A:1154:G:O2'	1:A:1155:G:H5'	2.10	0.51
1:A:1157:A:H1'	1:A:1181:G:N2	2.26	0.51
1:A:1251:A:H2'	1:A:1252:A:C8	2.45	0.51
1:A:302:G:H5''	12:L:13:LYS:HE2	1.92	0.51
1:A:666:G:H5'	1:A:726:C:H1'	1.92	0.51
5:E:76:ILE:H	5:E:76:ILE:HD13	1.74	0.51
11:K:100:ASP:OD2	18:R:73:LYS:NZ	2.33	0.51
1:A:1285:A:OP2	1:A:1285:A:H8	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:62:ARG:O	17:Q:64:ILE:HD12	2.10	0.51
1:A:1378:C:H2'	1:A:1379:G:H5'	1.92	0.51
7:G:5:ARG:O	7:G:6:ALA:C	2.48	0.51
4:D:186:ARG:HG3	4:D:187:LEU:N	2.26	0.51
1:A:1064:G:H1'	1:A:1190:G:H21	1.75	0.51
2:B:91:TRP:CH2	2:B:95:MET:HB2	2.45	0.51
1:A:1457:G:O2'	1:A:1458:G:H5'	2.11	0.51
1:A:1172:C:O2'	1:A:1173:G:H5'	2.11	0.51
3:C:9:PHE:CZ	3:C:177:LEU:HD13	2.46	0.51
2:B:71:ALA:CB	2:B:205:ILE:HD13	2.33	0.51
4:D:29:LYS:C	4:D:31:ALA:N	2.62	0.51
1:A:1368:G:O2'	1:A:1369:C:H5'	2.10	0.51
14:N:41:ILE:O	14:N:45:GLU:HG3	2.10	0.51
2:B:166:ILE:H	2:B:166:ILE:CD1	2.21	0.51
12:L:66:ILE:HD13	12:L:73:LEU:HD12	1.92	0.51
1:A:1251:A:H4'	9:I:11:GLU:CD	2.31	0.51
3:C:133:ILE:CG2	3:C:167:ALA:HB3	2.41	0.51
1:A:1152:A:O2'	1:A:1153:C:H5'	2.10	0.51
18:R:2:SER:HA	18:R:4:LYS:HZ2	1.74	0.51
8:H:121:ASP:OD2	8:H:125:ARG:NH2	2.43	0.51
1:A:433:C:O2'	1:A:434:U:H5'	2.11	0.51
1:A:928:G:O2'	1:A:929:G:H5'	2.11	0.51
10:J:19:GLN:OE1	10:J:22:VAL:HG11	2.11	0.51
19:S:63:GLU:O	19:S:66:VAL:HG23	2.11	0.51
2:B:70:GLN:NE2	2:B:70:GLN:O	2.43	0.51
3:C:99:ALA:O	3:C:100:LEU:HB2	2.09	0.51
7:G:52:LYS:H	7:G:52:LYS:HD2	1.76	0.51
3:C:90:LEU:HD12	3:C:90:LEU:C	2.31	0.51
13:M:2:ARG:HG2	13:M:8:ILE:HD12	1.93	0.51
1:A:542:G:H2'	1:A:543:C:H6	1.76	0.51
1:A:160:A:O2'	1:A:161:A:H5'	2.12	0.51
13:M:36:THR:O	13:M:36:THR:HG22	2.11	0.51
13:M:64:LYS:O	13:M:65:LEU:HD23	2.11	0.51
13:M:72:GLU:O	13:M:75:ALA:HB3	2.11	0.51
12:L:75:GLU:HG2	12:L:75:GLU:O	2.11	0.51
12:L:123:GLU:O	12:L:123:GLU:HG3	2.11	0.51
1:A:1023:G:N3	1:A:1023:G:H2'	2.26	0.50
9:I:110:ARG:HD2	14:N:60:TRP:OXT	2.10	0.50
1:A:376:G:OP2	16:P:67:THR:HG21	2.11	0.50
10:J:10:ASP:HB3	10:J:13:THR:HB	1.93	0.50
5:E:72:ILE:HG23	5:E:138:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:C:H4'	1:A:329:A:H5''	1.92	0.50
1:A:620:C:C1'	4:D:134:LEU:HD13	2.40	0.50
2:B:76:ARG:O	2:B:80:GLU:HG3	2.11	0.50
20:T:83:GLN:O	20:T:86:GLU:HB2	2.11	0.50
11:K:57:ASP:OD1	11:K:61:LYS:HE3	2.11	0.50
1:A:444:C:H2'	1:A:445:G:H8	1.77	0.50
1:A:358:U:O2'	1:A:359:U:H5'	2.11	0.50
10:J:1:LYS:N	10:J:73:ILE:HA	2.25	0.50
1:A:397:A:N3	1:A:397:A:H3'	2.26	0.50
1:A:837:G:H1	1:A:849:C:N4	2.09	0.50
13:M:19:THR:C	13:M:21:ILE:H	2.15	0.50
1:A:1425:U:H2'	1:A:1426:C:H6	1.70	0.50
19:S:76:THR:HG22	19:S:77:ARG:N	2.26	0.50
5:E:140:THR:O	5:E:144:VAL:HG23	2.11	0.50
11:K:106:HIS:O	11:K:107:ASN:HB2	2.12	0.50
23:Z:28:G:H2'	23:Z:29:G:H8	1.76	0.50
7:G:115:ALA:HA	7:G:118:ARG:NH2	2.26	0.50
4:D:2:ARG:NH1	4:D:117:ARG:HH22	2.09	0.50
4:D:77:LEU:HD22	4:D:95:LEU:HB3	1.93	0.50
4:D:193:LEU:HD22	4:D:193:LEU:H	1.76	0.50
17:Q:68:LYS:O	17:Q:69:ARG:HD2	2.11	0.50
9:I:3:TYR:CE2	9:I:87:TYR:HA	2.47	0.50
1:A:991:U:C2	1:A:1212:U:H1'	2.47	0.50
3:C:45:GLU:O	3:C:47:TYR:N	2.44	0.50
1:A:780:A:O2'	1:A:781:A:H5''	2.11	0.50
10:J:74:ASN:HB3	10:J:76:ASN:ND2	2.26	0.50
1:A:835:U:OP2	18:R:49:ARG:NH2	2.37	0.50
22:W:2:U:H2'	22:W:3:C:C6	2.47	0.50
2:B:135:GLU:O	2:B:138:ARG:HG3	2.10	0.50
12:L:55:ARG:NH1	12:L:61:GLU:HG2	2.27	0.50
17:Q:26:PHE:HB2	17:Q:27:PRO:HD2	1.94	0.50
1:A:1061:G:H1'	10:J:54:HIS:CE1	2.47	0.50
1:A:7:G:O2'	5:E:116:THR:O	2.29	0.50
1:A:1310:G:O2'	1:A:1311:G:H5'	2.12	0.50
9:I:120:ARG:HG3	9:I:120:ARG:HH11	1.76	0.50
1:A:1262:C:H2'	1:A:1263:C:C6	2.46	0.50
1:A:1070:U:OP2	5:E:16:GLN:HG3	2.11	0.50
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.11	0.50
11:K:74:VAL:HG21	11:K:85:ILE:HD11	1.94	0.50
20:T:50:ARG:HH12	20:T:93:ILE:HG21	1.77	0.50
20:T:93:ILE:O	20:T:95:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TRP:CZ2	2:B:95:MET:HB2	2.46	0.50
1:A:542:G:OP2	4:D:9:ARG:NH2	2.45	0.50
4:D:63:LEU:C	4:D:63:LEU:HD13	2.32	0.50
7:G:144:ALA:O	7:G:145:GLU:HB3	2.11	0.50
18:R:30:SER:C	18:R:32:THR:N	2.65	0.50
10:J:92:VAL:CG1	10:J:93:GLU:N	2.74	0.50
2:B:162:THR:OG1	2:B:186:SER:HB3	2.11	0.50
4:D:34:ARG:O	4:D:35:ARG:CB	2.59	0.50
3:C:69:VAL:CG1	3:C:70:ALA:N	2.75	0.50
2:B:156:ILE:CG2	2:B:158:VAL:HG23	2.41	0.50
2:B:96:LEU:HD21	2:B:156:ILE:CD1	2.36	0.50
13:M:87:ARG:HG3	13:M:97:VAL:HG13	1.93	0.50
1:A:293:G:H4'	1:A:609:A:N1	2.27	0.50
3:C:187:LEU:O	3:C:188:ALA:HB2	2.11	0.50
18:R:4:LYS:N	18:R:4:LYS:HD2	2.27	0.50
10:J:23:GLU:C	10:J:25:ALA:H	2.15	0.50
2:B:57:MET:HB3	2:B:219:ALA:O	2.12	0.50
1:A:1069:C:O2'	1:A:1192:C:H1'	2.11	0.50
3:C:66:THR:CG2	3:C:67:VAL:N	2.74	0.50
4:D:149:GLU:HA	4:D:152:ARG:CZ	2.42	0.50
23:Z:32:U:C2'	23:Z:33:U:C5'	2.88	0.50
10:J:80:ILE:HG22	10:J:80:ILE:O	2.12	0.50
1:A:689:C:H2'	1:A:690:G:O4'	2.12	0.50
1:A:443:C:H2'	1:A:444:C:H6	1.75	0.50
1:A:242:C:H2'	1:A:243:A:H5'	1.92	0.50
2:B:9:VAL:CG1	2:B:203:ARG:HB3	2.42	0.50
5:E:76:ILE:HD11	5:E:87:LEU:HD12	1.94	0.50
10:J:43:ARG:NH1	10:J:43:ARG:HB2	2.27	0.50
3:C:90:LEU:CD1	3:C:98:VAL:HG22	2.42	0.50
1:A:1343:G:H2'	1:A:1344:C:H6	1.71	0.50
1:A:19:C:H2'	1:A:20:U:C6	2.46	0.50
1:A:152:A:H5'	1:A:153:C:OP1	2.12	0.50
1:A:523:A:H61	12:L:88:ASP:HB2	1.77	0.50
1:A:229:U:H5''	16:P:33:ILE:HD13	1.94	0.50
1:A:1135:U:H2'	1:A:1135:U:O2	2.10	0.50
2:B:81:ARG:HH21	2:B:213:VAL:HB	1.77	0.49
1:A:145:G:H8	1:A:145:G:H5'	1.77	0.49
9:I:92:ARG:O	9:I:94:LYS:N	2.45	0.49
8:H:112:LEU:HD22	8:H:133:LEU:HD12	1.93	0.49
9:I:84:LEU:O	9:I:91:TYR:HD2	1.95	0.49
2:B:13:HIS:CE1	2:B:200:ASP:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:SER:HA	11:K:37:VAL:HG21	1.94	0.49
1:A:1241:G:H2'	1:A:1242:C:C6	2.46	0.49
1:A:268:C:O2'	1:A:269:C:H5'	2.12	0.49
1:A:1035:A:O2'	1:A:1036:G:H5'	2.12	0.49
1:A:325:A:OP1	20:T:63:SER:HB2	2.12	0.49
1:A:646:U:H2'	1:A:647:C:C6	2.47	0.49
1:A:1201:A:O2'	1:A:1202:G:OP2	2.27	0.49
3:C:206:VAL:CG1	3:C:207:ILE:N	2.74	0.49
1:A:1493:A:OP2	26:A:2759:ON0:HAO	2.11	0.49
1:A:1406:U:O2'	1:A:1407:C:H5'	2.11	0.49
10:J:45:PHE:CZ	14:N:36:PHE:HE1	2.30	0.49
13:M:104:THR:O	13:M:105:ASN:C	2.51	0.49
1:A:106:C:O2'	1:A:379:C:H5''	2.12	0.49
1:A:1417:G:H2'	1:A:1482:G:N2	2.28	0.49
1:A:1030:C:H6	1:A:1030:C:H5'	1.77	0.49
9:I:9:ARG:HG2	9:I:74:ASP:HB2	1.94	0.49
3:C:45:GLU:C	3:C:47:TYR:H	2.15	0.49
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.27	0.49
10:J:74:ASN:HB3	10:J:76:ASN:HD21	1.78	0.49
2:B:217:ILE:C	2:B:219:ALA:N	2.66	0.49
9:I:94:LYS:O	9:I:98:LEU:HD23	2.13	0.49
3:C:5:HIS:CD2	3:C:7:ILE:HB	2.47	0.49
3:C:12:GLY:CA	14:N:56:ARG:NH2	2.75	0.49
17:Q:66:LYS:HA	17:Q:69:ARG:NH1	2.19	0.49
1:A:1001:A:C3'	1:A:1001(A):G:H5'	2.42	0.49
7:G:135:LYS:HG2	7:G:139:ASP:OD1	2.13	0.49
1:A:190:U:C2	20:T:98:SER:HB2	2.47	0.49
18:R:4:LYS:O	18:R:5:ALA:CB	2.60	0.49
2:B:198:ASN:HD22	2:B:200:ASP:H	1.59	0.49
2:B:48:THR:O	2:B:51:PHE:HB3	2.12	0.49
4:D:2:ARG:NH2	4:D:73:GLN:OE1	2.45	0.49
4:D:175:LEU:HD12	4:D:181:LYS:O	2.12	0.49
1:A:545:C:H5''	4:D:71:GLU:HG3	1.93	0.49
1:A:263:A:OP1	20:T:72:ARG:NH1	2.46	0.49
12:L:36:VAL:HG12	12:L:36:VAL:O	2.11	0.49
1:A:1191:A:OP2	3:C:2:ASN:ND2	2.45	0.49
1:A:189(B):C:C3'	1:A:189(B):C:OP2	2.60	0.49
3:C:39:ARG:O	3:C:43:GLU:HG3	2.12	0.49
1:A:1259:C:H5'	1:A:1260:C:OP1	2.13	0.49
4:D:7:VAL:HG21	4:D:114:ARG:CZ	2.43	0.49
4:D:7:VAL:C	4:D:9:ARG:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:116:VAL:HG12	13:M:117:ALA:H	1.75	0.49
8:H:121:ASP:HB2	8:H:125:ARG:HH21	1.77	0.49
2:B:106:VAL:HG12	2:B:147:ARG:HD3	1.95	0.49
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.95	0.49
1:A:21:G:H2'	1:A:22:G:C8	2.47	0.49
2:B:116:PHE:O	2:B:117:ALA:HB2	2.12	0.49
2:B:9:VAL:HG11	2:B:203:ARG:C	2.33	0.49
1:A:663:A:H5'	1:A:836:G:OP2	2.13	0.49
13:M:76:ASN:O	13:M:80:LEU:HD23	2.13	0.49
19:S:16:GLU:HA	19:S:19:LEU:HD11	1.94	0.49
1:A:392:G:H2'	1:A:393:A:C8	2.47	0.49
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.45	0.49
8:H:126:LYS:C	8:H:128:GLY:H	2.16	0.49
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.49
4:D:116:ALA:O	4:D:120:VAL:HG23	2.13	0.49
15:O:41:HIS:O	15:O:44:VAL:O	2.31	0.49
2:B:1:VAL:HG11	2:B:215:LEU:HD23	1.95	0.49
3:C:135:GLN:O	3:C:138:GLN:N	2.46	0.49
18:R:32:THR:HG22	18:R:33:GLY:N	2.27	0.49
1:A:181:G:O2'	1:A:182:U:OP2	2.29	0.49
8:H:51:VAL:HG21	8:H:60:ARG:HG3	1.95	0.49
6:F:40:VAL:HG23	6:F:63:TYR:CD1	2.48	0.49
1:A:105:G:H2'	1:A:106:C:C6	2.47	0.49
1:A:920:U:H2'	1:A:921:U:C6	2.48	0.49
7:G:74:VAL:HG11	7:G:143:MET:HG2	1.94	0.49
13:M:84:GLY:O	13:M:85:CYS:O	2.31	0.49
3:C:187:LEU:CD1	3:C:194:VAL:HG13	2.43	0.49
9:I:10:LYS:O	9:I:10:LYS:HG2	2.13	0.49
3:C:122:GLN:NE2	3:C:139:ARG:HH22	2.10	0.49
9:I:7:GLY:HA2	9:I:78:LEU:HD13	1.94	0.49
1:A:1137:C:H6	1:A:1137:C:H5'	1.78	0.49
11:K:11:ILE:HD13	11:K:84:ALA:HB3	1.94	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
2:B:56:ALA:O	2:B:58:ARG:N	2.46	0.49
4:D:130:ARG:H	4:D:130:ARG:HD2	1.78	0.49
1:A:1346:A:C8	1:A:1348:U:N3	2.80	0.49
18:R:22:VAL:CG1	18:R:63:LEU:HB3	2.42	0.49
2:B:85:PRO:HG3	2:B:148:LEU:CB	2.39	0.49
1:A:734:G:H3'	1:A:735:C:H6	1.78	0.49
3:C:176:THR:O	3:C:176:THR:HG23	2.12	0.49
1:A:513:C:H2'	1:A:514:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:G:N3	20:T:98:SER:HB3	2.28	0.49
1:A:1060:C:H2'	1:A:1061:G:H8	1.78	0.49
14:N:25:ARG:NH2	14:N:46:LEU:HD21	2.28	0.49
5:E:8:LEU:HD13	5:E:27:LEU:HB2	1.94	0.49
8:H:58:TYR:O	8:H:59:LEU:HD23	2.12	0.49
1:A:160:A:H2'	1:A:161:A:O4'	2.12	0.49
3:C:14:THR:O	3:C:15:ARG:CB	2.55	0.48
13:M:18:LEU:O	13:M:21:ILE:HG13	2.13	0.48
13:M:7:GLU:HG3	13:M:21:ILE:HG23	1.95	0.48
2:B:91:TRP:CZ3	2:B:170:GLU:OE2	2.65	0.48
18:R:32:THR:HG23	18:R:68:GLU:H	1.78	0.48
10:J:88:LEU:HB2	10:J:89:PRO:HD3	1.94	0.48
1:A:1333:A:H2'	1:A:1334:G:O4'	2.13	0.48
1:A:1041:A:H2'	1:A:1042:G:C8	2.48	0.48
1:A:1130:A:H5'	1:A:1131:G:H5'	1.95	0.48
2:B:136:LEU:HD13	2:B:140:GLN:CD	2.33	0.48
1:A:1206:G:H1'	3:C:192:TYR:O	2.13	0.48
4:D:189:ASP:O	4:D:193:LEU:HD22	2.13	0.48
3:C:24:GLY:O	3:C:26:LYS:N	2.46	0.48
1:A:485:G:C2'	1:A:486:U:OP2	2.61	0.48
7:G:37:LEU:O	7:G:37:LEU:HD12	2.13	0.48
2:B:53:GLU:HG2	2:B:215:LEU:HD11	1.95	0.48
9:I:92:ARG:C	9:I:94:LYS:H	2.16	0.48
1:A:648:A:O2'	1:A:649:G:H5'	2.13	0.48
14:N:3:LYS:HA	14:N:6:ILE:HD12	1.94	0.48
3:C:22:TYR:CD2	10:J:8:GLY:HA2	2.48	0.48
1:A:1253:G:H2'	1:A:1254:C:C6	2.49	0.48
12:L:46:SER:O	12:L:47:ALA:HB2	2.13	0.48
9:I:92:ARG:HD3	9:I:96:LYS:HZ1	1.77	0.48
10:J:43:ARG:HH11	10:J:43:ARG:HB2	1.78	0.48
1:A:960:U:O2'	1:A:1223:C:H5''	2.13	0.48
1:A:1189:C:OP1	10:J:49:ARG:NH2	2.39	0.48
5:E:75:GLU:HG3	5:E:89:PRO:CD	2.43	0.48
7:G:145:GLU:C	7:G:147:ASN:N	2.67	0.48
1:A:1152:A:OP2	10:J:66:HIS:ND1	2.47	0.48
18:R:4:LYS:O	18:R:5:ALA:HB2	2.13	0.48
1:A:17:U:O4'	1:A:1080:A:H1'	2.13	0.48
2:B:198:ASN:ND2	2:B:200:ASP:H	2.10	0.48
1:A:995:C:O2'	1:A:996:A:H5''	2.13	0.48
16:P:26:ARG:HD3	16:P:31:LYS:N	2.28	0.48
1:A:1072:G:H2'	1:A:1073:U:C6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:118:ALA:O	11:K:119:SER:C	2.51	0.48
5:E:133:GLU:O	5:E:137:GLN:HG3	2.13	0.48
20:T:36:LEU:HD13	20:T:44:GLU:HG3	1.95	0.48
1:A:1227:A:C2'	1:A:1228:C:H5'	2.43	0.48
