



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 09:51 AM BST

PDB ID : 1K9M  
Title : Co-crystal structure of tylosin bound to the 50S ribosomal subunit of *Haloarcula marismortui*  
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2001-10-29  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

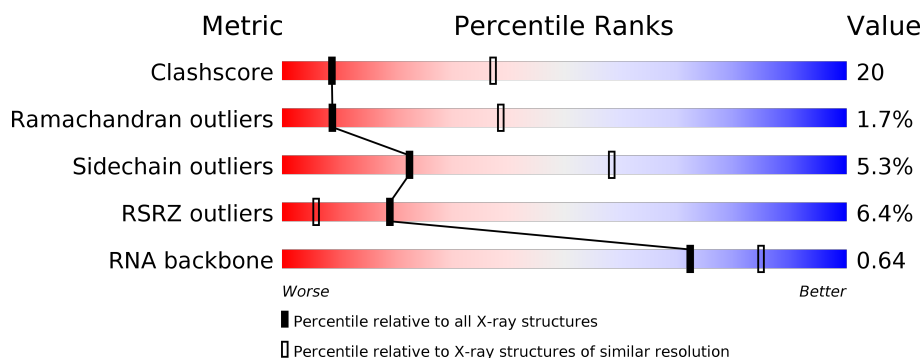
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div>2%</div> <div> <div>50%</div> <div>36%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>4%</div> <div> <div>45%</div> <div>39%</div> <div>10%</div> <div>6%</div> </div> </div>
3	C	239	<div> <div>7%</div> <div> <div>54%</div> <div>38%</div> <div>7%</div> </div> </div>
4	D	337	<div> <div>50%</div> <div>44%</div> <div>6%</div> </div>
5	E	246	<div> <div>%</div> <div> <div>61%</div> <div>34%</div> <div>6%</div> </div> </div>
6	F	176	<div> <div>23%</div> <div> <div>27%</div> <div>44%</div> <div>7%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	NA	A	8356	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	J	8322	-	-	-	X
33	NA	S	8386	-	-	-	X
33	NA	T	8312	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	A	8505	-	-	-	X
34	CL	O	8507	-	-	X	-
36	CD	4	8404	-	-	-	X
36	CD	V	8401	-	-	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	? 3377779

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O		0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.



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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

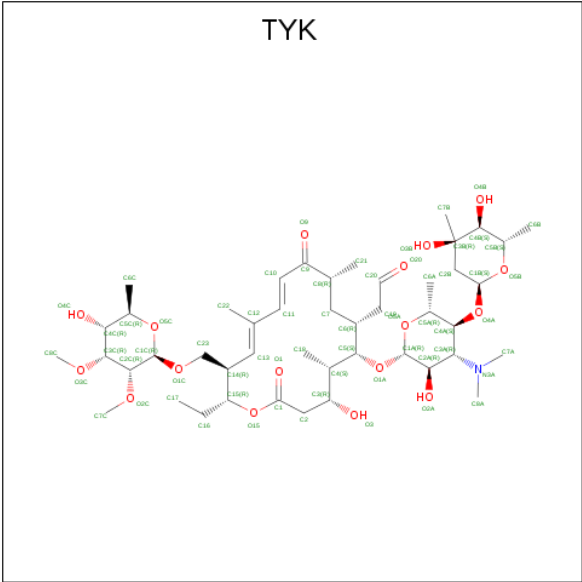
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is TYLOSIN (three-letter code: TYK) (formula: C<sub>46</sub>H<sub>77</sub>NO<sub>17</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total	Mg	0	0
			1	1		
32	D	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	111	Total	Mg	0	0
			111	111		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	A	72	Total Na 72 72	0	0
33	T	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	4	Total Cl 4 4	0	0
34	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	8	Total Cl 8 8	0	0
34	4	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5921	Total 5921	O 5921	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	146	Total 146	O 146	0	0
37	E	174	Total 174	O 174	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	26	Total 26	O 26	0	0
37	I	22	Total 22	O 22	0	0
37	J	79	Total 79	O 79	0	0
37	K	54	Total 54	O 54	0	0
37	L	60	Total 60	O 60	0	0
37	M	84	Total 84	O 84	0	0
37	N	127	Total 127	O 127	0	0
37	O	64	Total 64	O 64	0	0
37	P	42	Total 42	O 42	0	0
37	Q	66	Total 66	O 66	0	0
37	R	53	Total 53	O 53	0	0
37	S	84	Total 84	O 84	0	0
37	T	34	Total 34	O 34	0	0
37	U	39	Total 39	O 39	0	0
37	V	26	Total 26	O 26	0	0
37	W	12	Total 12	O 12	0	0
37	X	70	Total 70	O 70	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	96	Total 96	O 96	0	0
37	1	37	Total 37	O 37	0	0