14:N:13:PRO:C	14:N:15:PHE:H	2.16	0.48
7:G:77:ARG:HB2	7:G:155:TRP:CZ3	2.48	0.48
2:B:231:ALA:C	2:B:233:VAL:H	2.17	0.48
1:A:100:C:H2'	1:A:101:A:C8	2.48	0.48
2:B:82:ALA:C	2:B:84:MET:N	2.64	0.48
3:C:51:LEU:CD2	3:C:51:LEU:H	2.26	0.48
3:C:63:VAL:HB	3:C:98:VAL:HB	1.96	0.48
18:R:11:LEU:HD11	18:R:24:VAL:HG23	1.96	0.48
9:I:126:LYS:HB3	13:M:125:LYS:NZ	2.27	0.48
5:E:60:ARG:HH11	5:E:60:ARG:CG	2.26	0.48
1:A:1256:A:H61	1:A:1278:U:H3	1.58	0.48
2:B:12:GLY:CA	2:B:35:ILE:HA	2.44	0.48
1:A:1229:A:H2'	1:A:1230:C:H6	1.79	0.48
4:D:7:VAL:HG13	4:D:20:LEU:CD1	2.43	0.48
1:A:1015:A:H2'	1:A:1016:A:C8	2.49	0.48
5:E:7:ILE:HD12	5:E:27:LEU:HD13	1.95	0.48
1:A:181:G:O2'	1:A:182:U:P	2.71	0.48
11:K:94:GLN:OE1	11:K:96:LYS:HE2	2.14	0.48
1:A:572:A:H5''	1:A:917:G:H4'	1.95	0.48
2:B:31:ASN:N	2:B:31:ASN:HD22	2.09	0.48
10:J:76:ASN:O	10:J:78:LYS:N	2.40	0.48
1:A:402:G:C3'	1:A:403:C:H5''	2.43	0.48
22:W:2:U:H2'	22:W:3:C:H6	1.77	0.48
5:E:11:ARG:HD2	5:E:11:ARG:C	2.34	0.48
11:K:107:ASN:HD22	11:K:107:ASN:N	2.11	0.48
1:A:1080:A:C5'	5:E:12:THR:HG21	2.44	0.48
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.48
3:C:179:ALA:O	3:C:180:ASN:HB3	2.14	0.48
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.48
4:D:172:TRP:O	4:D:185:LEU:HB2	2.13	0.48
1:A:1063:C:C5'	1:A:1064:G:H5''	2.44	0.48
2:B:9:VAL:O	2:B:10:HIS:O	2.32	0.48
1:A:647:C:C2'	1:A:648:A:C5'	2.84	0.48
9:I:68:GLY:O	9:I:72:GLN:HG3	2.14	0.48
1:A:1301:U:H2'	1:A:1301:U:O2	2.14	0.48
13:M:122:ALA:O	13:M:124:ARG:N	2.46	0.48
13:M:123:PRO:HB3	13:M:125:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:C:O2	1:A:1539:C:H2'	2.13	0.48
1:A:948:C:OP1	13:M:108:THR:HG22	2.13	0.48
5:E:39:LEU:HD11	5:E:128:ALA:HB1	1.96	0.48
2:B:159:VAL:O	2:B:181:LEU:O	2.32	0.48
20:T:44:GLU:HA	20:T:47:LYS:HE2	1.96	0.48
16:P:6:LEU:CD2	16:P:19:ILE:HD13	2.43	0.48
5:E:145:GLU:O	5:E:149:LYS:HG3	2.14	0.48
10:J:84:MET:HA	10:J:84:MET:CE	2.43	0.48
1:A:1061:G:O2'	1:A:1062:U:H5'	2.13	0.48
2:B:10:HIS:CE1	2:B:204:SER:HA	2.49	0.48
1:A:1230:C:O2'	1:A:1231:G:H5'	2.14	0.48
20:T:88:ALA:O	20:T:89:GLY:C	2.52	0.48
13:M:22:TYR:HB3	13:M:66:GLU:HA	1.95	0.48
1:A:1134:G:N3	1:A:1134:G:H2'	2.28	0.48
1:A:1008:C:H2'	1:A:1009:G:C5'	2.21	0.47
1:A:1009:G:H2'	1:A:1010:G:C8	2.49	0.47
2:B:26:ILE:HD13	2:B:34:HIS:CD2	2.49	0.47
2:B:91:TRP:CZ3	2:B:92:LEU:O	2.67	0.47
1:A:1207:G:O2'	1:A:1208:C:H5'	2.14	0.47
20:T:87:ALA:O	20:T:88:ALA:CB	2.62	0.47
7:G:52:LYS:H	7:G:52:LYS:CD	2.27	0.47
1:A:794:A:H2'	1:A:795:C:C6	2.49	0.47
7:G:78:ARG:HB2	7:G:83:ASN:OD1	2.14	0.47
1:A:1371:G:O3'	9:I:68:GLY:HA3	2.15	0.47
13:M:16:VAL:O	13:M:19:THR:HB	2.13	0.47
15:O:24:THR:HG21	15:O:69:LEU:HG	1.95	0.47
19:S:4:LEU:O	19:S:5:LYS:CB	2.58	0.47
5:E:140:THR:HB	5:E:143:ASP:OD2	2.13	0.47
14:N:11:ARG:C	14:N:13:PRO:HD3	2.34	0.47
14:N:15:PHE:HB2	14:N:17:VAL:HG22	1.96	0.47
10:J:16:ALA:O	10:J:20:LYS:HD3	2.13	0.47
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.44	0.47
8:H:22:GLU:OE1	8:H:22:GLU:HA	2.14	0.47
2:B:9:VAL:HG11	2:B:204:SER:N	2.28	0.47
1:A:849:C:H3'	1:A:850:U:C5'	2.44	0.47
1:A:1123:A:C4'	10:J:34:GLY:HA3	2.38	0.47
2:B:101:THR:C	2:B:103:SER:N	2.68	0.47
2:B:91:TRP:HZ2	2:B:96:LEU:HD13	1.79	0.47
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.47
1:A:28:G:H2'	1:A:29:G:H5''	1.96	0.47
3:C:178:ARG:HD2	3:C:206:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:3:LEU:HD12	20:T:5:ALA:CB	2.43	0.47
7:G:112:GLU:HG2	7:G:118:ARG:HG2	1.95	0.47
2:B:13:HIS:CG	2:B:14:GLU:H	2.32	0.47
1:A:1515:C:O2'	1:A:1516:G:H5'	2.14	0.47
1:A:526:C:OP1	12:L:87:LYS:HE3	2.13	0.47
11:K:98:ILE:HG21	18:R:73:LYS:OXT	2.14	0.47
2:B:89:GLN:HG3	2:B:141:LYS:O	2.15	0.47
1:A:1052:U:C5'	1:A:1053:G:OP1	2.60	0.47
1:A:56:U:H2'	1:A:57:G:C8	2.49	0.47
1:A:1420:C:H2'	1:A:1421:G:H8	1.80	0.47
15:O:40:GLU:OE1	15:O:43:LYS:HE2	2.14	0.47
1:A:831:U:H2'	1:A:832:C:C6	2.50	0.47
1:A:1191:A:P	3:C:2:ASN:ND2	2.86	0.47
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.47
1:A:1366:C:C2	1:A:1367:C:C5	3.03	0.47
17:Q:66:LYS:CA	17:Q:69:ARG:NH1	2.77	0.47
18:R:10:THR:HG22	18:R:27:ARG:HH12	1.75	0.47
2:B:135:GLU:O	2:B:139:LEU:HG	2.14	0.47
19:S:15:LEU:O	19:S:18:VAL:HG12	2.15	0.47
7:G:114:ARG:HB2	7:G:117:VAL:HG23	1.96	0.47
2:B:109:LEU:HD23	2:B:109:LEU:C	2.35	0.47
20:T:69:ALA:O	20:T:73:ARG:HG3	2.15	0.47
10:J:3:ARG:H	10:J:98:THR:HA	1.80	0.47
3:C:21:TRP:CE3	3:C:21:TRP:O	2.67	0.47
1:A:1202:G:C2	14:N:41:ILE:HG21	2.50	0.47
1:A:157:G:O2'	1:A:158:G:H5'	2.14	0.47
18:R:6:LYS:HB3	18:R:42:GLY:HA3	1.95	0.47
1:A:216:G:H2'	1:A:217:C:C6	2.49	0.47
1:A:1102:A:H2'	1:A:1103:C:C6	2.49	0.47
1:A:976:G:C8	1:A:1358:U:O2	2.68	0.47
2:B:12:GLY:HA2	2:B:34:HIS:O	2.14	0.47
1:A:1286:A:C8	1:A:1287:A:H4'	2.50	0.47
1:A:502:G:H2'	1:A:503:C:C6	2.50	0.47
3:C:66:THR:CG2	3:C:67:VAL:H	2.25	0.47
1:A:254:G:OP1	17:Q:67:ARG:HB2	2.14	0.47
12:L:22:ALA:O	12:L:23:LEU:O	2.33	0.47
18:R:38:ARG:HA	18:R:41:THR:OG1	2.15	0.47
1:A:29:G:C2'	1:A:30:U:H5'	2.44	0.47
1:A:737:A:H2'	1:A:738:C:C6	2.49	0.47
17:Q:94:TYR:C	17:Q:96:SER:N	2.67	0.47
1:A:1351:U:O2'	1:A:1352:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442(A):G:H5'	1:A:1442(B):A:H3'	1.95	0.47
20:T:63:SER:HA	20:T:66:HIS:CD2	2.50	0.47
1:A:77:G:O2'	1:A:78:G:H5'	2.15	0.47
13:M:31:GLU:O	13:M:34:GLU:HB3	2.15	0.47
3:C:38:ILE:HG22	3:C:39:ARG:N	2.30	0.47
12:L:40:THR:HA	12:L:41:PRO:HD3	1.77	0.47
1:A:1074:G:O2'	2:B:97:THR:HG22	2.15	0.47
5:E:11:ARG:HD2	5:E:11:ARG:O	2.14	0.47
1:A:28:G:C2'	1:A:29:G:H5''	2.45	0.47
1:A:129(A):G:N1	1:A:189(E):U:O2'	2.41	0.47
5:E:7:ILE:HB	5:E:27:LEU:HB3	1.97	0.47
7:G:61:PHE:HA	7:G:123:LEU:HD22	1.96	0.47
16:P:6:LEU:HD22	16:P:19:ILE:HD13	1.95	0.47
5:E:24:PHE:O	5:E:43:LYS:HA	2.15	0.47
1:A:1411:C:O2'	1:A:1412:C:H5'	2.15	0.47
1:A:573:A:O2'	1:A:574:A:H5'	2.14	0.47
1:A:5:U:O4'	1:A:5:U:O2	2.32	0.47
3:C:133:ILE:HD11	3:C:152:VAL:HG21	1.96	0.47
15:O:13:GLU:HG3	15:O:14:PHE:CE1	2.50	0.47
1:A:1182:G:O2'	1:A:1183:A:OP2	2.31	0.47
1:A:1263:C:H2'	1:A:1264:C:C6	2.50	0.47
5:E:3:GLU:O	5:E:30:VAL:HA	2.15	0.47
1:A:132:C:O3'	20:T:67:LYS:HE3	2.13	0.47
2:B:78:GLU:HB3	2:B:213:VAL:CG2	2.26	0.47
3:C:90:LEU:HD22	3:C:98:VAL:HG22	1.96	0.47
3:C:90:LEU:HD12	3:C:91:ALA:N	2.30	0.47
1:A:1346:A:H61	1:A:1374:A:H3'	1.80	0.47
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.45	0.47
1:A:720:C:H3'	1:A:721:G:H5''	1.97	0.47
3:C:126:ARG:HH11	3:C:126:ARG:HG2	1.80	0.47
10:J:76:ASN:O	10:J:77:ARG:HB2	2.15	0.46
2:B:10:HIS:HE2	2:B:208:ILE:HG12	1.79	0.46
2:B:1:VAL:HG22	2:B:218:GLN:HE22	1.79	0.46
2:B:1:VAL:HG21	2:B:215:LEU:HD23	1.96	0.46
1:A:412:A:C4'	1:A:413:G:H8	2.28	0.46
1:A:1504:G:H4'	1:A:1505:G:C4	2.49	0.46
1:A:1367:C:C2	1:A:1368:G:C8	3.03	0.46
20:T:93:ILE:C	20:T:95:GLY:N	2.67	0.46
11:K:114:LYS:HD2	11:K:115:PHE:CZ	2.49	0.46
9:I:6:THR:HB	9:I:82:ARG:HH11	1.80	0.46
1:A:813:U:C2'	1:A:814:A:H5''	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:VAL:HG22	6:F:60:PHE:CD1	2.50	0.46
3:C:21:TRP:HB3	3:C:58:ARG:HB2	1.97	0.46
1:A:1201:A:HO2'	1:A:1202:G:P	2.38	0.46
2:B:118:SER:HB2	2:B:119:PRO:CD	2.42	0.46
1:A:1098:C:O2'	1:A:1099:G:H5'	2.14	0.46
5:E:11:ARG:HD3	5:E:22:PHE:CG	2.50	0.46
4:D:7:VAL:HG11	4:D:20:LEU:HB2	1.97	0.46
1:A:456:C:H2'	1:A:457:C:C6	2.50	0.46
1:A:631:G:H2'	1:A:632:A:H8	1.79	0.46
1:A:73:G:O2'	1:A:76:C:H5'	2.16	0.46
1:A:1132:C:H2'	1:A:1133:G:C8	2.50	0.46
1:A:1479:C:H2'	1:A:1480:G:H8	1.77	0.46
3:C:90:LEU:CD2	3:C:98:VAL:HG22	2.44	0.46
1:A:254:G:OP1	17:Q:66:LYS:O	2.32	0.46
1:A:981:U:O5'	1:A:982:U:H4'	2.14	0.46
3:C:194:VAL:C	3:C:195:LEU:HD22	2.36	0.46
6:F:101:ALA:HB1	18:R:13:GLU:HG3	1.97	0.46
9:I:7:GLY:HA2	9:I:78:LEU:HB3	1.97	0.46
1:A:16:A:C2'	1:A:17:U:H5'	2.45	0.46
1:A:165:C:O2'	1:A:166:G:H5'	2.15	0.46
8:H:91:ARG:HG3	8:H:91:ARG:O	2.15	0.46
7:G:92:PRO:HG2	7:G:93:ARG:H	1.80	0.46
13:M:18:LEU:HD11	13:M:33:LEU:HD21	1.96	0.46
1:A:1003:G:N2	1:A:1004:A:O3'	2.48	0.46
9:I:120:ARG:NH1	9:I:120:ARG:HG3	2.31	0.46
3:C:158:GLY:HA2	3:C:192:TYR:CE2	2.51	0.46
3:C:205:GLU:O	3:C:206:VAL:O	2.34	0.46
15:O:86:ILE:O	15:O:87:ARG:HB2	2.16	0.46
17:Q:91:ARG:O	17:Q:94:TYR:HB2	2.16	0.46
5:E:70:GLY:CA	5:E:112:THR:HG22	2.44	0.46
1:A:1499:A:O2'	1:A:1500:A:H5'	2.15	0.46
5:E:78:VAL:HG11	5:E:133:GLU:HB3	1.96	0.46
1:A:1271:G:H2'	1:A:1272:G:C5'	2.22	0.46
10:J:72:ILE:O	10:J:72:ILE:HG13	2.16	0.46
1:A:403:C:H6	1:A:403:C:C5'	2.29	0.46
1:A:1286:A:H2'	1:A:1287:A:C5'	2.46	0.46
7:G:140:VAL:O	7:G:143:MET:HB3	2.15	0.46
1:A:548:G:H2'	1:A:549:C:C6	2.51	0.46
9:I:96:LYS:CB	9:I:97:PRO:HD3	2.34	0.46
1:A:645:C:H2'	1:A:646:U:C6	2.50	0.46
18:R:27:ARG:O	18:R:27:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ALA:CB	5:E:116:THR:HG21	2.45	0.46
10:J:44:ARG:NH1	10:J:44:ARG:CG	2.76	0.46
6:F:69:GLU:O	6:F:72:VAL:HG23	2.15	0.46
15:O:13:GLU:HG3	15:O:14:PHE:CD1	2.50	0.46
1:A:182:U:O4	1:A:223:U:H1'	2.15	0.46
11:K:96:LYS:HD3	11:K:96:LYS:HA	1.71	0.46
3:C:78:ARG:HE	3:C:81:GLU:HG2	1.80	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.46
1:A:1030(D):A:H2'	1:A:1031:G:O4'	2.15	0.46
2:B:49:PHE:HE2	2:B:212:ALA:HA	1.81	0.46
1:A:1279:A:H5'	1:A:1280:A:OP2	2.14	0.46
1:A:1364:U:O2'	1:A:1365:G:H5''	2.16	0.46
11:K:100:ASP:HB2	18:R:73:LYS:HE2	1.97	0.46
1:A:1346:A:C8	1:A:1348:U:C2	3.04	0.46
1:A:1086:U:C2'	1:A:1087:G:H5'	2.45	0.46
13:M:79:ARG:O	13:M:83:ILE:HG13	2.15	0.46
2:B:18:TRP:CG	2:B:19:ASN:N	2.83	0.46
1:A:1314:C:OP2	19:S:5:LYS:HD3	2.15	0.46
1:A:1435:G:H2'	1:A:1436:U:H6	1.75	0.46
7:G:145:GLU:C	7:G:147:ASN:H	2.16	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.80	0.46
1:A:485:G:O2'	1:A:486:U:P	2.73	0.46
5:E:79:GLU:HG2	5:E:84:LYS:HG3	1.98	0.46
1:A:669:U:H2'	1:A:670:G:C8	2.51	0.46
1:A:1030:C:H42	1:A:1031:G:H1	1.64	0.46
1:A:1178:G:OP2	9:I:96:LYS:NZ	2.48	0.46
1:A:1305:G:O2'	1:A:1331:G:N2	2.49	0.46
2:B:172:ARG:HH22	8:H:74:PRO:HB3	1.80	0.46
12:L:37:ARG:NH1	12:L:53:LYS:CE	2.78	0.46
9:I:9:ARG:HD3	9:I:104:ASP:HB3	1.97	0.46
3:C:118:ARG:NE	3:C:139:ARG:NH1	2.63	0.46
9:I:5:GLY:HA3	9:I:82:ARG:HB2	1.98	0.46
1:A:1378:C:C2'	1:A:1379:G:H5'	2.45	0.46
4:D:18:LEU:HD22	4:D:66:ILE:HG12	1.97	0.46
10:J:28:SER:HB3	10:J:78:LYS:HG3	1.97	0.46
2:B:213:VAL:HA	2:B:216:ILE:HD12	1.97	0.46
4:D:23:GLU:O	4:D:24:ARG:CB	2.64	0.46
7:G:74:VAL:HG21	7:G:85:GLN:CB	2.32	0.46
3:C:90:LEU:HD21	3:C:98:VAL:O	2.14	0.46
11:K:77:THR:HG23	11:K:77:THR:O	2.15	0.46
1:A:1343:G:H1'	9:I:120:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:ARG:NE	3:C:139:ARG:HH12	2.14	0.46
3:C:107:ASN:HD21	3:C:143:SER:CB	2.28	0.46
1:A:538:G:H2'	1:A:539:A:C8	2.50	0.46
13:M:96:PRO:HB3	13:M:100:GLN:OE1	2.16	0.46
1:A:304:U:H2'	1:A:305:G:C8	2.51	0.46
1:A:1315:U:H2'	1:A:1316:G:O4'	2.16	0.46
10:J:69:LEU:O	10:J:70:VAL:HB	2.16	0.46
1:A:1195:C:H3'	1:A:1196:U:H5''	1.91	0.46
1:A:1195:C:C3'	1:A:1196:U:C5'	2.84	0.46
3:C:31:LEU:HD22	3:C:58:ARG:HH11	1.79	0.46
2:B:136:LEU:O	2:B:140:GLN:HG3	2.15	0.46
2:B:189:ASP:O	8:H:74:PRO:HG3	2.15	0.46
3:C:194:VAL:HG12	3:C:195:LEU:N	2.31	0.46
15:O:87:ARG:NH1	15:O:87:ARG:CB	2.79	0.46
17:Q:103:LYS:HA	17:Q:103:LYS:NZ	2.28	0.46
2:B:13:HIS:CG	2:B:14:GLU:N	2.84	0.46
2:B:108:ARG:HD3	2:B:112:LEU:HG	1.97	0.46
1:A:639:G:O2'	1:A:640:A:H5'	2.16	0.46
15:O:4:LYS:O	15:O:8:GLN:HG2	2.16	0.46
3:C:106:GLN:H	3:C:106:GLN:CD	2.19	0.46
19:S:32:THR:CG2	19:S:33:TRP:N	2.79	0.46
1:A:412:A:H4'	1:A:413:G:H8	1.81	0.46
1:A:502:G:H2'	1:A:503:C:H6	1.81	0.46
13:M:4:ALA:O	13:M:5:GLY:C	2.54	0.46
1:A:1284:C:C3'	1:A:1285:A:H5''	2.39	0.46
3:C:119:VAL:O	3:C:123:ILE:HG12	2.15	0.46
6:F:26:ILE:O	6:F:30:LEU:HG	2.16	0.46
1:A:1151:A:O2'	1:A:1152:A:H8	1.98	0.46
1:A:22:G:H4'	1:A:885:G:C8	2.51	0.46
1:A:1307:U:H5'	13:M:100:GLN:HE22	1.81	0.46
4:D:56:ARG:HD3	4:D:204:GLU:CB	2.46	0.46
1:A:942:G:H2'	1:A:943:U:H6	1.81	0.46
1:A:1125:U:OP2	10:J:36:ILE:HD13	2.16	0.45
3:C:94:THR:C	3:C:96:LYS:H	2.19	0.45
1:A:1302:U:C5	13:M:16:VAL:HG21	2.51	0.45
14:N:2:ARG:O	14:N:3:LYS:C	2.53	0.45
13:M:81:MET:CE	13:M:91:HIS:HB3	2.47	0.45
1:A:1091:U:O2	1:A:1093:A:C8	2.69	0.45
18:R:13:GLU:OE1	18:R:13:GLU:N	2.49	0.45
16:P:67:THR:CG2	16:P:68:ASP:N	2.78	0.45
3:C:138:GLN:CA	3:C:138:GLN:HE21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:155:TRP:CD1	7:G:155:TRP:OXT	2.69	0.45
1:A:883:C:C2'	1:A:884:U:H5'	2.46	0.45
6:F:43:LEU:N	6:F:43:LEU:CD2	2.80	0.45
1:A:1214:C:O2'	1:A:1215:G:OP2	2.32	0.45
1:A:488:C:O2'	1:A:489:C:H5'	2.16	0.45
1:A:1283:G:O2'	1:A:1284:C:H5'	2.16	0.45
4:D:64:ARG:CD	4:D:69:ILE:O	2.61	0.45
5:E:27:LEU:HD22	5:E:39:LEU:HD22	1.98	0.45
6:F:43:LEU:H	6:F:43:LEU:HD22	1.82	0.45
10:J:14:LEU:HD23	10:J:92:VAL:HG22	1.99	0.45
1:A:1329:A:OP2	13:M:27:ALA:HB3	2.16	0.45
12:L:107:LYS:O	12:L:108:ASP:HB2	2.16	0.45
20:T:4:SER:C	20:T:6:LEU:H	2.19	0.45
1:A:783:C:O2'	1:A:784:C:H5'	2.15	0.45
1:A:1272:G:H2'	1:A:1273:G:C5'	2.45	0.45
14:N:28:ARG:HB3	14:N:39:CYS:HB3	1.98	0.45
18:R:22:VAL:O	18:R:26:LYS:HG2	2.16	0.45
11:K:70:VAL:HG23	11:K:93:LEU:HB3	1.97	0.45
2:B:21:LYS:HD2	2:B:187:ASP:OD1	2.16	0.45
5:E:31:GLY:HA3	5:E:108:LEU:HB3	1.97	0.45
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.50	0.45
7:G:119:ILE:O	7:G:123:LEU:HB2	2.16	0.45
7:G:61:PHE:HA	7:G:123:LEU:HD21	1.97	0.45
1:A:995:C:C2'	1:A:996:A:H5''	2.46	0.45
1:A:176:C:O2'	1:A:177:C:H5'	2.15	0.45
1:A:1112:C:N3	3:C:177:LEU:N	2.58	0.45
3:C:4:ILE:O	3:C:4:ILE:HD13	2.15	0.45
2:B:211:ARG:HA	2:B:214:ASP:OD2	2.16	0.45
2:B:224:VAL:HG12	2:B:225:GLU:N	2.31	0.45
4:D:149:GLU:CG	4:D:152:ARG:HH22	2.20	0.45
1:A:1343:G:H1'	9:I:120:ARG:HH12	1.80	0.45
11:K:19:ILE:HD13	11:K:19:ILE:O	2.16	0.45
4:D:198:ASN:C	4:D:198:ASN:ND2	2.69	0.45
1:A:1407:C:O2'	1:A:1408:A:H5'	2.17	0.45
3:C:100:LEU:CD2	3:C:100:LEU:O	2.64	0.45
20:T:60:ALA:O	20:T:66:HIS:ND1	2.49	0.45
1:A:279:A:H5'	1:A:281:G:O4'	2.17	0.45
2:B:45:LEU:CD2	2:B:49:PHE:HE1	2.29	0.45
3:C:35:ASP:O	3:C:38:ILE:HB	2.16	0.45
9:I:63:THR:HG22	9:I:64:VAL:N	2.32	0.45
12:L:23:LEU:C	12:L:25:GLY:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:PRO:HA	2:B:148:LEU:HD12	1.98	0.45
1:A:1229:A:H2'	1:A:1230:C:C6	2.52	0.45
1:A:738:C:H5''	6:F:69:GLU:HB3	1.99	0.45
7:G:144:ALA:O	7:G:146:ALA:N	2.46	0.45
15:O:6:GLU:OE2	15:O:37:ARG:NH2	2.49	0.45
7:G:76:SER:O	7:G:155:TRP:HZ3	1.98	0.45
8:H:6:ILE:O	8:H:10:LEU:HG	2.16	0.45
1:A:813:U:H2'	1:A:814:A:C5'	2.47	0.45
1:A:359:U:O2'	1:A:360:A:H5'	2.16	0.45
3:C:115:VAL:HG21	3:C:201:ILE:HD11	1.97	0.45
13:M:95:LEU:O	13:M:109:ARG:NH1	2.49	0.45
3:C:82:ARG:C	3:C:84:ARG:N	2.69	0.45
18:R:20:ARG:O	18:R:22:VAL:HG13	2.16	0.45
1:A:1311:G:O6	19:S:1:PRO:HB3	2.16	0.45
5:E:47:VAL:HB	5:E:48:PRO:CD	2.40	0.45
18:R:25:LEU:HB3	18:R:64:LEU:HD11	1.97	0.45
4:D:4:ILE:HA	4:D:114:ARG:NH2	2.30	0.45
19:S:14:LEU:HA	19:S:17:LYS:HB3	1.99	0.45
7:G:71:ARG:HH12	7:G:137:LYS:HZ1	1.63	0.45
1:A:791:G:C6	1:A:792:A:N7	2.84	0.45
1:A:26:A:H2'	1:A:27:G:H5'	1.98	0.45
3:C:10:ARG:HG3	3:C:177:LEU:HD12	1.98	0.45
1:A:1194:U:H4'	5:E:18:GLY:HA2	1.98	0.45
3:C:25:LYS:HD2	10:J:43:ARG:NH2	2.31	0.45
3:C:75:VAL:O	3:C:82:ARG:HB3	2.17	0.45
1:A:1365:G:O2'	1:A:1366:C:H5'	2.17	0.45
18:R:18:ASP:OD2	18:R:21:ASN:HB2	2.17	0.45
1:A:1086:U:O2'	1:A:1087:G:H5'	2.17	0.45
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.85	0.45
9:I:10:LYS:O	9:I:11:GLU:CB	2.64	0.45
7:G:119:ILE:N	7:G:119:ILE:HD12	2.32	0.45
1:A:686:U:O4	1:A:703:G:H1'	2.16	0.45
1:A:243:A:H4'	1:A:244:U:H5''	1.98	0.45
1:A:1513:A:H2'	1:A:1514:C:C6	2.52	0.45
11:K:4:VAL:O	11:K:5:ALA:HB3	2.17	0.45
3:C:34:GLU:OE2	3:C:58:ARG:NH2	2.50	0.45
14:N:23:CYS:SG	14:N:42:CYS:SG	3.15	0.45
1:A:953:G:H1'	13:M:124:ARG:CA	2.42	0.45
5:E:144:VAL:HG21	8:H:107:LEU:HB3	1.99	0.45
7:G:25:PHE:CE2	7:G:29:ILE:HD11	2.51	0.45
1:A:1237:C:C4'	1:A:1334:G:N2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:A:O2'	1:A:432:A:H5'	2.17	0.45
13:M:78:LYS:HG2	13:M:82:ASP:OD2	2.16	0.45
9:I:27:VAL:O	9:I:28:ASN:HB2	2.17	0.45
1:A:858:G:O6	1:A:869:G:H3'	2.17	0.45
1:A:1427:U:O2'	1:A:1428:A:H5'	2.17	0.45
11:K:89:GLN:HG2	11:K:95:VAL:CG2	2.34	0.45
5:E:74:HIS:CE1	5:E:76:ILE:CG2	3.00	0.45
3:C:46:LEU:HD12	3:C:46:LEU:N	2.31	0.45
2:B:17:ARG:HB2	2:B:17:ARG:NH1	2.32	0.45
6:F:97:PHE:CB	18:R:17:ARG:HH21	2.28	0.45
12:L:37:ARG:CG	12:L:38:THR:H	2.28	0.45
19:S:18:VAL:CG1	19:S:19:LEU:N	2.79	0.45
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.45
1:A:337:C:H2'	1:A:338:A:C8	2.52	0.45
8:H:11:THR:HG23	8:H:14:ARG:NH1	2.32	0.45
14:N:35:PHE:C	14:N:35:PHE:CD1	2.90	0.45
10:J:81:GLU:C	10:J:83:LEU:H	2.21	0.45
1:A:424:G:O2'	1:A:425:G:H5'	2.16	0.45
1:A:998:G:C2'	1:A:999:C:H5''	2.47	0.45
2:B:138:ARG:C	2:B:140:GLN:N	2.69	0.45
2:B:64:PHE:O	2:B:86:TYR:HA	2.17	0.45
1:A:1074:G:O3'	2:B:97:THR:CG2	2.65	0.45
1:A:953:G:C1'	13:M:124:ARG:HA	2.42	0.45
19:S:73:PHE:N	19:S:73:PHE:CD1	2.85	0.45
18:R:58:ALA:HB3	18:R:64:LEU:HD12	1.99	0.45
4:D:69:ILE:HD11	4:D:99:ARG:NE	2.32	0.45
13:M:116:VAL:CG1	13:M:117:ALA:N	2.80	0.45
4:D:150:LYS:CD	4:D:150:LYS:N	2.80	0.45
2:B:128:GLU:C	2:B:130:VAL:H	2.19	0.45
13:M:36:THR:HG23	13:M:54:ARG:HB3	1.98	0.45
1:A:325:A:OP1	20:T:63:SER:CB	2.65	0.45
1:A:1132:C:H2'	1:A:1133:G:H8	1.82	0.45
7:G:8:VAL:HG13	7:G:93:ARG:NH1	2.31	0.45
1:A:339:C:H2'	1:A:340:U:C6	2.52	0.45
5:E:106:LEU:HD13	5:E:114:ILE:HG21	1.97	0.45
2:B:152:LEU:HB3	2:B:176:ILE:HD11	1.99	0.45
10:J:28:SER:HB3	10:J:82:GLN:NE2	2.32	0.44
10:J:81:GLU:C	10:J:83:LEU:N	2.70	0.44
1:A:189(B):C:N3	1:A:189(J):G:C2	2.85	0.44
1:A:474:G:C8	1:A:474:G:H5'	2.43	0.44
1:A:952:U:O2'	1:A:953:G:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:VAL:HG12	12:L:37:ARG:H	1.83	0.44
1:A:407:G:H2'	1:A:408:A:H8	1.82	0.44
12:L:115:LYS:O	12:L:116:TYR:CB	2.64	0.44
10:J:40:THR:HG22	10:J:41:ARG:N	2.31	0.44
9:I:107:VAL:HG12	9:I:108:VAL:N	2.32	0.44
1:A:1417:G:H2'	1:A:1482:G:H22	1.82	0.44
1:A:720:C:H3'	1:A:721:G:C5'	2.46	0.44
5:E:26:ALA:O	5:E:41:PHE:HA	2.17	0.44
1:A:1303:C:H2'	1:A:1304:G:H5'	1.98	0.44
1:A:1459:C:O2'	1:A:1460:A:H5'	2.16	0.44
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.53	0.44
2:B:10:HIS:HE1	2:B:207:LEU:HB3	1.82	0.44
3:C:63:VAL:HG12	3:C:65:VAL:HG23	2.00	0.44
2:B:138:ARG:C	2:B:140:GLN:H	2.19	0.44
1:A:319:G:C3'	1:A:320:C:C5'	2.95	0.44
1:A:965:A:C2	1:A:969:A:C2	3.05	0.44
7:G:45:ALA:O	7:G:49:ILE:HG13	2.16	0.44
4:D:63:LEU:HD11	4:D:96:LEU:CD1	2.47	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:629:G:H5''	1:A:629:G:H8	1.82	0.44
11:K:48:PRO:O	11:K:51:ALA:HB3	2.17	0.44
10:J:21:ILE:HA	10:J:83:LEU:HD22	1.99	0.44
2:B:49:PHE:HD2	2:B:215:LEU:HG	1.81	0.44
4:D:29:LYS:O	4:D:31:ALA:N	2.51	0.44
9:I:64:VAL:HG21	9:I:72:GLN:HB3	1.99	0.44
14:N:25:ARG:HD3	14:N:42:CYS:HB3	1.99	0.44
19:S:5:LYS:HB3	19:S:6:LYS:H	1.56	0.44
1:A:1206:G:C6	1:A:1207:G:C5	3.06	0.44
12:L:120:LYS:HD2	12:L:121:PRO:HD2	1.99	0.44
1:A:417:C:H2'	1:A:418:C:C6	2.52	0.44
13:M:66:GLU:HB3	13:M:67:GLY:H	1.54	0.44
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.44
1:A:403:C:C6	1:A:403:C:H5'	2.50	0.44
1:A:1191:A:OP1	3:C:2:ASN:ND2	2.51	0.44
19:S:40:VAL:HB	19:S:41:PRO:HD2	1.98	0.44
3:C:153:SER:HB3	3:C:196:GLY:H	1.82	0.44
5:E:11:ARG:HD3	5:E:22:PHE:CB	2.48	0.44
3:C:144:GLY:O	3:C:145:ALA:HB3	2.16	0.44
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.44
1:A:247:G:OP1	17:Q:98:SER:HB2	2.18	0.44
11:K:2:ARG:HG2	11:K:2:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:36:ASN:HA	7:G:36:ASN:HD22	1.69	0.44
4:D:23:GLU:C	4:D:25:CYS:N	2.69	0.44
1:A:944:G:O5'	1:A:944:G:O2'	2.27	0.44
11:K:89:GLN:CG	11:K:95:VAL:HG21	2.36	0.44
1:A:579:G:H5'	1:A:728:A:C1'	2.40	0.44
3:C:37:ARG:HG3	3:C:37:ARG:NH1	2.30	0.44
1:A:1310:G:O6	19:S:1:PRO:HG3	2.18	0.44
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.99	0.44
1:A:1169:A:H2'	1:A:1170:A:H8	1.79	0.44
3:C:166:TRP:O	3:C:167:ALA:CB	2.65	0.44
1:A:16:A:O2'	1:A:17:U:H5'	2.17	0.44
2:B:183:ASP:HB2	2:B:199:ASP:OD1	2.16	0.44
2:B:125:PRO:C	2:B:127:LYS:H	2.20	0.44
9:I:35:TYR:HD2	9:I:36:PHE:CE1	2.35	0.44
21:V:9:ARG:HH11	21:V:22:ARG:HA	1.83	0.44
1:A:781:A:C5	1:A:802:A:C2	3.05	0.44
1:A:1121:U:C4	1:A:1122:U:C4	3.06	0.44
1:A:184:G:O2'	1:A:185:A:H5'	2.17	0.44
1:A:389:A:H2'	1:A:389:A:N3	2.33	0.44
2:B:16:LYS:HG3	2:B:32:GLY:O	2.17	0.44
2:B:17:ARG:O	2:B:18:TRP:O	2.36	0.44
3:C:190:THR:CG2	3:C:191:THR:N	2.79	0.44
4:D:7:VAL:CG2	4:D:114:ARG:NH1	2.78	0.44
19:S:27:LYS:CG	19:S:28:ARG:N	2.80	0.44
3:C:138:GLN:CA	3:C:138:GLN:NE2	2.77	0.44
4:D:161:LEU:HD13	4:D:180:MET:SD	2.57	0.44
18:R:40:ARG:HH11	18:R:40:ARG:HA	1.82	0.44
2:B:126:LYS:C	2:B:128:GLU:N	2.71	0.44
1:A:1263:C:H2'	1:A:1264:C:H6	1.82	0.44
8:H:114:THR:HG21	8:H:129:VAL:HG23	1.99	0.44
3:C:86:LEU:HA	3:C:89:GLU:HB2	1.99	0.44
14:N:30:ARG:O	14:N:31:SER:HB2	2.17	0.44
9:I:31:ASP:HB3	9:I:34:GLU:HB2	1.99	0.44
1:A:1126:U:H2'	1:A:1126:U:O2	2.17	0.44
4:D:35:ARG:N	4:D:36:PRO:CD	2.70	0.44
1:A:1196:U:H4'	1:A:1197:G:O5'	2.18	0.44
3:C:35:ASP:HB3	3:C:39:ARG:NH1	2.32	0.44
2:B:15:ARG:HB2	2:B:16:LYS:H	1.68	0.44
1:A:1313:U:OP2	19:S:5:LYS:HA	2.17	0.44
7:G:51:GLU:O	7:G:53:THR:N	2.51	0.44
5:E:140:THR:HG22	5:E:142:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:A:H2'	1:A:540:G:H8	1.81	0.44
1:A:106:C:HO2'	1:A:107:G:H5'	1.82	0.44
1:A:335:C:H2'	1:A:336:C:H6	1.82	0.44
1:A:895:G:H2'	1:A:896:C:C6	2.53	0.44
8:H:18:ARG:NH2	8:H:81:HIS:O	2.50	0.44
13:M:15:ASP:OD1	13:M:15:ASP:N	2.51	0.44
4:D:31:ALA:C	4:D:33:GLU:N	2.70	0.44
1:A:1054:C:C5'	1:A:1054:C:H6	2.29	0.44
4:D:61:GLN:HE22	4:D:64:ARG:NH1	2.13	0.44
4:D:157:ILE:HG23	4:D:161:LEU:HD12	2.00	0.44
8:H:68:ARG:NH1	8:H:68:ARG:HG2	2.32	0.44
1:A:1485:U:O2'	1:A:1486:G:H5'	2.18	0.44
15:O:60:GLY:O	15:O:63:ARG:HG2	2.17	0.44
1:A:1158:C:C5	1:A:1160:G:H1'	2.53	0.44
6:F:48:LEU:HD13	6:F:52:ILE:HG13	2.00	0.44
1:A:1060:C:H2'	1:A:1061:G:C8	2.53	0.44
1:A:836:G:C6	1:A:851:G:C6	3.06	0.44
5:E:86:VAL:HB	5:E:117:LYS:HB3	2.00	0.44
1:A:1424:C:C2'	1:A:1425:U:H5'	2.48	0.44
9:I:16:VAL:HG11	9:I:80:ILE:HA	2.00	0.44
1:A:1182:G:C4'	1:A:1183:A:H5'	2.48	0.44
1:A:1309:G:C5	1:A:1329:A:C2	3.06	0.44
1:A:106:C:O2	1:A:379:C:H4'	2.17	0.44
1:A:22:G:H2'	1:A:23:C:C6	2.53	0.44
1:A:76:C:O2'	1:A:77:G:H5'	2.18	0.44
1:A:335:C:H2'	1:A:336:C:C6	2.53	0.44
16:P:75:ARG:O	16:P:78:GLY:N	2.48	0.44
4:D:190:ARG:HD2	4:D:190:ARG:O	2.18	0.44
2:B:11:PHE:HD1	2:B:35:ILE:HG23	1.83	0.43
1:A:733:A:H4'	1:A:734:G:OP2	2.18	0.43
3:C:138:GLN:HA	3:C:138:GLN:HE21	1.79	0.43