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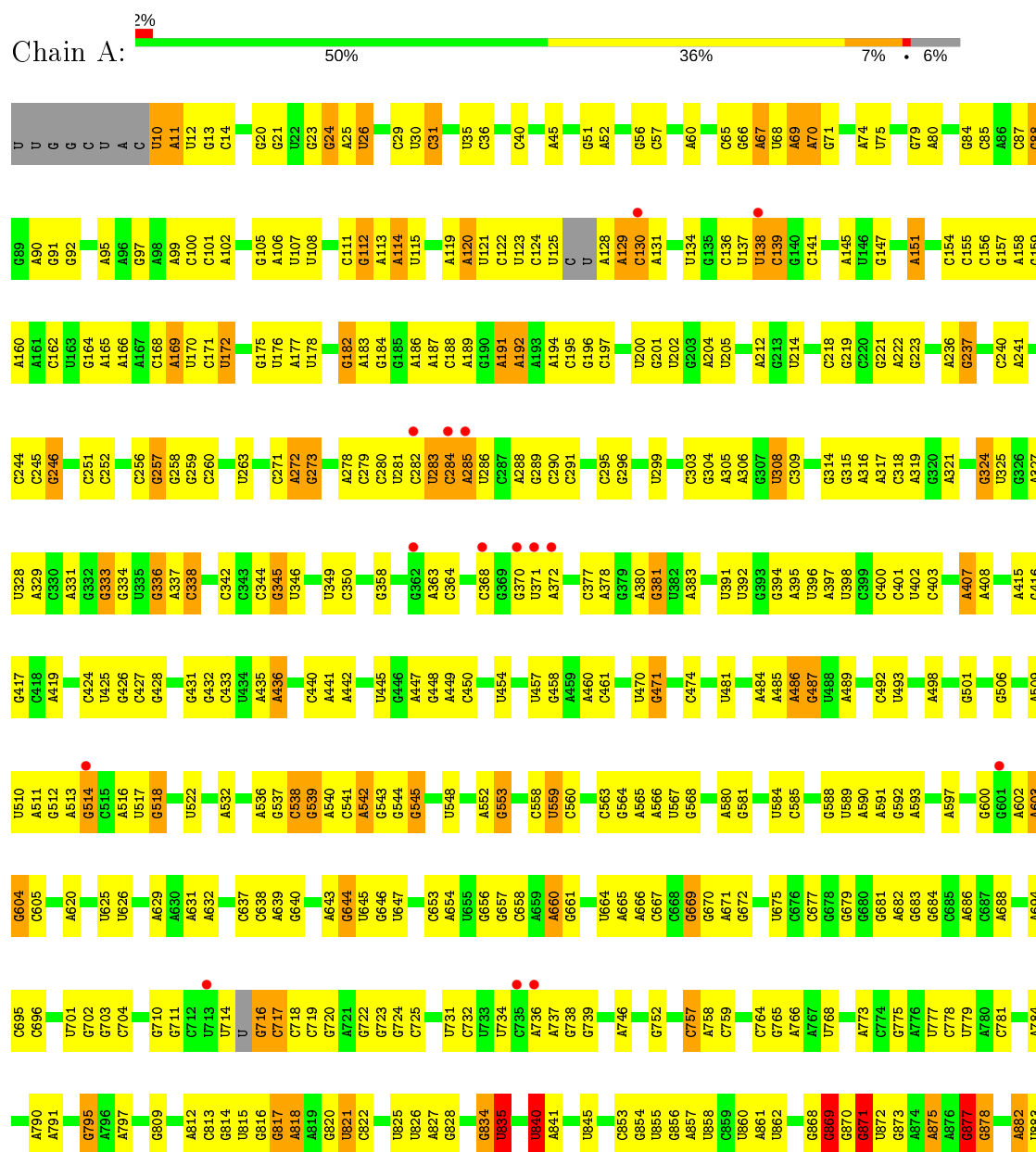
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	56	Total 56	O 56	0	0
37	3	43	Total 43	O 43	0	0
37	4	72	Total 72	O 72	0	0