1:A:882:C:O2'	1:A:883:C:H5'	2.18	0.43
1:A:392:G:H2'	1:A:393:A:H8	1.83	0.43
7:G:115:ALA:HA	7:G:118:ARG:CZ	2.48	0.43
2:B:13:HIS:CD2	2:B:183:ASP:OD2	2.71	0.43
20:T:60:ALA:O	20:T:66:HIS:CE1	2.71	0.43
16:P:51:VAL:O	16:P:53:VAL:N	2.51	0.43
10:J:21:ILE:O	10:J:21:ILE:CG2	2.66	0.43
1:A:1190:G:P	3:C:4:ILE:HD12	2.58	0.43
2:B:4:LEU:HD12	2:B:4:LEU:N	2.33	0.43
11:K:38:ILE:HD11	11:K:54:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:HD22	3:C:67:VAL:HG21	2.00	0.43
12:L:23:LEU:C	12:L:25:GLY:H	2.21	0.43
7:G:22:VAL:HG13	7:G:42:PHE:CE2	2.53	0.43
1:A:1221:G:O3'	19:S:76:THR:HG21	2.18	0.43
5:E:11:ARG:CD	5:E:22:PHE:CD1	2.99	0.43
1:A:29:G:C5'	1:A:29:G:H8	2.25	0.43
1:A:1353:G:H2'	1:A:1354:C:C6	2.53	0.43
20:T:3:LEU:O	20:T:5:ALA:N	2.51	0.43
1:A:533:A:O2'	1:A:534:U:P	2.76	0.43
6:F:55:ASP:CB	6:F:86:ARG:HH12	2.31	0.43
2:B:76:ARG:HB3	2:B:88:ASN:HD22	1.82	0.43
20:T:65:LEU:HD21	20:T:73:ARG:CZ	2.48	0.43
7:G:121:HIS:HD2	7:G:124:MET:CE	2.31	0.43
2:B:1:VAL:O	2:B:2:LYS:HB3	2.18	0.43
2:B:9:VAL:HG11	2:B:203:ARG:HB3	2.01	0.43
1:A:1054:C:OP2	1:A:1197:G:OP1	2.35	0.43
1:A:1198:G:C8	1:A:1198:G:H5'	2.48	0.43
3:C:74:VAL:O	3:C:82:ARG:HD3	2.18	0.43
11:K:81:ARG:CZ	18:R:73:LYS:HZ2	2.31	0.43
2:B:16:LYS:C	2:B:17:ARG:HG3	2.39	0.43
1:A:1342:C:O2'	1:A:1343:G:H5'	2.18	0.43
19:S:54:LYS:HG2	19:S:55:GLN:NE2	2.29	0.43
5:E:89:PRO:HG2	8:H:105:ARG:CZ	2.48	0.43
7:G:145:GLU:HA	7:G:148:ARG:HB2	1.99	0.43
15:O:32:THR:HG23	15:O:62:ARG:HH12	1.83	0.43
15:O:62:ARG:NH1	15:O:86:ILE:HD12	2.33	0.43
13:M:57:GLU:OE1	13:M:57:GLU:HA	2.18	0.43
15:O:9:LYS:HZ1	15:O:13:GLU:HB2	1.83	0.43
19:S:79:TYR:CZ	19:S:80:ARG:HG2	2.52	0.43
1:A:334:C:H2'	1:A:335:C:C6	2.53	0.43
1:A:933:G:OP1	7:G:2:ARG:HB3	2.19	0.43
9:I:54:ALA:O	9:I:56:GLY:N	2.51	0.43
1:A:1124:G:H3'	1:A:1145:C:H41	1.84	0.43
19:S:40:VAL:N	19:S:43:MET:HE3	2.07	0.43
3:C:46:LEU:CD1	3:C:46:LEU:H	2.31	0.43
20:T:93:ILE:C	20:T:95:GLY:H	2.22	0.43
1:A:1305:G:H5''	21:V:4:GLY:C	2.38	0.43
4:D:7:VAL:HG11	4:D:20:LEU:CB	2.48	0.43
1:A:376:G:P	16:P:67:THR:HG21	2.58	0.43
14:N:8:LYS:HD3	14:N:8:LYS:O	2.19	0.43
7:G:119:ILE:HG22	7:G:123:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:H8	1.84	0.43
3:C:89:GLU:HA	3:C:89:GLU:OE1	2.19	0.43
1:A:722:A:O3'	1:A:723:U:C6	2.72	0.43
2:B:37:ASP:OD1	2:B:39:GLN:HB2	2.19	0.43
2:B:47:ARG:NH1	2:B:47:ARG:HG2	2.33	0.43
10:J:28:SER:O	10:J:76:ASN:CB	2.67	0.43
1:A:1130:A:C5'	1:A:1131:G:H5'	2.48	0.43
1:A:1397:C:C5	22:W:5:A:N7	2.87	0.43
1:A:522:C:N4	12:L:49:ARG:HH22	2.06	0.43
13:M:123:PRO:C	13:M:125:LYS:N	2.72	0.43
15:O:69:LEU:HD23	15:O:69:LEU:HA	1.88	0.43
15:O:81:ILE:O	15:O:82:GLU:C	2.56	0.43
19:S:79:TYR:CE2	19:S:80:ARG:HG2	2.54	0.43
1:A:831:U:H2'	1:A:832:C:H6	1.82	0.43
11:K:56:LEU:HB3	11:K:60:LYS:HE3	2.00	0.43
15:O:31:LEU:O	15:O:35:ILE:HG13	2.18	0.43
1:A:972:C:H4'	10:J:55:LYS:CG	2.40	0.43
1:A:983:A:H5'	14:N:2:ARG:HH12	1.84	0.43
1:A:1017:G:H2'	1:A:1018:C:C6	2.53	0.43
5:E:20:ARG:HG2	5:E:20:ARG:NH1	2.32	0.43
10:J:63:LEU:HG	14:N:55:VAL:HG22	2.00	0.43
5:E:8:LEU:HD13	5:E:8:LEU:O	2.18	0.43
7:G:58:LEU:O	7:G:62:LYS:HG2	2.19	0.43
1:A:938:A:C6	1:A:939:G:C5	3.07	0.43
1:A:518:C:H2'	1:A:530:G:N3	2.33	0.43
1:A:1314:C:OP2	19:S:5:LYS:HG2	2.18	0.43
3:C:187:LEU:HA	3:C:187:LEU:HD22	1.73	0.43
19:S:22:ASN:HA	19:S:25:GLY:O	2.19	0.43
1:A:1320:C:N4	19:S:35:ARG:HB2	2.34	0.43
10:J:88:LEU:H	10:J:89:PRO:CD	2.31	0.43
4:D:120:VAL:O	4:D:133:ASP:HA	2.19	0.43
1:A:430:A:C2'	1:A:431:A:H5'	2.49	0.43
5:E:51:VAL:O	5:E:54:ALA:HB3	2.19	0.43
4:D:125:ILE:HG22	4:D:126:THR:N	2.34	0.43
1:A:1020:U:O2'	1:A:1021:G:H5'	2.19	0.43
1:A:1061:G:C6	1:A:1062:U:N3	2.87	0.43
1:A:1130:A:H5'	1:A:1131:G:P	2.59	0.43
3:C:69:VAL:HG12	3:C:71:LYS:N	2.29	0.43
11:K:70:VAL:HG22	11:K:93:LEU:HD22	2.00	0.43
1:A:1223:C:OP1	19:S:77:ARG:NH1	2.52	0.43
3:C:129:VAL:HG13	3:C:133:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:U:O2'	4:D:122:HIS:CD2	2.71	0.43
2:B:200:ASP:O	2:B:201:ALA:CB	2.66	0.43
23:Z:34:G:H2'	23:Z:35:A:C8	2.54	0.43
9:I:85:VAL:HG13	9:I:89:PRO:HA	2.00	0.43
1:A:1226:C:N4	13:M:103:ARG:HG3	2.34	0.43
21:V:24:ARG:O	21:V:26:LYS:N	2.51	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.53	0.43
10:J:38:LEU:HD11	10:J:69:LEU:HD23	2.00	0.43
2:B:11:PHE:O	2:B:12:GLY:O	2.37	0.43
2:B:45:LEU:HD22	2:B:49:PHE:CE1	2.52	0.43
9:I:115:LYS:O	9:I:117:LYS:N	2.52	0.43
14:N:56:ARG:HG2	14:N:57:LYS:N	2.31	0.43
9:I:126:LYS:CB	13:M:125:LYS:NZ	2.81	0.43
1:A:841:U:H6	1:A:848:C:O4'	2.02	0.43
7:G:76:SER:O	7:G:155:TRP:CZ3	2.72	0.43
17:Q:75:LEU:HD21	17:Q:78:SER:HB2	2.01	0.43
6:F:43:LEU:H	6:F:43:LEU:CD2	2.32	0.43
1:A:942:G:H2'	1:A:943:U:C6	2.53	0.43
10:J:19:GLN:HA	10:J:22:VAL:CG1	2.48	0.43
1:A:1427:U:H2'	1:A:1428:A:C8	2.54	0.43
1:A:188:C:C3'	1:A:189:G:C5'	2.93	0.43
17:Q:68:LYS:C	17:Q:69:ARG:HD2	2.39	0.43
15:O:25:GLU:CG	15:O:80:LEU:HG	2.39	0.43
9:I:42:ALA:O	9:I:43:VAL:C	2.56	0.43
4:D:64:ARG:HG2	4:D:74:PHE:CG	2.54	0.43
16:P:67:THR:HG22	16:P:68:ASP:N	2.34	0.43
1:A:824:C:H2'	1:A:825:G:C8	2.53	0.43
5:E:78:VAL:HG21	5:E:134:ALA:HA	2.01	0.43
1:A:562:C:H3'	12:L:11:ARG:HB3	2.01	0.43
3:C:54:VAL:O	3:C:54:VAL:HG12	2.19	0.43
1:A:1125:U:H3	10:J:3:ARG:NH2	2.14	0.42
1:A:834:C:H2'	1:A:835:U:C6	2.54	0.42
1:A:1228:C:H2'	1:A:1229:A:C8	2.50	0.42
3:C:190:THR:HG22	3:C:191:THR:H	1.84	0.42
1:A:1292:U:H5'	9:I:37:GLN:HE22	1.84	0.42
1:A:625:G:H2'	1:A:626:U:H6	1.81	0.42
4:D:155:GLU:HG2	4:D:159:GLN:NE2	2.33	0.42
11:K:69:SER:OG	11:K:96:LYS:HG2	2.19	0.42
2:B:31:ASN:N	2:B:31:ASN:ND2	2.67	0.42
5:E:103:ARG:HG3	5:E:104:ALA:N	2.34	0.42
2:B:12:GLY:HA3	2:B:35:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:62:THR:CG2	19:S:63:GLU:N	2.77	0.42
1:A:189(B):C:C4'	1:A:189(C):C:OP1	2.66	0.42
19:S:52:ASN:ND2	19:S:55:GLN:HB2	2.27	0.42
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.54	0.42
4:D:145:ILE:N	4:D:145:ILE:CD1	2.79	0.42
7:G:154:ARG:HA	7:G:154:ARG:HD3	1.90	0.42
9:I:6:THR:H	9:I:79:GLY:HA2	1.84	0.42
15:O:81:ILE:HG22	15:O:82:GLU:N	2.33	0.42
1:A:366:C:C2'	1:A:366:C:O2	2.67	0.42
16:P:26:ARG:HD3	16:P:31:LYS:H	1.82	0.42
15:O:44:VAL:O	15:O:45:HIS:HB2	2.19	0.42
22:W:4:A:C2	23:Z:34:G:C6	3.07	0.42
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.42
1:A:357:G:OP1	1:A:367:U:H5''	2.19	0.42
7:G:64:ALA:O	7:G:68:VAL:HG23	2.19	0.42
1:A:1357:A:N7	1:A:1358:U:C5	2.87	0.42
2:B:11:PHE:C	2:B:11:PHE:CD1	2.92	0.42
1:A:411:A:C5	1:A:429:U:C5	3.06	0.42
1:A:1281:U:H3'	1:A:1282:C:C6	2.54	0.42
3:C:64:ALA:O	3:C:65:VAL:CB	2.67	0.42
1:A:1302:U:H5	13:M:16:VAL:HG21	1.84	0.42
2:B:19:ASN:ND2	2:B:19:ASN:C	2.71	0.42
4:D:3:TYR:O	4:D:4:ILE:HB	2.18	0.42
7:G:144:ALA:C	7:G:146:ALA:H	2.22	0.42
3:C:22:TYR:OH	10:J:7:ARG:HD3	2.18	0.42
3:C:22:TYR:CG	3:C:23:ALA:N	2.86	0.42
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.99	0.42
4:D:75:ARG:HG3	4:D:75:ARG:NH1	2.33	0.42
2:B:128:GLU:O	2:B:132:LEU:HG	2.20	0.42
1:A:1275:A:H2'	1:A:1276:G:O4'	2.18	0.42
19:S:30:ILE:HG22	19:S:31:LYS:H	1.84	0.42
2:B:76:ARG:HB3	2:B:88:ASN:ND2	2.34	0.42
8:H:114:THR:HG22	8:H:130:GLY:O	2.18	0.42
20:T:82:ARG:HB2	20:T:97:LEU:HD13	2.00	0.42
1:A:453:A:H4'	16:P:72:ARG:HG3	2.01	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
1:A:1009:G:H2'	1:A:1010:G:H8	1.84	0.42
2:B:57:MET:CE	2:B:57:MET:O	2.68	0.42
2:B:82:ALA:CB	2:B:84:MET:HG2	2.48	0.42
1:A:1178:G:H2'	1:A:1179:A:H5''	2.01	0.42
9:I:92:ARG:C	9:I:94:LYS:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:C:H5''	19:S:5:LYS:HD3	2.02	0.42
1:A:1250:A:H2'	1:A:1251:A:C8	2.55	0.42
19:S:14:LEU:O	19:S:18:VAL:N	2.53	0.42
3:C:176:THR:O	3:C:176:THR:CG2	2.68	0.42
10:J:10:ASP:OD1	10:J:12:LYS:N	2.45	0.42
18:R:19:TYR:CA	18:R:54:THR:HG23	2.49	0.42
1:A:1456:G:H2'	1:A:1457:G:O4'	2.20	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.18	0.42
1:A:1149:C:OP2	9:I:8:ARG:NH1	2.48	0.42
1:A:485:G:H2'	1:A:486:U:OP2	2.20	0.42
1:A:795:C:H5''	1:A:796:C:OP2	2.20	0.42
1:A:892:A:H2'	1:A:893:C:C6	2.55	0.42
1:A:370:C:O2'	1:A:371:G:H5'	2.20	0.42
1:A:644:G:O2'	1:A:645:C:H5'	2.19	0.42
13:M:39:ASN:C	13:M:39:ASN:HD22	2.22	0.42
6:F:75:LEU:O	6:F:78:GLU:HB3	2.19	0.42
12:L:51:VAL:CG1	12:L:52:ALA:N	2.83	0.42
12:L:71:HIS:HD2	12:L:73:LEU:N	2.08	0.42
1:A:1057:G:H2'	1:A:1058:G:O4'	2.18	0.42
7:G:135:LYS:O	7:G:138:GLU:N	2.52	0.42
1:A:653:A:C8	8:H:56:LYS:HG2	2.54	0.42
3:C:100:LEU:HD23	3:C:100:LEU:O	2.19	0.42
1:A:93:G:H2'	1:A:96:U:C6	2.54	0.42
10:J:46:THR:OG1	10:J:60:HIS:CD2	2.71	0.42
18:R:46:LYS:O	18:R:50:ILE:HG13	2.19	0.42
2:B:12:GLY:H	2:B:36:ILE:H	1.65	0.42
9:I:112:LYS:H	9:I:118:ALA:HA	1.84	0.42
18:R:23:GLU:O	18:R:26:LYS:HE2	2.20	0.42
2:B:99:PHE:O	2:B:103:SER:HB3	2.19	0.42
3:C:154:GLY:O	3:C:195:LEU:HD13	2.20	0.42
1:A:1162:C:H2'	1:A:1163:C:C6	2.53	0.42
4:D:63:LEU:O	4:D:63:LEU:HD13	2.20	0.42
9:I:10:LYS:O	9:I:11:GLU:HB3	2.19	0.42
19:S:15:LEU:HA	19:S:18:VAL:HG12	2.00	0.42
19:S:28:ARG:HD2	19:S:28:ARG:N	2.35	0.42
10:J:63:LEU:HD21	14:N:53:PRO:O	2.19	0.42
1:A:697:U:C2'	1:A:698:G:H5'	2.49	0.42
7:G:62:LYS:O	7:G:63:GLN:C	2.58	0.42
2:B:160:ASP:HB3	2:B:163:LYS:HB2	2.02	0.42
19:S:30:ILE:HG22	19:S:31:LYS:N	2.33	0.42
9:I:8:ARG:HA	9:I:12:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:G:H2'	1:A:634:C:C6	2.54	0.42
4:D:87:VAL:O	4:D:91:VAL:HG23	2.19	0.42
1:A:663:A:O2'	1:A:664:G:H5'	2.20	0.42
1:A:530:G:HO2'	1:A:531:U:P	2.42	0.42
5:E:98:ALA:HB1	5:E:116:THR:HG21	2.01	0.42
1:A:734:G:H3'	1:A:735:C:C6	2.54	0.42
8:H:104:ARG:O	8:H:107:LEU:N	2.49	0.42
8:H:82:HIS:HB3	8:H:138:TRP:CD2	2.55	0.42
1:A:1251:A:H4'	9:I:11:GLU:OE2	2.20	0.42
14:N:8:LYS:HD3	14:N:8:LYS:C	2.40	0.42
2:B:110:GLU:HA	2:B:147:ARG:NH2	2.35	0.42
1:A:1238:A:C8	1:A:1303:C:H1'	2.55	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.42
4:D:168:LYS:HG3	4:D:169:VAL:N	2.34	0.42
6:F:47:ARG:N	6:F:47:ARG:HD3	2.35	0.42
8:H:30:ARG:NH1	8:H:30:ARG:HG2	2.34	0.42
3:C:35:ASP:HB3	3:C:39:ARG:HH12	1.84	0.42
3:C:13:ILE:CG2	3:C:14:THR:H	2.11	0.42
14:N:26:CYS:SG	14:N:28:ARG:CB	3.08	0.42
17:Q:65:SER:O	17:Q:69:ARG:NH1	2.52	0.42
1:A:1346:A:H61	1:A:1374:A:C5'	2.20	0.42
1:A:983:A:H2	1:A:984:C:C6	2.37	0.42
1:A:1237:C:C4'	1:A:1334:G:H21	2.32	0.42
2:B:109:LEU:O	2:B:112:LEU:N	2.53	0.42
1:A:66:G:N2	1:A:172:A:C2	2.87	0.42
1:A:986:A:C2	1:A:1220:G:C2	3.08	0.42
1:A:1239:A:H2'	1:A:1298:C:H42	1.84	0.42
1:A:1012:U:H2'	1:A:1013:G:C8	2.55	0.42
3:C:92:LYS:HA	3:C:92:LYS:HD3	1.86	0.42
1:A:1060:C:O2'	1:A:1061:G:H5'	2.19	0.42
13:M:38:ILE:HD12	13:M:55:LEU:HG	2.02	0.42
5:E:47:VAL:O	5:E:50:ALA:HB3	2.20	0.42
1:A:734:G:OP1	1:A:734:G:H8	2.02	0.42
4:D:60:LYS:HG2	4:D:74:PHE:HE2	1.84	0.42
1:A:1188:A:C2'	1:A:1189:C:H5'	2.49	0.42
1:A:1090:U:O2'	1:A:1091:U:H5'	2.19	0.42
9:I:7:GLY:HA2	9:I:78:LEU:CD1	2.49	0.42
1:A:393:A:C2'	1:A:394:G:H5'	2.50	0.42
1:A:865:A:C2	1:A:918:A:H4'	2.55	0.42
2:B:108:ARG:HG2	2:B:108:ARG:HH11	1.84	0.42
10:J:22:VAL:O	10:J:26:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:C:O2'	1:A:1060:C:H5'	2.20	0.42
9:I:124:TYR:CE2	9:I:127:ARG:NE	2.88	0.42
13:M:79:ARG:C	13:M:81:MET:N	2.73	0.42
13:M:79:ARG:HB3	13:M:79:ARG:NH1	2.34	0.42
1:A:738:C:OP2	6:F:92:LYS:HD3	2.20	0.42
23:Z:28:G:C2'	23:Z:29:G:H8	2.33	0.42
20:T:89:GLY:O	20:T:90:ALA:CB	2.68	0.42
8:H:50:ARG:O	8:H:51:VAL:HG23	2.19	0.42
7:G:52:LYS:N	7:G:52:LYS:HD2	2.34	0.42
7:G:68:VAL:HG11	7:G:133:ALA:HB1	2.02	0.42
1:A:1298:C:OP2	7:G:113:ARG:NH2	2.53	0.42
7:G:98:LEU:HA	7:G:98:LEU:HD23	1.90	0.42
11:K:38:ILE:HD11	11:K:54:ALA:CA	2.49	0.41
1:A:472:A:O4'	16:P:82:GLN:NE2	2.45	0.41
22:W:5:A:H5'	22:W:6:A:OP2	2.20	0.41
10:J:47:VAL:HG22	14:N:40:ARG:HB2	2.01	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
1:A:631:G:O2'	1:A:632:A:O5'	2.38	0.41
1:A:1442(A):G:H5''	1:A:1442(B):A:H3'	2.00	0.41
1:A:1521:G:H2'	1:A:1522:U:H6	1.83	0.41
19:S:50:VAL:O	19:S:57:VAL:N	2.53	0.41
5:E:37:VAL:HG21	5:E:109:ALA:HB2	2.01	0.41
4:D:101:ASP:OD1	4:D:102:ASN:N	2.52	0.41
2:B:161:PRO:O	2:B:165:ALA:N	2.52	0.41
1:A:1119:C:O2'	1:A:1120:G:H5'	2.19	0.41
1:A:1124:G:O2'	1:A:1125:U:P	2.78	0.41
10:J:30:ALA:C	10:J:32:VAL:H	2.24	0.41
2:B:208:ILE:HA	2:B:208:ILE:HD13	1.90	0.41
1:A:1502:A:C2	1:A:1504:G:C2	3.08	0.41
1:A:644:G:C5	1:A:645:C:C5	3.08	0.41
11:K:85:ILE:O	11:K:89:GLN:HG3	2.20	0.41
14:N:5:LEU:C	14:N:7:GLU:H	2.22	0.41
13:M:83:ILE:HG22	13:M:84:GLY:N	2.35	0.41
1:A:1314:C:OP2	19:S:5:LYS:CD	2.68	0.41
14:N:17:VAL:O	14:N:19:ALA:N	2.53	0.41
3:C:166:TRP:HB3	3:C:167:ALA:H	1.46	0.41
14:N:20:TYR:HE2	14:N:22:ARG:NE	2.17	0.41
6:F:19:LEU:C	6:F:19:LEU:HD23	2.40	0.41
1:A:928:G:O2'	1:A:1533:C:OP2	2.38	0.41
7:G:124:MET:C	7:G:126:ALA:N	2.72	0.41
2:B:171:ALA:O	2:B:174:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:GLN:HA	7:G:50:GLN:OE1	2.20	0.41
2:B:11:PHE:CD1	2:B:35:ILE:HG23	2.55	0.41
1:A:980:C:H2'	1:A:981:U:O4'	2.20	0.41
13:M:121:LYS:O	13:M:122:ALA:CB	2.67	0.41
2:B:44:GLU:OE2	2:B:194:ILE:HB	2.20	0.41
1:A:275:G:C5'	17:Q:13:LYS:HB3	2.43	0.41
4:D:61:GLN:NE2	4:D:64:ARG:NH1	2.65	0.41
5:E:140:THR:CG2	5:E:142:ALA:H	2.34	0.41
7:G:142:ARG:O	7:G:146:ALA:HB2	2.20	0.41
9:I:9:ARG:HD2	9:I:10:LYS:H	1.84	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.55	0.41
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.41
1:A:925:G:C6	1:A:927:G:N7	2.88	0.41
9:I:101:LEU:N	9:I:101:LEU:HD22	2.35	0.41
9:I:1:GLU:O	9:I:2:GLN:HB2	2.21	0.41
1:A:876:G:H2'	1:A:877:C:C6	2.55	0.41
1:A:1273:G:H2'	1:A:1274:G:C8	2.55	0.41
1:A:834:C:H2'	1:A:835:U:H6	1.85	0.41
3:C:90:LEU:HD11	3:C:98:VAL:H	1.85	0.41
1:A:1369:C:H2'	1:A:1370:G:H8	1.74	0.41
14:N:28:ARG:HG2	14:N:28:ARG:NH1	2.34	0.41
12:L:23:LEU:O	12:L:25:GLY:N	2.53	0.41
2:B:101:THR:C	2:B:103:SER:H	2.24	0.41
3:C:33:LEU:C	3:C:33:LEU:HD23	2.37	0.41
1:A:1039:C:H2'	1:A:1040:U:O4'	2.20	0.41
1:A:946:A:C2	1:A:1236:A:C2	3.09	0.41
1:A:631:G:HO2'	1:A:632:A:C5'	2.34	0.41
2:B:125:PRO:C	2:B:127:LYS:N	2.72	0.41
2:B:70:GLN:O	2:B:202:ILE:HG12	2.20	0.41
1:A:99:U:O2'	1:A:100:C:H5'	2.21	0.41
11:K:5:ALA:HA	11:K:66:GLY:O	2.20	0.41
1:A:1175:G:O2'	1:A:1176:A:H5'	2.21	0.41
2:B:222:GLY:O	2:B:223:VAL:C	2.59	0.41
19:S:32:THR:CG2	19:S:34:SER:HB2	2.51	0.41
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.47	0.41
17:Q:94:TYR:O	17:Q:96:SER:N	2.53	0.41
12:L:122:LYS:HZ3	12:L:122:LYS:HB2	1.85	0.41
1:A:443:C:H2'	1:A:444:C:C6	2.54	0.41
3:C:24:GLY:C	3:C:26:LYS:H	2.23	0.41
1:A:938:A:N6	1:A:939:G:C6	2.88	0.41
3:C:72:PRO:O	3:C:73:GLY:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:49:LYS:HD3	14:N:51:GLN:NE2	2.35	0.41
4:D:16:VAL:N	4:D:32:MET:HE2	2.36	0.41
7:G:15:LEU:HD22	7:G:15:LEU:N	2.35	0.41
10:J:77:ARG:O	10:J:81:GLU:HG3	2.21	0.41
1:A:1474:G:C6	1:A:1475:G:N7	2.88	0.41
1:A:849:C:C3'	1:A:850:U:C5'	2.90	0.41
9:I:4:TYR:CD1	9:I:4:TYR:C	2.94	0.41
1:A:974:A:P	14:N:40:ARG:HH12	2.43	0.41
2:B:85:PRO:HG2	2:B:149:LEU:HD23	2.02	0.41
1:A:1074:G:O3'	2:B:97:THR:HG23	2.20	0.41
1:A:1310:G:OP1	13:M:87:ARG:NH2	2.51	0.41
13:M:10:ARG:CG	13:M:11:ASN:H	2.34	0.41
19:S:19:LEU:HA	19:S:22:ASN:HD22	1.86	0.41
1:A:1090:U:H2'	1:A:1091:U:C6	2.55	0.41
1:A:1068:G:OP1	1:A:1388:C:H5'	2.20	0.41
1:A:129(A):G:C6	1:A:189(E):U:O2'	2.61	0.41
2:B:106:VAL:CG1	2:B:147:ARG:HD3	2.51	0.41
6:F:40:VAL:CG2	6:F:41:GLU:N	2.84	0.41
1:A:434:U:H2'	1:A:435:C:C6	2.56	0.41
19:S:30:ILE:HG13	19:S:48:ILE:CD1	2.50	0.41
1:A:1410:G:H2'	1:A:1411:C:C6	2.56	0.41
1:A:448:A:C4	1:A:487:A:C2	3.09	0.41
12:L:56:LEU:HB2	12:L:60:TYR:O	2.20	0.41
4:D:90:SER:O	4:D:93:LEU:N	2.54	0.41
1:A:1110:A:H8	1:A:1110:A:O5'	2.03	0.41
1:A:501:C:H1'	1:A:549:C:H1'	2.01	0.41
1:A:740:U:O2'	1:A:741:G:H5'	2.21	0.41
3:C:42:LEU:O	3:C:46:LEU:HB2	2.20	0.41
1:A:977:A:N6	1:A:1224:G:O5'	2.54	0.41
12:L:37:ARG:NH1	12:L:53:LYS:HE2	2.36	0.41
1:A:819:A:O2'	1:A:819:A:O5'	2.39	0.41
1:A:614:A:C2	1:A:627:G:C2	3.09	0.41
1:A:189(D):C:H2'	1:A:189(E):U:O2'	2.21	0.41
2:B:13:HIS:NE2	2:B:200:ASP:HB3	2.35	0.41
3:C:174:LEU:N	3:C:174:LEU:HD23	2.35	0.41
16:P:43:LYS:HD3	16:P:48:TRP:CZ2	2.55	0.41
18:R:31:GLU:N	18:R:31:GLU:CD	2.74	0.41
2:B:120:GLU:HG2	2:B:123:GLU:OE1	2.21	0.41
8:H:23:SER:HA	8:H:61:VAL:O	2.21	0.41
1:A:1115:C:H2'	1:A:1116:C:H6	1.86	0.41
2:B:217:ILE:O	2:B:219:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:C:O2'	1:A:648:A:H5''	2.20	0.41
18:R:72:ARG:HB3	18:R:73:LYS:H	1.53	0.41
9:I:32:PHE:CZ	9:I:46:LEU:HD21	2.56	0.41
5:E:27:LEU:HA	5:E:27:LEU:HD23	1.89	0.41
11:K:24:ASP:O	11:K:26:ASP:N	2.54	0.41
1:A:1405:G:O2'	1:A:1406:U:H5'	2.20	0.41
21:V:24:ARG:HG3	21:V:24:ARG:HH11	1.85	0.41
1:A:911:U:OP1	12:L:91:GLY:HA2	2.20	0.41
6:F:37:VAL:HA	6:F:65:VAL:HG12	2.02	0.41
13:M:28:ARG:HG2	13:M:63:TRP:CZ2	2.56	0.41
1:A:1494:G:H2'	1:A:1494:G:N3	2.36	0.41
19:S:32:THR:HG21	19:S:34:SER:HB2	2.03	0.41
2:B:207:LEU:O	2:B:211:ARG:HG2	2.20	0.41
4:D:22:GLY:O	4:D:25:CYS:HB2	2.21	0.41
19:S:62:THR:CG2	19:S:63:GLU:H	2.29	0.41
3:C:34:GLU:O	3:C:38:ILE:HD13	2.21	0.41
18:R:71:VAL:O	18:R:72:ARG:CG	2.58	0.41
19:S:21:LEU:HD11	19:S:27:LYS:HD3	2.03	0.41
10:J:88:LEU:H	10:J:89:PRO:HD2	1.85	0.41
11:K:105:PRO:C	11:K:107:ASN:H	2.24	0.41
13:M:61:ASN:O	13:M:62:THR:CB	2.69	0.41
15:O:14:PHE:CZ	15:O:83:LYS:HE2	2.56	0.41
20:T:7:LYS:HA	20:T:10:ARG:HG2	2.02	0.41
3:C:149:LYS:HG2	3:C:150:VAL:N	2.36	0.41
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.36	0.41
19:S:79:TYR:CE2	19:S:80:ARG:CG	3.04	0.41
4:D:186:ARG:HG3	4:D:187:LEU:H	1.86	0.41
1:A:1418:A:N6	1:A:1482:G:O2'	2.53	0.41
1:A:1041:A:H2'	1:A:1042:G:H8	1.84	0.41
1:A:382:A:O2'	1:A:383:A:H5'	2.21	0.41
3:C:86:LEU:O	3:C:89:GLU:HB2	2.21	0.41
3:C:53:ARG:O	3:C:54:VAL:HG23	2.20	0.41
19:S:9:PHE:CD1	19:S:10:VAL:N	2.89	0.41
1:A:593:G:O2'	1:A:594:G:H5'	2.21	0.41
2:B:150:LYS:HD3	2:B:150:LYS:O	2.21	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.21	0.41
19:S:40:VAL:HG22	19:S:43:MET:HE2	2.02	0.41
9:I:111:LYS:HD3	9:I:112:LYS:O	2.19	0.41
9:I:41:ARG:O	9:I:42:ALA:C	2.59	0.41
8:H:121:ASP:CB	8:H:125:ARG:HH21	2.34	0.41
2:B:126:LYS:C	2:B:128:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.50	0.41
1:A:1262:C:H2'	1:A:1263:C:H6	1.85	0.41
3:C:78:ARG:HG3	3:C:78:ARG:O	2.21	0.41
4:D:126:THR:HG23	4:D:146:ALA:HB3	2.03	0.41
15:O:65:LEU:O	15:O:68:TYR:HB3	2.21	0.41
1:A:1447:A:O2'	1:A:1452:C:OP2	2.33	0.41
21:V:7:ARG:HG3	21:V:7:ARG:O	2.21	0.41
1:A:402:G:H2'	1:A:403:C:C5'	2.23	0.40
4:D:35:ARG:HH11	4:D:35:ARG:CG	2.31	0.40
1:A:998:G:C3'	1:A:999:C:C5'	2.94	0.40
9:I:126:LYS:HG2	13:M:125:LYS:HZ3	1.85	0.40
2:B:108:ARG:CD	2:B:112:LEU:HG	2.50	0.40
1:A:633:G:H2'	1:A:634:C:H6	1.86	0.40
1:A:285:G:O2'	1:A:286:G:H5'	2.21	0.40
1:A:413:G:H1'	1:A:428:G:H21	1.86	0.40
13:M:9:PRO:HB3	13:M:17:ALA:O	2.22	0.40
13:M:48:THR:O	13:M:52:VAL:HG23	2.21	0.40
18:R:21:ASN:OD1	18:R:24:VAL:HG12	2.21	0.40
2:B:138:ARG:HA	2:B:141:LYS:HG3	2.02	0.40
2:B:95:MET:O	2:B:99:PHE:HA	2.22	0.40
13:M:123:PRO:O	13:M:125:LYS:N	2.55	0.40
15:O:20:ASP:OD2	15:O:23:SER:OG	2.33	0.40
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.04	0.40
1:A:832:C:O2'	1:A:833:U:H5'	2.21	0.40
2:B:112:LEU:HA	2:B:112:LEU:HD23	1.94	0.40
6:F:50:TYR:CE1	18:R:62:GLY:HA2	2.56	0.40
1:A:619:U:O2	4:D:132:VAL:HA	2.21	0.40
1:A:1464:G:O2'	1:A:1465:C:H5'	2.22	0.40
4:D:109:PHE:N	4:D:109:PHE:CD1	2.88	0.40
1:A:994:A:N3	1:A:994:A:H2'	2.36	0.40
13:M:101:ARG:HB2	13:M:101:ARG:HH11	1.86	0.40
3:C:21:TRP:CB	3:C:58:ARG:HB2	2.52	0.40
14:N:25:ARG:HH12	14:N:45:GLU:HB2	1.86	0.40
2:B:101:THR:O	2:B:103:SER:N	2.53	0.40
5:E:5:LYS:HD3	5:E:108:LEU:HG	2.03	0.40
8:H:104:ARG:O	8:H:105:ARG:C	2.58	0.40
11:K:24:ASP:HB2	11:K:25:PRO:HD2	2.04	0.40
2:B:70:GLN:HE22	2:B:202:ILE:N	2.20	0.40
4:D:2:ARG:HG3	4:D:117:ARG:CZ	2.52	0.40
5:E:127:ILE:HD13	5:E:127:ILE:HA	1.94	0.40
10:J:36:ILE:HA	10:J:37:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLU:CB	2:B:226:PRO:CD	2.99	0.40
1:A:1473:A:C2	1:A:1474:G:H1'	2.57	0.40
10:J:55:LYS:C	10:J:55:LYS:HD2	2.41	0.40
12:L:21:PRO:C	12:L:23:LEU:N	2.74	0.40
18:R:20:ARG:O	18:R:22:VAL:N	2.51	0.40
18:R:21:ASN:CG	18:R:24:VAL:HG12	2.42	0.40
5:E:36:ARG:NH1	5:E:64:GLU:OE1	2.54	0.40
12:L:52:ALA:HB2	12:L:66:ILE:HD11	2.04	0.40
17:Q:4:VAL:HA	17:Q:58:ILE:O	2.22	0.40
8:H:65:TYR:CD1	8:H:65:TYR:N	2.90	0.40
4:D:60:LYS:HD2	4:D:60:LYS:C	2.42	0.40
11:K:114:LYS:HG2	11:K:114:LYS:O	2.21	0.40
1:A:1090:U:O4'	1:A:1170:A:H2	2.04	0.40
4:D:200:GLN:HE21	4:D:200:GLN:CA	2.26	0.40
8:H:6:ILE:N	8:H:6:ILE:HD12	2.36	0.40
18:R:2:SER:HB2	18:R:39:ARG:HH21	1.86	0.40
1:A:16:A:H2'	1:A:17:U:H5'	2.03	0.40
1:A:1182:G:O2'	1:A:1183:A:P	2.79	0.40
5:E:72:ILE:CG2	5:E:138:LEU:CD2	3.00	0.40
1:A:861:G:O2'	1:A:862:C:H5'	2.22	0.40
2:B:47:ARG:HG2	2:B:47:ARG:HH11	1.86	0.40
3:C:114:LEU:HD23	3:C:117:GLN:OE1	2.22	0.40
1:A:682:G:O2'	1:A:683:G:H5'	2.21	0.40
2:B:133:LYS:HA	2:B:133:LYS:HD2	1.91	0.40
1:A:1192:C:C5	1:A:1193:G:C8	3.10	0.40
1:A:838:G:C3'	1:A:839:U:H5''	2.51	0.40
13:M:83:ILE:CG2	19:S:73:PHE:HE2	2.34	0.40
2:B:16:LYS:HD2	2:B:29:GLU:OE1	2.20	0.40
11:K:49:TYR:O	11:K:52:GLN:HB3	2.21	0.40
19:S:18:VAL:CG1	19:S:19:LEU:H	2.27	0.40
16:P:42:ARG:O	16:P:43:LYS:C	2.60	0.40
1:A:857:C:H2'	1:A:858:G:O4'	2.21	0.40
3:C:53:ARG:HG2	3:C:54:VAL:H	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	166 (71%)	45 (19%)	22 (9%)	1	2
3	C	205/239 (86%)	145 (71%)	38 (18%)	22 (11%)	0	1
4	D	206/208 (99%)	172 (84%)	22 (11%)	12 (6%)	2	6
5	E	149/161 (92%)	139 (93%)	9 (6%)	1 (1%)	26	63
6	F	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
7	G	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	3	11
8	H	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	6	23
9	I	125/128 (98%)	99 (79%)	14 (11%)	12 (10%)	1	2
10	J	97/104 (93%)	69 (71%)	15 (16%)	13 (13%)	0	1
11	K	117/129 (91%)	96 (82%)	18 (15%)	3 (3%)	7	26
12	L	123/132 (93%)	106 (86%)	10 (8%)	7 (6%)	2	6
13	M	123/126 (98%)	94 (76%)	17 (14%)	12 (10%)	1	2
14	N	58/60 (97%)	43 (74%)	7 (12%)	8 (14%)	0	0
15	O	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	8	30
16	P	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	16	48
17	Q	102/104 (98%)	86 (84%)	9 (9%)	7 (7%)	1	4
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	6	24
19	S	79/92 (86%)	61 (77%)	12 (15%)	6 (8%)	1	3
20	T	97/106 (92%)	76 (78%)	12 (12%)	9 (9%)	1	2
21	V	23/26 (88%)	18 (78%)	4 (17%)	1 (4%)	3	13
All	All	2364/2529 (94%)	1921 (81%)	292 (12%)	151 (6%)	2	5