### 3 Residue-property plots

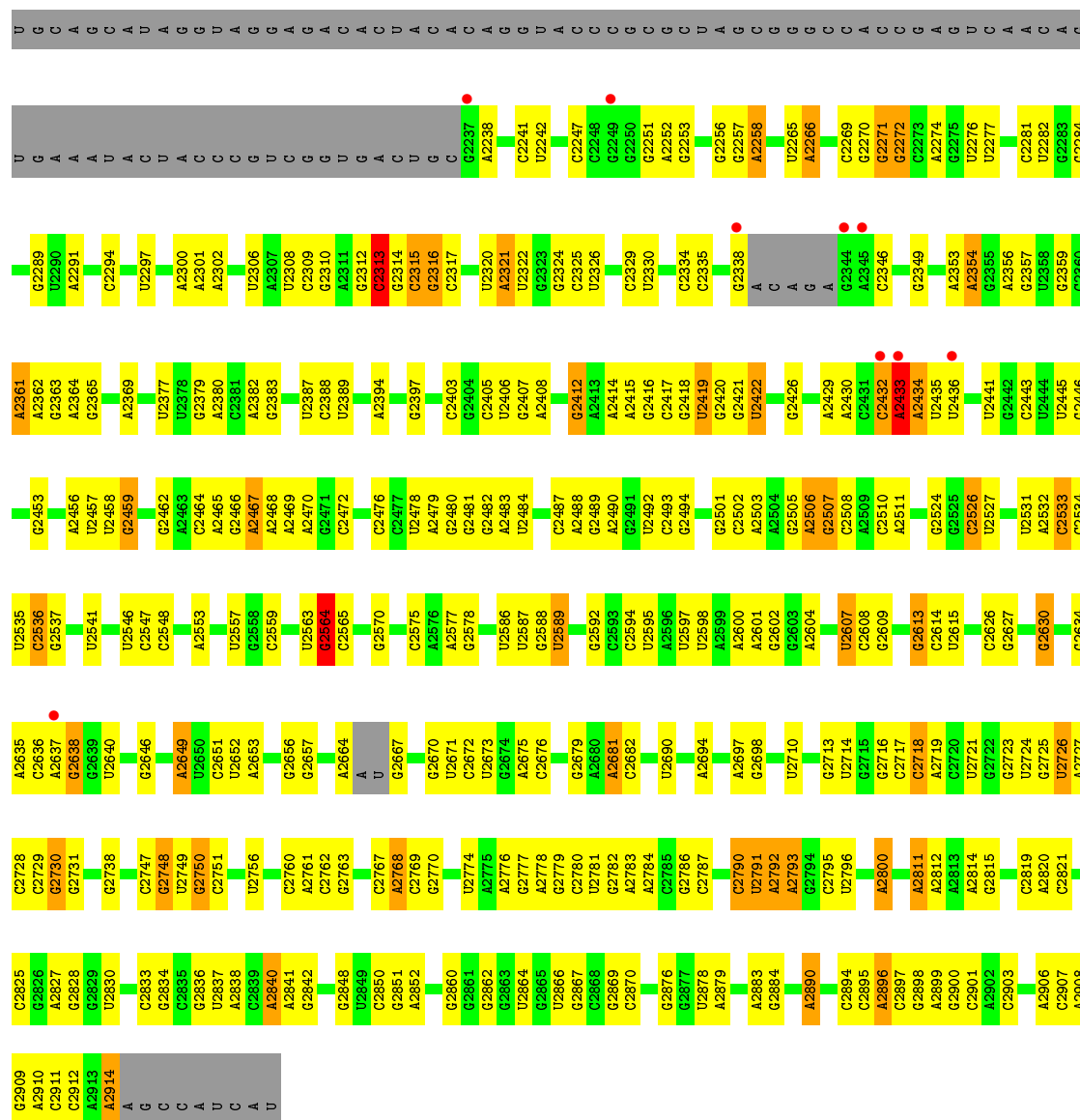
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 23S rRNA

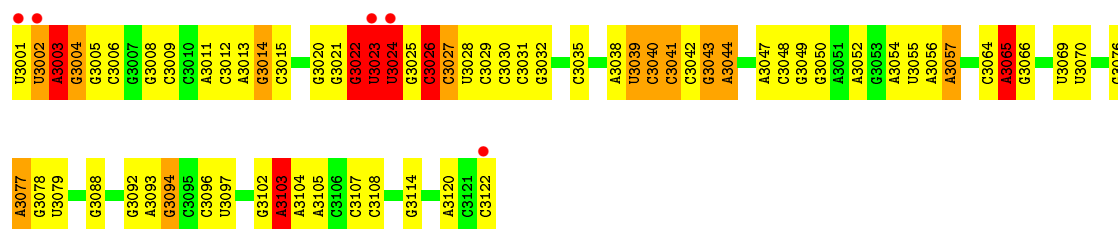
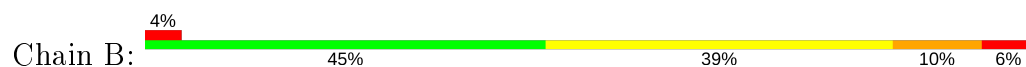