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	HIS

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Mol	Chain	Res	Type
2	B	11	PHE
2	B	12	GLY
2	B	18	TRP
2	B	117	ALA
2	B	223	VAL
3	C	14	THR
3	C	15	ARG
3	C	25	LYS
3	C	46	LEU
3	C	60	ALA
3	C	65	VAL
3	C	100	LEU
3	C	153	SER
3	C	178	ARG
3	C	188	ALA
3	C	206	VAL
4	D	35	ARG
4	D	178	GLU
5	E	149	LYS
7	G	4	ARG
7	G	6	ALA
7	G	51	GLU
7	G	154	ARG
8	H	91	ARG
9	I	57	ARG
9	I	116	HIS
9	I	126	LYS
10	J	32	VAL
10	J	58	ARG
12	L	23	LEU
12	L	37	ARG
13	M	62	THR
13	M	66	GLU
13	M	85	CYS
13	M	122	ALA
14	N	4	ALA
14	N	31	SER
16	P	83	GLU
17	Q	79	GLY
17	Q	80	ARG
17	Q	98	SER
18	R	5	ALA

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Mol	Chain	Res	Type
19	S	5	LYS
2	B	3	GLU
2	B	5	LEU
2	B	9	VAL
2	B	14	GLU
2	B	82	ALA
2	B	89	GLN
2	B	221	GLY
3	C	54	VAL
3	C	64	ALA
3	C	67	VAL
3	C	76	ILE
3	C	99	ALA
3	C	155	ARG
4	D	2	ARG
4	D	28	PRO
4	D	170	GLY
7	G	52	LYS
8	H	24	THR
8	H	105	ARG
9	I	45	ALA
9	I	93	ALA
10	J	28	SER
10	J	34	GLY
10	J	53	LYS
10	J	70	VAL
10	J	80	ILE
10	J	88	LEU
12	L	22	ALA
12	L	25	GLY
13	M	58	TYR
13	M	105	ASN
13	M	123	PRO
14	N	16	LYS
14	N	22	ARG
18	R	72	ARG
19	S	42	GLU
20	T	2	ASN
20	T	87	ALA
20	T	89	GLY
20	T	95	GLY
2	B	15	ARG

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Mol	Chain	Res	Type
2	B	58	ARG
3	C	167	ALA
4	D	3	TYR
4	D	29	LYS
7	G	5	ARG
9	I	42	ALA
10	J	37	PRO
10	J	98	THR
11	K	3	GLN
12	L	70	GLY
12	L	75	GLU
13	M	124	ARG
14	N	3	LYS
14	N	18	ARG
14	N	21	THR
17	Q	67	ARG
17	Q	96	SER
17	Q	97	LEU
20	T	4	SER
20	T	91	PRO
2	B	17	ARG
2	B	56	ALA
2	B	109	LEU
2	B	218	GLN
3	C	118	ARG
4	D	177	VAL
9	I	23	GLY
9	I	54	ALA
10	J	38	LEU
11	K	40	TYR
13	M	5	GLY
20	T	88	ALA
21	V	3	LYS
3	C	145	ALA
4	D	4	ILE
4	D	30	CYS
4	D	38	PRO
9	I	6	THR
10	J	30	ALA
11	K	25	PRO
12	L	24	LYS
15	O	87	ARG

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Mol	Chain	Res	Type
17	Q	33	LYS
19	S	4	LEU
19	S	29	LEU
19	S	80	ARG
2	B	68	LYS
2	B	226	PRO
7	G	62	LYS
9	I	22	ASN
9	I	43	VAL
13	M	20	TYR
13	M	35	LYS
19	S	7	GLY
20	T	90	ALA
3	C	13	ILE
4	D	6	PRO
9	I	40	VAL
13	M	3	ILE
20	T	94	GLY
3	C	80	GLY
8	H	83	ILE
14	N	6	ILE
10	J	74	ASN
15	O	81	ILE
2	B	124	ARG

### 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	202/220 (92%)	174 (86%)	28 (14%)	4	12
3	C	160/188 (85%)	148 (92%)	12 (8%)	17	44
4	D	180/180 (100%)	168 (93%)	12 (7%)	20	50
5	E	115/122 (94%)	104 (90%)	11 (10%)	10	31
6	F	90/90 (100%)	88 (98%)	2 (2%)	60	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	126/126 (100%)	123 (98%)	3 (2%)	57	86
8	H	119/119 (100%)	110 (92%)	9 (8%)	16	43
9	I	98/99 (99%)	93 (95%)	5 (5%)	29	65
10	J	88/91 (97%)	84 (96%)	4 (4%)	34	70
11	K	90/99 (91%)	82 (91%)	8 (9%)	12	35
12	L	104/109 (95%)	99 (95%)	5 (5%)	31	67
13	M	100/101 (99%)	89 (89%)	11 (11%)	8	23
14	N	49/49 (100%)	42 (86%)	7 (14%)	4	12
15	O	79/79 (100%)	74 (94%)	5 (6%)	22	54
16	P	72/74 (97%)	65 (90%)	7 (10%)	10	30
17	Q	96/96 (100%)	90 (94%)	6 (6%)	22	54
18	R	64/77 (83%)	61 (95%)	3 (5%)	32	68
19	S	71/79 (90%)	67 (94%)	4 (6%)	26	60
20	T	76/82 (93%)	67 (88%)	9 (12%)	6	19
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1998/2101 (95%)	1847 (92%)	151 (8%)	16	43

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2	LYS
2	B	3	GLU
2	B	6	GLU
2	B	11	PHE
2	B	15	ARG
2	B	17	ARG
2	B	18	TRP
2	B	19	ASN
2	B	46	GLU
2	B	70	GLN
2	B	76	ARG
2	B	97	THR
2	B	106	VAL
2	B	108	ARG
2	B	133	LYS
2	B	138	ARG
2	B	147	ARG

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Mol	Chain	Res	Type
2	B	151	ARG
2	B	156	ILE
2	B	163	LYS
2	B	179	ILE
2	B	181	LEU
2	B	184	THR
2	B	198	ASN
2	B	199	ASP
2	B	218	GLN
2	B	225	GLU
2	B	230	TYR
3	C	2	ASN
3	C	4	ILE
3	C	10	ARG
3	C	25	LYS
3	C	89	GLU
3	C	90	LEU
3	C	98	VAL
3	C	166	TRP
3	C	171	ARG
3	C	187	LEU
3	C	191	THR
3	C	203	LEU
4	D	8	CYS
4	D	24	ARG
4	D	35	ARG
4	D	57	LEU
4	D	60	LYS
4	D	64	ARG
4	D	71	GLU
4	D	75	ARG
4	D	121	ARG
4	D	189	ASP
4	D	193	LEU
4	D	198	ASN
5	E	8	LEU
5	E	27	LEU
5	E	37	VAL
5	E	39	LEU
5	E	60	ARG
5	E	69	ASN
5	E	71	THR

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Mol	Chain	Res	Type
5	E	75	GLU
5	E	76	ILE
5	E	116	THR
5	E	140	THR
6	F	10	LEU
6	F	27	GLN
7	G	7	GLU
7	G	52	LYS
7	G	123	LEU
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	92	ARG
8	H	112	LEU
8	H	119	LEU
8	H	125	ARG
9	I	4	TYR
9	I	37	GLN
9	I	78	LEU
9	I	103	ARG
9	I	126	LYS
10	J	36	ILE
10	J	55	LYS
10	J	69	LEU
10	J	71	ASP
11	K	17	ASN
11	K	19	ILE
11	K	25	PRO
11	K	30	ILE
11	K	71	ASP
11	K	82	GLU
11	K	83	GLN
11	K	110	ARG
12	L	38	THR
12	L	44	PRO
12	L	49	ARG
12	L	63	THR
12	L	109	ARG
13	M	8	ILE
13	M	39	ASN

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Mol	Chain	Res	Type
13	M	69	LEU
13	M	80	LEU
13	M	87	ARG
13	M	101	ARG
13	M	105	ASN
13	M	109	ARG
13	M	114	LYS
13	M	120	LYS
13	M	124	ARG
14	N	11	ARG
14	N	16	LYS
14	N	26	CYS
14	N	31	SER
14	N	40	ARG
14	N	42	CYS
14	N	43	LEU
15	O	30	LEU
15	O	33	LEU
15	O	56	LEU
15	O	69	LEU
15	O	80	LEU
16	P	1	MET
16	P	2	VAL
16	P	42	ARG
16	P	43	LYS
16	P	45	THR
16	P	55	ARG
16	P	81	ARG
17	Q	25	GLN
17	Q	37	ARG
17	Q	58	ILE
17	Q	73	LEU
17	Q	97	LEU
17	Q	103	LYS
18	R	13	GLU
18	R	21	ASN
18	R	22	VAL
19	S	6	LYS
19	S	11	ASP
19	S	14	LEU
19	S	61	ILE
20	T	3	LEU