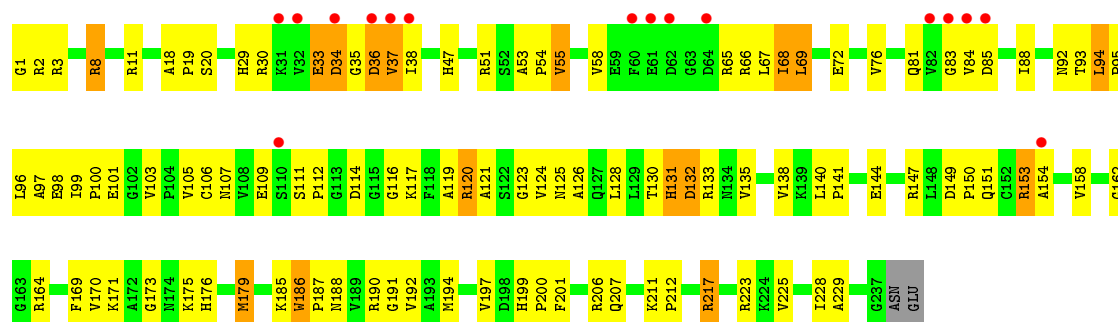


- Molecule 2: 5S RRNA



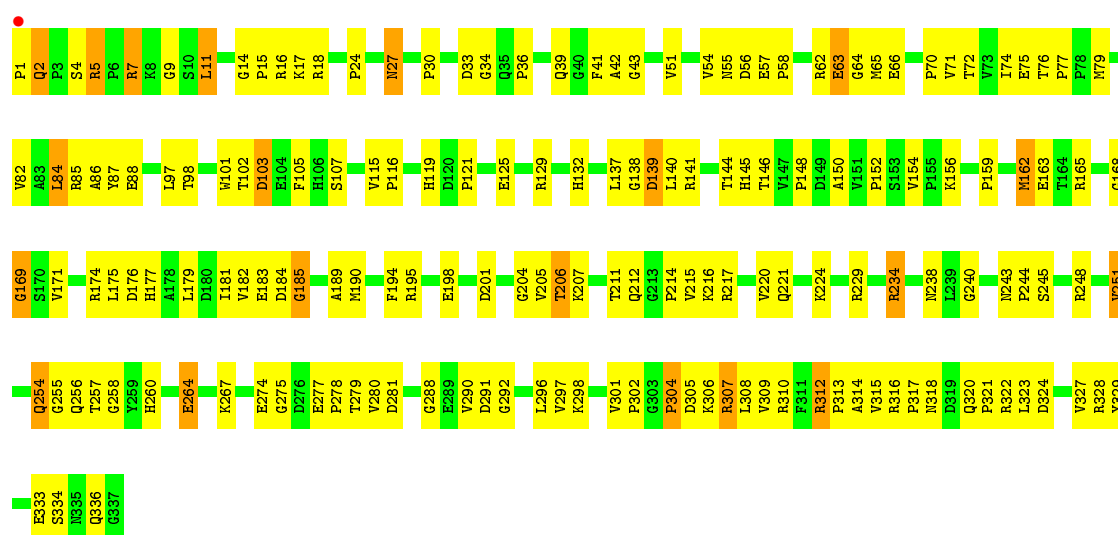
- Molecule 3: RIBOSOMAL PROTEIN L2





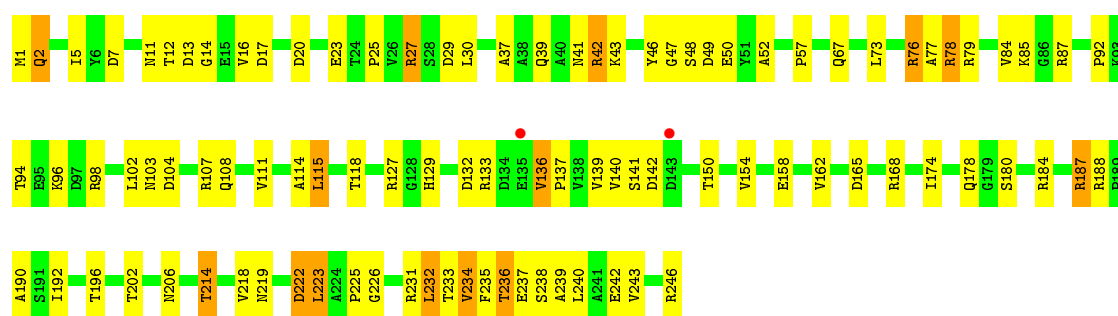
### • Molecule 4: RIBOSOMAL PROTEIN L3

Chain D: 50% 44% 6%



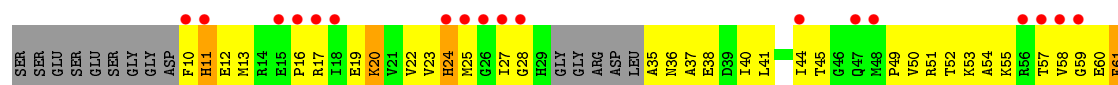
### • Molecule 5: RIBOSOMAL PROTEIN L4

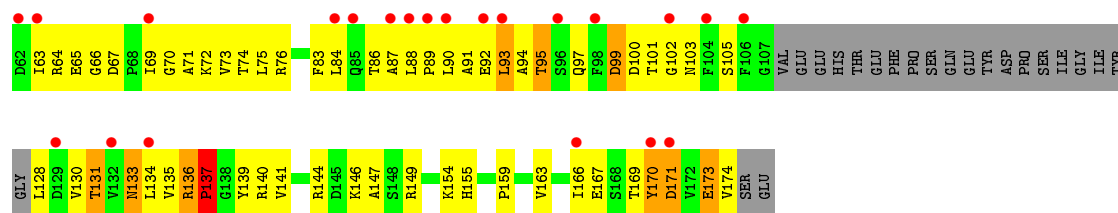
Chain E: 61% 34% 6%



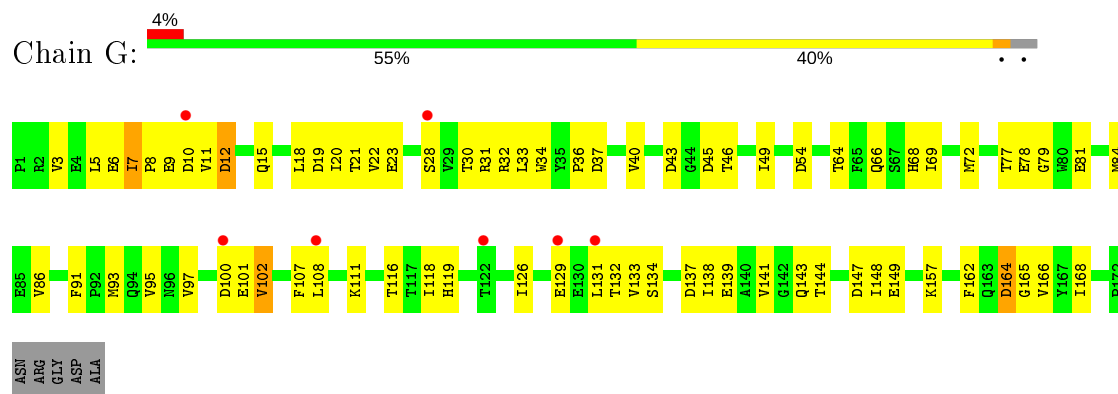