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Mol	Chain	Res	Type
20	T	6	LEU
20	T	35	GLN
20	T	50	ARG
20	T	66	HIS
20	T	68	ASN
20	T	77	LEU
20	T	86	GLU
20	T	93	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	HIS
2	B	19	ASN
2	B	31	ASN
2	B	34	HIS
2	B	70	GLN
2	B	72	GLN
2	B	198	ASN
2	B	206	GLN
2	B	218	GLN
2	B	234	GLN
3	C	5	HIS
3	C	30	HIS
3	C	36	GLN
3	C	68	HIS
3	C	106	GLN
3	C	122	GLN
3	C	138	GLN
3	C	169	GLN
3	C	175	HIS
4	D	41	GLN
4	D	61	GLN
4	D	122	HIS
4	D	159	GLN
4	D	160	ASN
4	D	198	ASN
4	D	200	GLN
5	E	69	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN

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Mol	Chain	Res	Type
6	F	94	GLN
7	G	36	ASN
7	G	55	GLN
7	G	121	HIS
7	G	147	ASN
9	I	30	GLN
9	I	37	GLN
9	I	72	GLN
10	J	54	HIS
10	J	60	HIS
10	J	74	ASN
10	J	76	ASN
10	J	82	GLN
11	K	12	HIS
11	K	17	ASN
11	K	52	GLN
11	K	83	GLN
11	K	107	ASN
12	L	45	ASN
12	L	71	HIS
13	M	11	ASN
13	M	39	ASN
15	O	36	ASN
15	O	45	HIS
15	O	70	GLN
17	Q	15	GLN
17	Q	25	GLN
18	R	21	ASN
19	S	22	ASN
19	S	46	HIS
19	S	52	ASN
19	S	55	GLN
20	T	83	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1521 (99%)	262 (17%)	61 (4%)
22	W	5/6 (83%)	0	0
23	Z	15/16 (93%)	2 (13%)	0
All	All	1530/1543 (99%)	264 (17%)	61 (3%)

All (264) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	29	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	52	G
1	A	60	A
1	A	61	G
1	A	82	U
1	A	115	G
1	A	116	A
1	A	121	C
1	A	131	C
1	A	145	G
1	A	163	C
1	A	174	C
1	A	182	U
1	A	183	G
1	A	189	G
1	A	189(B)	C
1	A	189(C)	C
1	A	189(E)	U
1	A	189(F)	U
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	231	G
1	A	245	C
1	A	246	A
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	275	G
1	A	279	A
1	A	289	G

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Mol	Chain	Res	Type
1	A	319	G
1	A	320	C
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	397	A
1	A	403	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	426	G
1	A	429	U
1	A	439	A
1	A	441	A
1	A	452	A
1	A	453	A
1	A	470	C
1	A	471	G
1	A	474	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	498	U
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	G
1	A	530	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	548	G
1	A	559	A
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	596	C
1	A	607	A
1	A	629	G
1	A	630	G
1	A	631	G
1	A	632	A
1	A	648	A
1	A	653	A
1	A	654	G
1	A	661	G
1	A	665	A
1	A	688	G
1	A	703	G
1	A	721	G
1	A	722	A
1	A	723	U
1	A	734	G
1	A	735	C
1	A	749	C
1	A	755	G
1	A	776	G
1	A	777	A
1	A	781	A
1	A	793	U
1	A	794	A
1	A	809	G
1	A	810	C
1	A	814	A
1	A	817	C

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Mol	Chain	Res	Type
1	A	819	A
1	A	820	U
1	A	821	G
1	A	839	U
1	A	840	C
1	A	848	C
1	A	850	U
1	A	859	A
1	A	865	A
1	A	872	A
1	A	874	G
1	A	885	G
1	A	889	A
1	A	914	A
1	A	934	C
1	A	935	A
1	A	944	G
1	A	945	G
1	A	960	U
1	A	961	U
1	A	968	A
1	A	969	A
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	983	A
1	A	992	U
1	A	993	G
1	A	996	A
1	A	998	G
1	A	999	C
1	A	1001(A)	G
1	A	1004	A
1	A	1009	G
1	A	1018	C
1	A	1019	C
1	A	1020	U
1	A	1024	G
1	A	1025	U
1	A	1030	C

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Mol	Chain	Res	Type
1	A	1040	U
1	A	1045	C
1	A	1049	U
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1159	U
1	A	1160	G
1	A	1179	A
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1227	A
1	A	1238	A

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Mol	Chain	Res	Type
1	A	1245	A
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1272	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1324	A
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1357	A
1	A	1363(A)	A
1	A	1364	U
1	A	1365	G
1	A	1400	C
1	A	1441	G
1	A	1442	G
1	A	1442(B)	A
1	A	1452	C
1	A	1463	C
1	A	1474	G
1	A	1475	G
1	A	1476	G
1	A	1478	C
1	A	1481	U

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Mol	Chain	Res	Type
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1540	U
1	A	1541	U
23	Z	28	G
23	Z	33	U

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	29	G
1	A	51	A
1	A	60	A
1	A	115	G
1	A	181	G
1	A	189	G
1	A	189(B)	C
1	A	189(E)	U
1	A	196	A
1	A	244	U
1	A	246	A
1	A	250	A
1	A	320	C
1	A	353	A
1	A	366	C
1	A	485	G
1	A	495	A
1	A	496	A
1	A	517	G
1	A	530	G
1	A	533	A
1	A	562	C
1	A	572	A
1	A	629	G
1	A	631	G
1	A	653	A

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Mol	Chain	Res	Type
1	A	721	G
1	A	734	G
1	A	748	C
1	A	776	G
1	A	793	U
1	A	819	A
1	A	884	U
1	A	944	G
1	A	968	A
1	A	974	A
1	A	982	U
1	A	1017	G
1	A	1019	C
1	A	1054	C
1	A	1064	G
1	A	1067	A
1	A	1124	G
1	A	1135	U
1	A	1145	C
1	A	1181	G
1	A	1182	G
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1214	C
1	A	1278	U
1	A	1285	A
1	A	1298	C
1	A	1336	C
1	A	1346	A
1	A	1363(A)	A
1	A	1442(A)	G
1	A	1447	A
1	A	1475	G
1	A	1529	G

## 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 260 ligands modelled in this entry, 259 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	ON0	A	2759	-	54,54,54	1.41	6 (11%)	73,80,80	0.78	3 (4%)

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	ON0	A	2759	-	-	0/20/105/105	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2759	ON0	CBC-CBP	-5.06	1.41	1.50
26	A	2759	ON0	CAP-CBC	2.26	1.42	1.39
26	A	2759	ON0	CAO-CBC	2.45	1.43	1.39
26	A	2759	ON0	CBW-CBT	2.58	1.57	1.52
26	A	2759	ON0	O4-CBP	3.44	1.47	1.42
26	A	2759	ON0	O6-CBP	3.70	1.48	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2759	ON0	CBQ-O3'-C3'	-2.20	112.25	118.01
26	A	2759	ON0	OAV-CBM-CAQ	2.00	110.01	106.10
26	A	2759	ON0	O1-CBT-CBW	2.33	113.59	107.49