### • Molecule 6: RIBOSOMAL PROTEIN L5

Chain F: 27% 44% 7% 20%

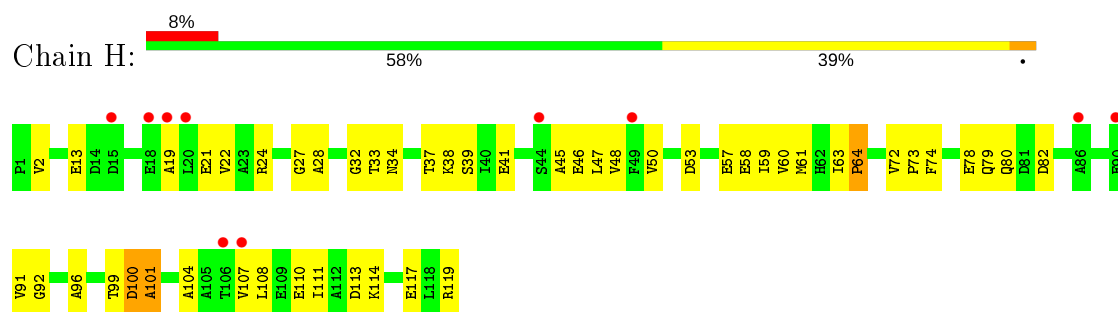




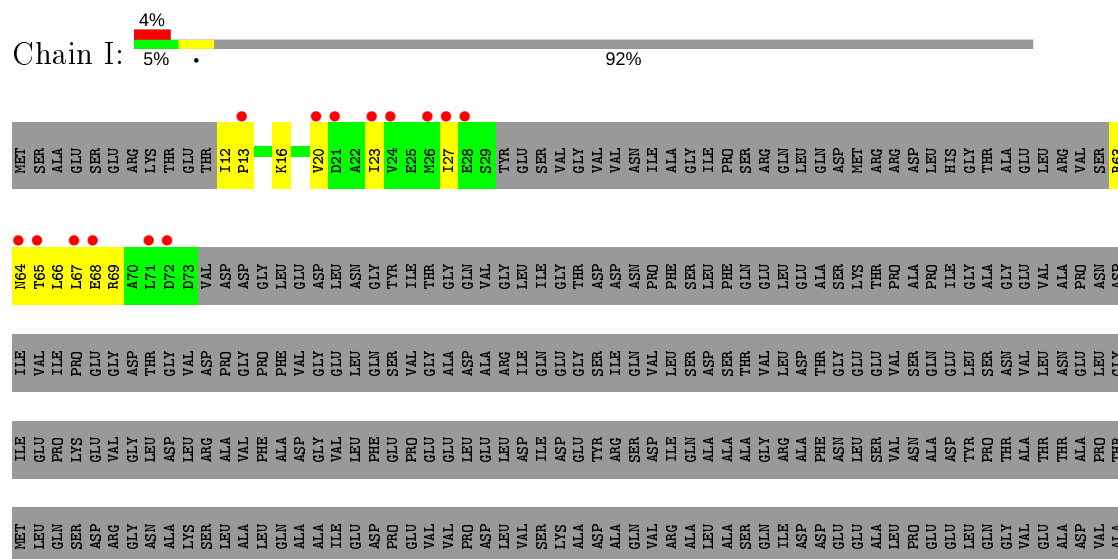
- Molecule 7: RIBOSOMAL PROTEIN L6



- Molecule 8: RIBOSOMAL PROTEIN L7AE



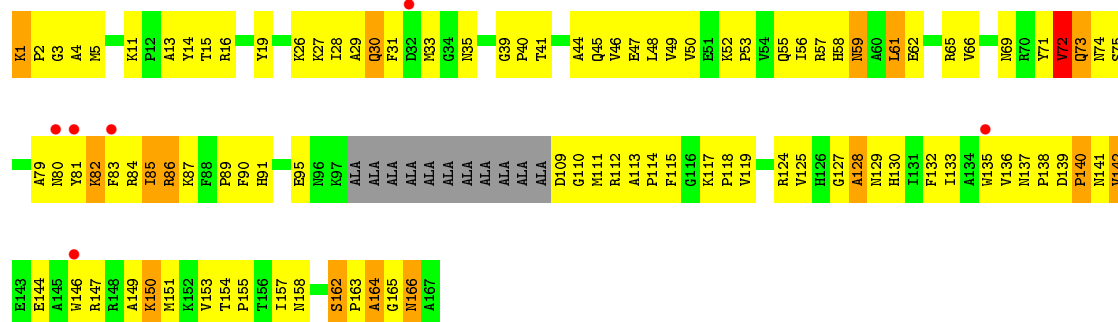
- Molecule 9: RIBOSOMAL PROTEIN L10



THR  
GLU  
GLU  
GLU  
PHE  
THR  
ASP  
ASP  
GLN  
ASP  
ASP  
ASP  
ASP  
THR  
ALA  
SER  
GLU  
ASP  
ASP  
ALA  
ASP  
ALA  
ASP  
ASP  
ASP  
ALA  
ALA  
GLU  
GLU  
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ASP  
ALA  
ALA  
LEU  
GLY  
MET  
PHE

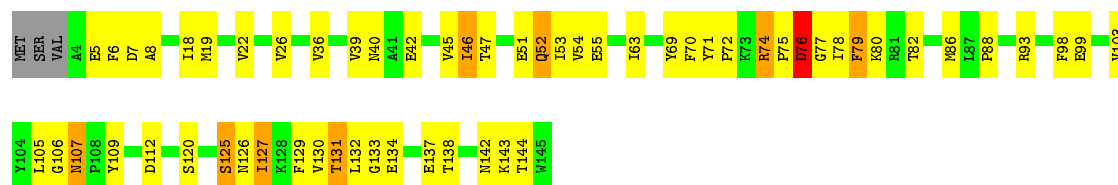
• Molecule 10: RIBOSOMAL PROTEIN L10E

Chain J: 4% 33% 51% 9% 7%



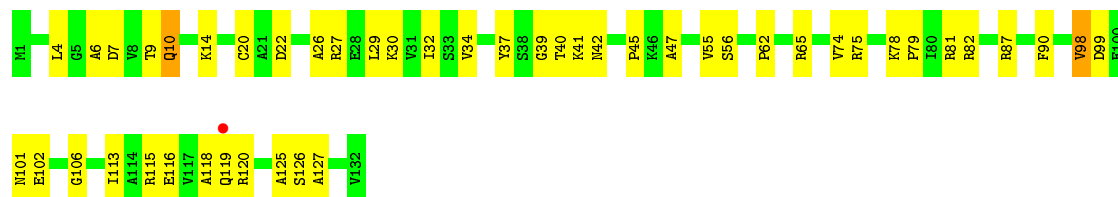
• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 57% 34% 6%



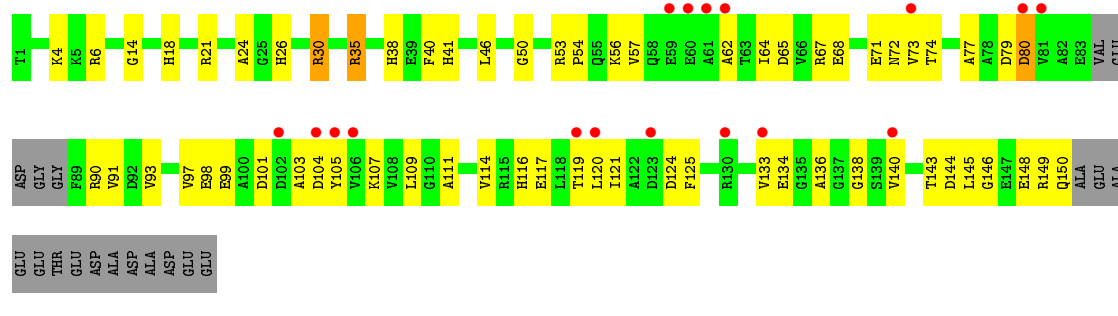
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 64% 34% 2%