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2759	ON0	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1512/1521 (99%)	0.05	22 (1%) 76 74	44, 74, 145, 201	0
2	B	235/256 (91%)	0.36	21 (8%) 12 7	62, 110, 166, 189	0
3	C	207/239 (86%)	0.23	6 (2%) 55 49	62, 101, 148, 173	0
4	D	208/208 (100%)	0.14	11 (5%) 30 23	58, 85, 139, 194	0
5	E	151/161 (93%)	-0.14	0 100 100	44, 68, 102, 157	0
6	F	101/101 (100%)	0.06	2 (1%) 68 64	74, 104, 133, 159	0
7	G	155/155 (100%)	0.04	7 (4%) 37 31	65, 91, 146, 175	0
8	H	138/138 (100%)	-0.22	1 (0%) 89 88	45, 66, 93, 145	0
9	I	127/128 (99%)	0.40	6 (4%) 35 29	59, 110, 146, 196	0
10	J	99/104 (95%)	1.43	24 (24%) 1 0	55, 127, 184, 198	0
11	K	119/129 (92%)	0.24	4 (3%) 49 41	42, 80, 120, 179	0
12	L	125/132 (94%)	0.10	5 (4%) 42 35	41, 72, 110, 167	0
13	M	125/126 (99%)	0.90	15 (12%) 6 3	63, 94, 154, 187	0
14	N	60/60 (100%)	0.58	4 (6%) 21 15	61, 93, 133, 175	0
15	O	88/88 (100%)	0.06	2 (2%) 64 59	52, 81, 117, 171	0
16	P	84/88 (95%)	-0.07	0 100 100	52, 68, 101, 168	0
17	Q	104/104 (100%)	0.44	5 (4%) 34 28	40, 69, 132, 201	0
18	R	73/88 (82%)	0.27	2 (2%) 58 52	64, 87, 145, 196	0
19	S	81/92 (88%)	0.49	7 (8%) 13 8	72, 111, 153, 172	0
20	T	99/106 (93%)	0.15	5 (5%) 32 25	49, 74, 111, 148	0
21	V	25/26 (96%)	0.75	2 (8%) 15 10	63, 81, 121, 154	0
22	W	6/6 (100%)	0.81	2 (33%) 0 0	78, 87, 144, 171	0
23	Z	16/16 (100%)	0.61	1 (6%) 23 17	78, 111, 186, 191	0
All	All	3938/4072 (96%)	0.19	154 (3%) 43 36	40, 83, 151, 201	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	123	PRO	21.6
13	M	122	ALA	21.4
17	Q	104	ALA	20.3
11	K	119	SER	15.6
17	Q	103	LYS	12.5
17	Q	102	GLY	12.4
13	M	121	LYS	10.3
17	Q	101	GLY	9.7
13	M	124	ARG	9.4
13	M	119	LYS	9.1
1	A	1129	C	8.6
10	J	31	GLN	8.1
13	M	120	LYS	7.7
2	B	125	PRO	7.3
13	M	125	LYS	7.2
1	A	1001(A)	G	7.2
2	B	127	LYS	6.7
13	M	6	VAL	6.5
10	J	22	VAL	6.3
10	J	70	VAL	6.2
19	S	2	ARG	6.2
2	B	126	LYS	5.9
11	K	118	ALA	5.9
2	B	124	ARG	5.6
4	D	34	ARG	5.6
9	I	127	ARG	5.4
15	O	88	GLY	5.1
4	D	22	GLY	5.0
2	B	128	GLU	4.9
10	J	72	ILE	4.8
2	B	232	LEU	4.8
10	J	32	VAL	4.8
13	M	118	GLY	4.7
11	K	117	LYS	4.5
10	J	83	LEU	4.3
10	J	97	LYS	4.3
1	A	1539	C	4.3
10	J	73	ILE	4.2
13	M	117	ALA	4.2
10	J	68	ARG	4.1
10	J	3	ARG	4.0
17	Q	100	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
10	J	69	LEU	3.9
21	V	25	LYS	3.9
20	T	96	GLY	3.8
12	L	124	ALA	3.7
2	B	10	HIS	3.7
19	S	26	GLU	3.7
4	D	46	ARG	3.7
10	J	96	ILE	3.6
18	R	2	SER	3.6
7	G	155	TRP	3.6
10	J	20	LYS	3.5
1	A	630	G	3.5
1	A	1531	A	3.5
2	B	116	PHE	3.5
10	J	35	PRO	3.4
8	H	1	MET	3.4
10	J	71	ASP	3.4
10	J	4	ILE	3.3
2	B	123	GLU	3.2
10	J	33	SER	3.2
1	A	1533	C	3.2
20	T	93	ILE	3.2
2	B	130	VAL	3.2
1	A	631	G	3.2
4	D	37	TYR	3.2
14	N	5	LEU	3.2
1	A	1034	G	3.1
7	G	78	ARG	3.1
12	L	14	VAL	3.1
12	L	15	ARG	3.1
10	J	2	ILE	3.0
10	J	34	GLY	3.0
18	R	1	PRO	3.0
21	V	24	ARG	2.9
1	A	1003	G	2.9
13	M	116	VAL	2.9
14	N	3	LYS	2.9
23	Z	27	G	2.8
1	A	1031	G	2.8
10	J	57	SER	2.8
2	B	13	HIS	2.8
1	A	1027	C	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	35	ARG	2.7
10	J	94	ILE	2.7
4	D	8	CYS	2.7
19	S	48	ILE	2.7
15	O	87	ARG	2.7
10	J	17	SER	2.6
1	A	1035	A	2.6
10	J	98	THR	2.6
10	J	76	ASN	2.6
22	W	6	A	2.6
2	B	131	ARG	2.5
2	B	112	LEU	2.5
2	B	115	LEU	2.5
9	I	114	GLY	2.5
4	D	48	ARG	2.5
4	D	36	PRO	2.5
2	B	121	ILE	2.5
2	B	134	HIS	2.5
2	B	29	GLU	2.5
19	S	28	ARG	2.4
1	A	1033	G	2.4
3	C	171	ARG	2.4
12	L	23	LEU	2.4
20	T	92	LEU	2.4
9	I	113	TYR	2.4
3	C	75	VAL	2.4
1	A	202	U	2.4
14	N	16	LYS	2.4
13	M	7	GLU	2.4
4	D	178	GLU	2.3
7	G	149	ALA	2.3
11	K	22	ILE	2.3
3	C	195	LEU	2.3
1	A	1045	C	2.3
12	L	123	GLU	2.3
7	G	82	ALA	2.2
3	C	59	ALA	2.2
1	A	1030(B)	C	2.2
7	G	153	TYR	2.2
6	F	35	ALA	2.2
2	B	129	GLN	2.2
9	I	91	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1029	C	2.2
14	N	2	ARG	2.2
20	T	97	LEU	2.2
20	T	67	LYS	2.1
1	A	1030(A)	G	2.1
13	M	99	GLY	2.1
2	B	83	GLY	2.1
19	S	33	TRP	2.1
19	S	14	LEU	2.1
1	A	1026	G	2.1
13	M	10	ARG	2.1
19	S	38	THR	2.1
9	I	124	TYR	2.1
13	M	5	GLY	2.1
4	D	12	ARG	2.1
7	G	154	ARG	2.1
3	C	166	TRP	2.1
9	I	93	ALA	2.1
2	B	205	ILE	2.1
6	F	14	LEU	2.1
3	C	93	LEU	2.0
1	A	412	A	2.0
22	W	5	A	2.0
1	A	1140	C	2.0
4	D	30	CYS	2.0
2	B	119	PRO	2.0
7	G	25	PHE	2.0
1	A	1030(D)	A	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	2555	1/1	0.73	0.87	132.40	68,68,68,68	0
24	MG	A	2770	1/1	0.93	0.98	56.88	68,68,68,68	0
24	MG	A	2735	1/1	0.98	0.75	52.15	69,69,69,69	0
24	MG	A	2733	1/1	0.97	0.62	38.58	63,63,63,63	0
24	MG	A	2560	1/1	0.99	0.50	36.66	45,45,45,45	0
24	MG	A	2604	1/1	0.93	0.41	30.49	63,63,63,63	0
24	MG	A	2716	1/1	0.96	0.73	28.19	77,77,77,77	0
24	MG	A	2611	1/1	0.88	0.44	22.79	51,51,51,51	0
24	MG	A	2684	1/1	0.87	0.50	21.61	63,63,63,63	0
24	MG	A	2766	1/1	0.98	0.75	21.29	60,60,60,60	0
24	MG	A	2571	1/1	0.95	0.47	20.76	57,57,57,57	0
24	MG	A	2718	1/1	0.47	0.52	19.34	75,75,75,75	0
24	MG	A	2562	1/1	0.97	0.43	19.16	53,53,53,53	0
24	MG	A	2599	1/1	0.77	0.98	18.77	90,90,90,90	0
24	MG	E	1152	1/1	0.90	0.68	14.87	71,71,71,71	0
24	MG	A	2639	1/1	0.89	0.64	14.80	65,65,65,65	0
24	MG	A	2587	1/1	0.92	0.73	13.75	64,64,64,64	0
24	MG	H	1140	1/1	0.63	0.47	12.63	74,74,74,74	0
24	MG	A	2569	1/1	0.89	0.35	12.18	55,55,55,55	0
24	MG	A	2742	1/1	0.93	0.45	11.83	60,60,60,60	0
24	MG	A	2657	1/1	0.97	0.30	11.69	28,28,28,28	0
25	K	A	2673	1/1	0.67	0.42	11.31	129,129,129,129	0
24	MG	A	2696	1/1	0.98	0.30	10.79	41,41,41,41	0
24	MG	A	2661	1/1	0.78	0.81	10.30	75,75,75,75	0
24	MG	A	2601	1/1	0.95	0.44	9.36	61,61,61,61	0
24	MG	A	2647	1/1	0.97	0.28	8.05	35,35,35,35	0
24	MG	A	2572	1/1	0.95	0.38	7.89	71,71,71,71	0
24	MG	A	2615	1/1	0.88	0.27	7.58	60,60,60,60	0
24	MG	H	1139	1/1	0.77	0.33	7.18	75,75,75,75	0
24	MG	A	2706	1/1	0.95	0.41	7.15	67,67,67,67	0
24	MG	A	2632	1/1	0.86	0.29	6.77	75,75,75,75	0
24	MG	A	2713	1/1	0.84	0.25	6.24	70,70,70,70	0
24	MG	A	2591	1/1	0.46	0.31	5.73	83,83,83,83	0
24	MG	E	1151	1/1	0.94	0.38	5.47	72,72,72,72	0
24	MG	A	2747	1/1	0.49	0.31	5.36	66,66,66,66	0
24	MG	A	2577	1/1	0.81	0.22	4.78	45,45,45,45	0
24	MG	A	2616	1/1	0.92	0.24	4.37	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	2628	1/1	0.69	0.39	4.29	68,68,68,68	0
24	MG	A	2697	1/1	0.97	0.20	3.93	99,99,99,99	0
24	MG	A	2662	1/1	0.64	0.45	3.84	64,64,64,64	0
24	MG	A	2586	1/1	0.82	0.27	3.51	70,70,70,70	0
24	MG	T	1100	1/1	0.86	0.33	3.51	60,60,60,60	0
24	MG	A	2594	1/1	0.92	0.20	3.40	61,61,61,61	0
24	MG	A	2749	1/1	0.55	0.19	3.32	66,66,66,66	0
24	MG	A	2584	1/1	0.95	0.28	3.19	54,54,54,54	0
24	MG	A	2612	1/1	0.83	0.22	3.15	59,59,59,59	0
24	MG	A	2740	1/1	0.85	0.44	3.05	66,66,66,66	0
24	MG	A	2659	1/1	0.65	0.21	3.04	66,66,66,66	0
24	MG	N	1062	1/1	0.73	0.37	3.01	111,111,111,111	0
24	MG	A	2738	1/1	0.95	0.31	2.82	67,67,67,67	0
26	ON0	A	2759	49/49	0.95	0.21	2.81	56,64,79,80	0
25	K	A	2675	1/1	0.95	0.18	2.61	105,105,105,105	0
24	MG	A	2588	1/1	0.97	0.31	2.61	55,55,55,55	0
24	MG	A	2641	1/1	0.89	0.21	2.09	49,49,49,49	0
24	MG	A	2619	1/1	0.83	0.24	2.07	54,54,54,54	0
24	MG	A	2609	1/1	0.92	0.19	2.06	91,91,91,91	0
24	MG	I	1128	1/1	0.97	0.34	2.06	128,128,128,128	0
25	K	A	2672	1/1	0.65	0.20	2.02	97,97,97,97	0
24	MG	A	2688	1/1	0.95	0.20	1.91	79,79,79,79	0
24	MG	A	2610	1/1	0.94	0.24	1.87	55,55,55,55	0
24	MG	A	2699	1/1	0.87	0.19	1.87	78,78,78,78	0
24	MG	A	2550	1/1	0.83	0.26	1.75	60,60,60,60	0
24	MG	A	2646	1/1	0.95	0.17	1.29	50,50,50,50	0
24	MG	K	1120	1/1	0.93	0.17	1.20	59,59,59,59	0
24	MG	A	2651	1/1	0.79	0.19	0.94	69,69,69,69	0
24	MG	A	2751	1/1	0.89	0.21	0.94	64,64,64,64	0
24	MG	A	2745	1/1	0.81	0.20	0.65	57,57,57,57	0
24	MG	A	2649	1/1	0.87	0.19	0.47	54,54,54,54	0
24	MG	A	2640	1/1	0.92	0.17	0.38	58,58,58,58	0
24	MG	A	2631	1/1	0.85	0.14	0.29	54,54,54,54	0
27	ZN	D	1209	1/1	0.99	0.28	0.24	103,103,103,103	0
24	MG	A	2658	1/1	0.71	0.15	-0.12	59,59,59,59	0
24	MG	A	2687	1/1	0.83	0.16	-0.14	65,65,65,65	0
24	MG	A	2549	1/1	0.83	0.14	-0.15	57,57,57,57	0
24	MG	A	2643	1/1	0.88	0.15	-0.15	55,55,55,55	0
24	MG	B	1235	1/1	0.87	0.16	-0.45	95,95,95,95	0
24	MG	D	1210	1/1	0.87	0.15	-0.86	59,59,59,59	0
24	MG	M	1126	1/1	0.91	0.13	-1.00	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	2600	1/1	0.95	0.14	-1.30	60,60,60,60	0
24	MG	A	2635	1/1	0.92	0.13	-1.44	49,49,49,49	0
24	MG	Q	1105	1/1	0.83	0.10	-1.93	69,69,69,69	0
24	MG	A	2605	1/1	0.88	0.13	-1.94	43,43,43,43	0
24	MG	A	2573	1/1	0.88	0.10	-2.39	57,57,57,57	0
24	MG	A	2648	1/1	0.70	0.14	-2.53	52,52,52,52	0
27	ZN	N	1061	1/1	0.99	0.12	-3.22	98,98,98,98	0
24	MG	A	2645	1/1	0.95	0.10	-3.27	34,34,34,34	0
24	MG	A	2625	1/1	0.87	0.12	-3.67	49,49,49,49	0
25	K	A	2668	1/1	0.92	0.09	-4.13	99,99,99,99	0
24	MG	A	2644	1/1	0.99	0.10	-4.31	26,26,26,26	0
24	MG	A	2626	1/1	0.97	0.07	-5.22	49,49,49,49	0
24	MG	A	2613	1/1	0.67	0.84	-	73,73,73,73	0
24	MG	A	2581	1/1	0.96	0.47	-	59,59,59,59	0
24	MG	A	2624	1/1	0.69	0.14	-	59,59,59,59	0
24	MG	A	2655	1/1	0.82	0.23	-	57,57,57,57	0
24	MG	A	2705	1/1	0.89	0.40	-	77,77,77,77	0
24	MG	A	2282	1/1	0.88	1.03	-	82,82,82,82	0
24	MG	A	2698	1/1	0.96	0.08	-	66,66,66,66	0
24	MG	A	2650	1/1	0.80	0.17	-	55,55,55,55	0
24	MG	A	2602	1/1	0.75	0.21	-	78,78,78,78	0
24	MG	A	2736	1/1	0.68	0.28	-	82,82,82,82	0
24	MG	A	2617	1/1	0.46	0.98	-	119,119,119,119	0
24	MG	A	2630	1/1	0.65	0.18	-	62,62,62,62	0
25	K	A	2679	1/1	0.92	0.49	-	120,120,120,120	0
24	MG	A	2545	1/1	0.83	0.13	-	64,64,64,64	0
24	MG	A	2690	1/1	0.98	0.16	-	36,36,36,36	0
24	MG	A	2756	1/1	0.91	0.22	-	83,83,83,83	0
24	MG	A	2614	1/1	0.89	0.55	-	80,80,80,80	0
24	MG	A	2570	1/1	0.92	0.57	-	72,72,72,72	0
24	MG	A	2772	1/1	0.91	0.27	-	95,95,95,95	0
24	MG	A	2757	1/1	0.76	0.39	-	92,92,92,92	0
24	MG	A	2748	1/1	0.53	0.24	-	80,80,80,80	0
24	MG	A	2284	1/1	0.92	0.48	-	98,98,98,98	0
24	MG	A	2633	1/1	0.80	0.16	-	92,92,92,92	0
24	MG	A	2739	1/1	0.52	0.27	-	83,83,83,83	0
24	MG	A	2575	1/1	0.50	0.65	-	91,91,91,91	0
24	MG	A	2654	1/1	0.80	0.29	-	63,63,63,63	0
24	MG	A	2771	1/1	0.92	0.87	-	89,89,89,89	0
24	MG	A	2565	1/1	0.83	0.21	-	60,60,60,60	0
24	MG	A	2732	1/1	0.88	0.39	-	87,87,87,87	0
24	MG	A	2606	1/1	0.96	0.23	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	2707	1/1	0.67	0.24	-	74,74,74,74	0
25	K	A	2773	1/1	0.67	0.48	-	132,132,132,132	0
24	MG	A	2589	1/1	0.94	0.24	-	55,55,55,55	0
25	K	A	2669	1/1	0.44	0.32	-	113,113,113,113	0
24	MG	A	2579	1/1	0.64	0.38	-	75,75,75,75	0
24	MG	A	2767	1/1	0.78	0.39	-	66,66,66,66	0
24	MG	A	2548	1/1	0.75	0.31	-	63,63,63,63	0
24	MG	A	2722	1/1	0.53	0.91	-	88,88,88,88	0
24	MG	A	2755	1/1	0.84	0.22	-	63,63,63,63	0
24	MG	A	2546	1/1	0.63	0.74	-	111,111,111,111	0
24	MG	A	2709	1/1	0.86	0.37	-	75,75,75,75	0
24	MG	A	2764	1/1	0.86	0.43	-	84,84,84,84	0
24	MG	A	2725	1/1	0.84	0.19	-	67,67,67,67	0
24	MG	A	2559	1/1	0.84	1.32	-	83,83,83,83	0
24	MG	A	2598	1/1	0.91	0.30	-	66,66,66,66	0
24	MG	A	2656	1/1	0.91	0.13	-	72,72,72,72	0
25	K	A	2674	1/1	0.70	0.22	-	114,114,114,114	0
24	MG	A	2666	1/1	0.68	0.46	-	96,96,96,96	0
24	MG	A	2563	1/1	0.83	0.20	-	86,86,86,86	0
24	MG	A	2597	1/1	0.94	0.29	-	53,53,53,53	0
24	MG	A	2567	1/1	0.82	0.36	-	64,64,64,64	0
24	MG	A	2689	1/1	0.91	0.34	-	96,96,96,96	0
24	MG	A	2580	1/1	0.88	0.22	-	115,115,115,115	0
24	MG	A	2726	1/1	0.92	0.29	-	89,89,89,89	0
24	MG	A	2660	1/1	0.51	0.46	-	125,125,125,125	0
24	MG	A	2712	1/1	0.98	0.13	-	84,84,84,84	0
24	MG	A	2566	1/1	0.63	0.42	-	73,73,73,73	0
24	MG	A	2568	1/1	0.94	0.32	-	52,52,52,52	0
24	MG	A	2623	1/1	0.61	0.12	-	69,69,69,69	0
24	MG	A	2561	1/1	0.93	0.49	-	44,44,44,44	0
25	K	A	2683	1/1	0.68	0.12	-	111,111,111,111	0
24	MG	A	2746	1/1	0.60	0.20	-	69,69,69,69	0
24	MG	A	2281	1/1	0.93	0.77	-	72,72,72,72	0
24	MG	A	2694	1/1	0.69	0.16	-	94,94,94,94	0
24	MG	A	2721	1/1	0.45	0.17	-	88,88,88,88	0
24	MG	A	2578	1/1	0.81	0.34	-	53,53,53,53	0
24	MG	A	2761	1/1	0.93	0.93	-	86,86,86,86	0
24	MG	A	2637	1/1	0.70	0.20	-	70,70,70,70	0
24	MG	A	2760	1/1	0.83	0.50	-	73,73,73,73	0
24	MG	A	2769	1/1	0.92	0.50	-	85,85,85,85	0
24	MG	A	2622	1/1	0.97	0.12	-	66,66,66,66	0
24	MG	A	2754	1/1	0.65	0.65	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	2762	1/1	0.94	0.57	-	53,53,53,53	0
24	MG	A	2753	1/1	0.74	0.17	-	80,80,80,80	0
24	MG	A	2618	1/1	0.85	0.85	-	76,76,76,76	0
24	MG	A	2685	1/1	0.83	0.14	-	50,50,50,50	0
25	K	A	2680	1/1	0.43	0.35	-	115,115,115,115	0
24	MG	A	2763	1/1	0.96	0.54	-	56,56,56,56	0
24	MG	A	2715	1/1	0.69	0.41	-	74,74,74,74	0
24	MG	H	1142	1/1	0.85	0.31	-	72,72,72,72	0
24	MG	A	2629	1/1	0.87	0.17	-	53,53,53,53	0
24	MG	A	2564	1/1	0.71	0.20	-	94,94,94,94	0
24	MG	A	2741	1/1	0.84	0.70	-	86,86,86,86	0
24	MG	A	2701	1/1	0.88	0.16	-	86,86,86,86	0
24	MG	A	2620	1/1	0.77	0.17	-	60,60,60,60	0
24	MG	E	1153	1/1	0.95	0.38	-	57,57,57,57	0
24	MG	A	2717	1/1	0.60	0.46	-	83,83,83,83	0
24	MG	A	2727	1/1	0.93	0.36	-	70,70,70,70	0
24	MG	A	2737	1/1	0.79	1.23	-	100,100,100,100	0
24	MG	A	2758	1/1	0.35	0.40	-	93,93,93,93	0
24	MG	A	2277	1/1	0.92	0.82	-	69,69,69,69	0
24	MG	A	2652	1/1	0.72	0.19	-	66,66,66,66	0
24	MG	A	2695	1/1	0.82	0.21	-	76,76,76,76	0
24	MG	A	2551	1/1	0.79	0.19	-	60,60,60,60	0
24	MG	A	2554	1/1	0.61	0.43	-	78,78,78,78	0
24	MG	A	2627	1/1	0.81	0.13	-	63,63,63,63	0
24	MG	A	2558	1/1	0.84	0.85	-	58,58,58,58	0
24	MG	A	2700	1/1	0.96	0.12	-	61,61,61,61	0
24	MG	A	2714	1/1	0.72	0.42	-	91,91,91,91	0
24	MG	H	1141	1/1	0.96	0.43	-	70,70,70,70	0
24	MG	A	2278	1/1	0.91	0.27	-	72,72,72,72	0
24	MG	A	2642	1/1	0.99	0.25	-	51,51,51,51	0
24	MG	A	2752	1/1	0.79	0.21	-	67,67,67,67	0
24	MG	A	2553	1/1	0.66	1.03	-	94,94,94,94	0
24	MG	A	2667	1/1	0.90	0.22	-	108,108,108,108	0
24	MG	A	2765	1/1	0.93	0.56	-	61,61,61,61	0
24	MG	A	2743	1/1	0.51	0.52	-	84,84,84,84	0
25	K	A	2676	1/1	0.77	0.12	-	100,100,100,100	0
24	MG	A	2710	1/1	0.90	0.58	-	76,76,76,76	0
24	MG	A	2557	1/1	0.94	0.47	-	67,67,67,67	0
24	MG	A	2731	1/1	0.80	0.34	-	77,77,77,77	0
24	MG	A	2702	1/1	0.89	0.35	-	65,65,65,65	0
24	MG	A	2664	1/1	0.91	0.64	-	69,69,69,69	0
25	K	A	2670	1/1	0.65	0.26	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	2704	1/1	0.70	0.21	-	83,83,83,83	0
24	MG	A	2665	1/1	0.69	0.33	-	82,82,82,82	0
24	MG	A	2728	1/1	0.81	0.23	-	80,80,80,80	0
24	MG	A	2729	1/1	0.66	0.59	-	82,82,82,82	0
24	MG	A	2279	1/1	0.90	0.65	-	80,80,80,80	0
24	MG	A	2723	1/1	0.70	0.39	-	90,90,90,90	0
24	MG	A	2556	1/1	0.72	0.23	-	102,102,102,102	0
24	MG	A	2719	1/1	0.69	0.67	-	81,81,81,81	0
24	MG	A	2768	1/1	0.89	0.53	-	83,83,83,83	0
24	MG	A	2607	1/1	0.74	0.57	-	89,89,89,89	0
24	MG	A	2744	1/1	0.46	0.77	-	85,85,85,85	0
24	MG	L	1125	1/1	0.84	0.41	-	63,63,63,63	0
24	MG	A	2720	1/1	0.94	0.58	-	90,90,90,90	0
24	MG	A	2636	1/1	0.82	0.21	-	71,71,71,71	0
24	MG	A	2711	1/1	0.84	0.66	-	95,95,95,95	0
24	MG	A	2547	1/1	0.64	0.41	-	43,43,43,43	0
25	K	A	2671	1/1	0.90	0.22	-	90,90,90,90	0
24	MG	A	2583	1/1	0.94	0.54	-	59,59,59,59	0
24	MG	A	2595	1/1	0.92	0.37	-	61,61,61,61	0
25	K	A	2678	1/1	0.87	0.26	-	102,102,102,102	0
24	MG	A	2280	1/1	0.97	0.45	-	72,72,72,72	0
24	MG	A	2730	1/1	0.93	0.43	-	75,75,75,75	0
24	MG	A	2285	1/1	0.84	0.69	-	84,84,84,84	0
24	MG	A	2585	1/1	0.98	0.39	-	56,56,56,56	0
25	K	A	2677	1/1	0.75	0.34	-	135,135,135,135	0
24	MG	A	2686	1/1	0.65	0.31	-	87,87,87,87	0
24	MG	A	2621	1/1	0.86	0.19	-	68,68,68,68	0
24	MG	A	2724	1/1	0.77	0.92	-	84,84,84,84	0
24	MG	A	2593	1/1	0.72	0.36	-	89,89,89,89	0
24	MG	A	2275	1/1	0.80	0.71	-	69,69,69,69	0
24	MG	A	2663	1/1	0.89	0.37	-	70,70,70,70	0
24	MG	A	2603	1/1	0.97	0.89	-	63,63,63,63	0
24	MG	A	2590	1/1	0.94	0.24	-	80,80,80,80	0
24	MG	A	2750	1/1	0.29	0.94	-	97,97,97,97	0
24	MG	A	2653	1/1	0.84	0.19	-	68,68,68,68	0
24	MG	Z	1043	1/1	0.63	0.49	-	96,96,96,96	0
24	MG	A	2608	1/1	0.84	0.39	-	60,60,60,60	0
24	MG	A	2596	1/1	0.96	0.28	-	45,45,45,45	0
24	MG	A	2574	1/1	0.99	0.18	-	40,40,40,40	0
24	MG	A	2692	1/1	0.77	0.21	-	90,90,90,90	0
24	MG	A	2708	1/1	0.89	0.97	-	82,82,82,82	0
24	MG	A	2283	1/1	0.88	0.34	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	K	A	2682	1/1	0.89	0.37	-	117,117,117,117	0
24	MG	A	2734	1/1	0.57	0.23	-	92,92,92,92	0
24	MG	A	2582	1/1	0.97	0.43	-	56,56,56,56	0
24	MG	A	2274	1/1	0.92	0.59	-	62,62,62,62	0
24	MG	A	2638	1/1	0.94	0.19	-	68,68,68,68	0
24	MG	A	2576	1/1	0.81	0.36	-	75,75,75,75	0
24	MG	A	2552	1/1	0.90	0.36	-	46,46,46,46	0
24	MG	A	2634	1/1	0.74	0.18	-	66,66,66,66	0
24	MG	A	2592	1/1	0.54	0.13	-	77,77,77,77	0
24	MG	A	2693	1/1	0.86	0.44	-	75,75,75,75	0
24	MG	A	2276	1/1	0.93	0.39	-	74,74,74,74	0
24	MG	A	2703	1/1	0.30	0.67	-	87,87,87,87	0
25	K	A	2681	1/1	0.67	0.18	-	118,118,118,118	0
24	MG	A	2691	1/1	0.80	0.72	-	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.