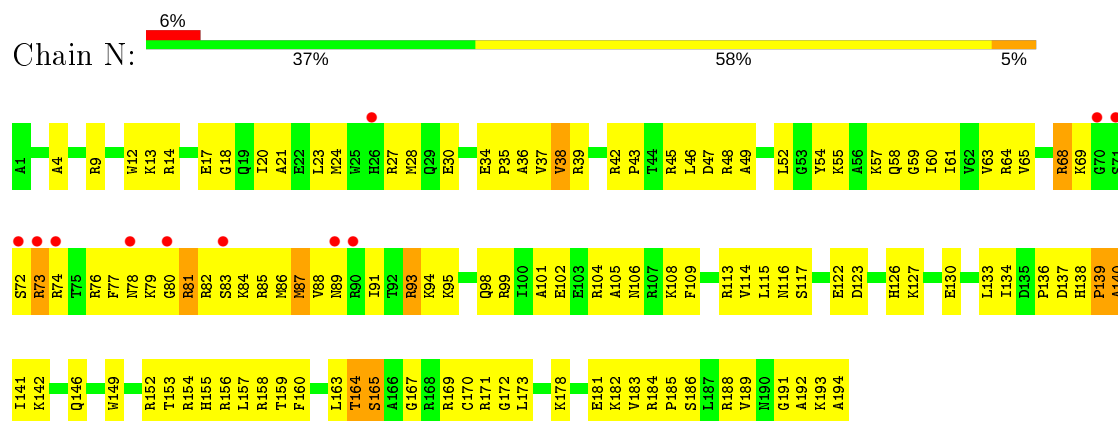


• Molecule 13: RIBOSOMAL PROTEIN L15

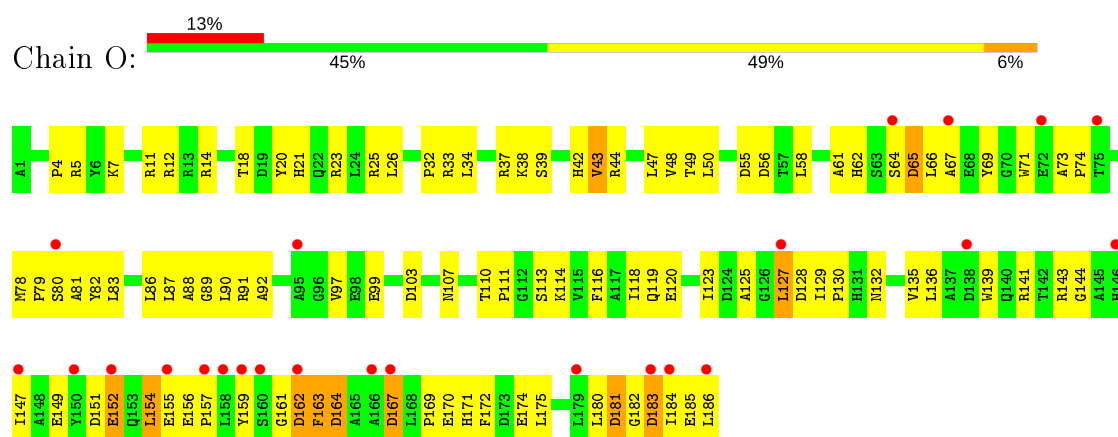
Chain M: 10% 50% 37% 12%



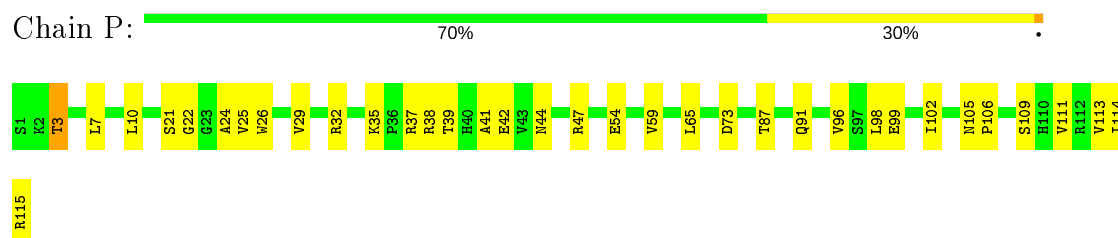
- Molecule 14: RIBOSOMAL PROTEIN L15E



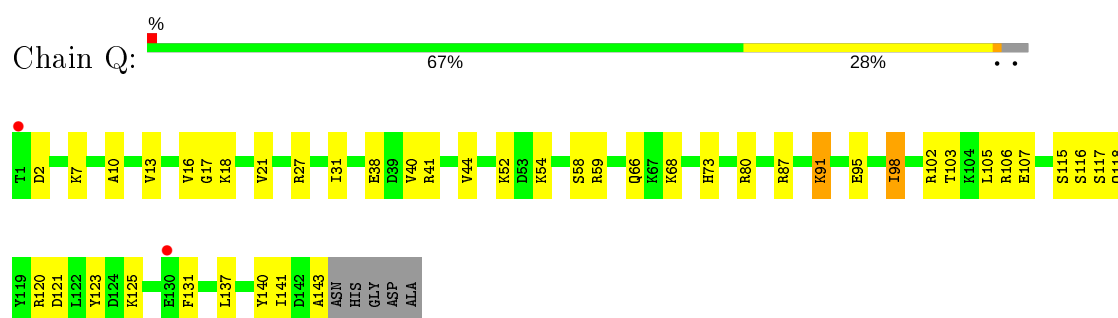
- Molecule 15: RIBOSOMAL PROTEIN L18



- Molecule 16: RIBOSOMAL PROTEIN L18E



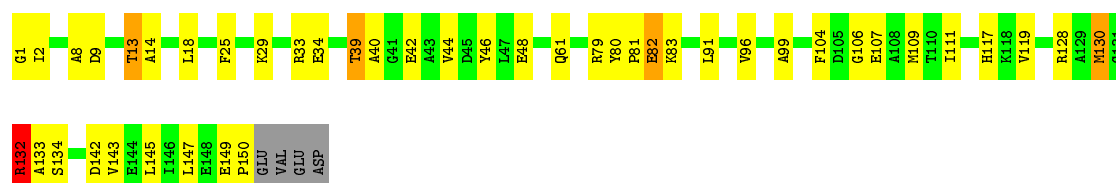
- Molecule 17: RIBOSOMAL PROTEIN L19E



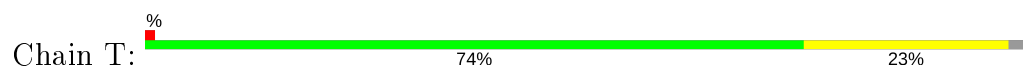
- Molecule 18: RIBOSOMAL PROTEIN L21E



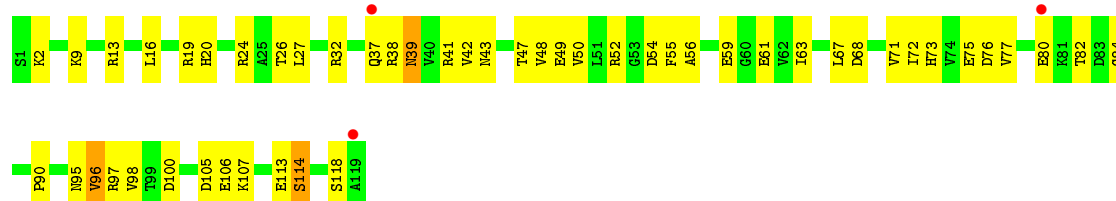
• Molecule 19: RIBOSOMAL PROTEIN L22



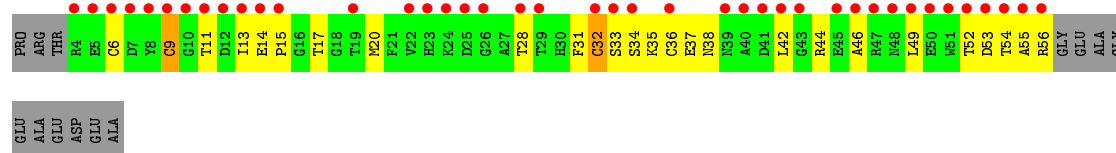
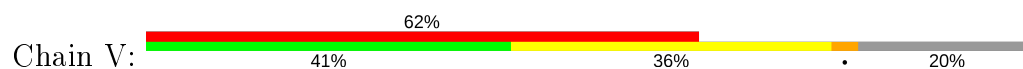
• Molecule 20: RIBOSOMAL PROTEIN L23



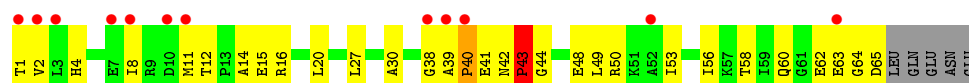
• Molecule 21: RIBOSOMAL PROTEIN L24



• Molecule 22: RIBOSOMAL PROTEIN L24E

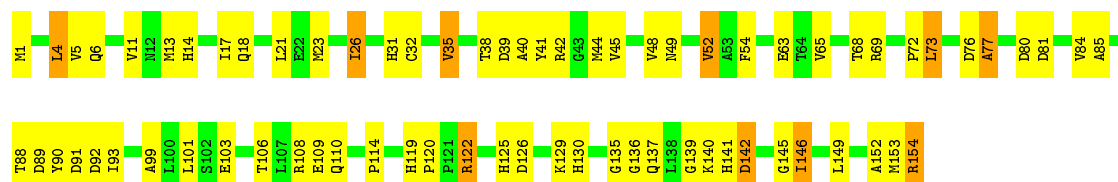


• Molecule 23: RIBOSOMAL PROTEIN L29



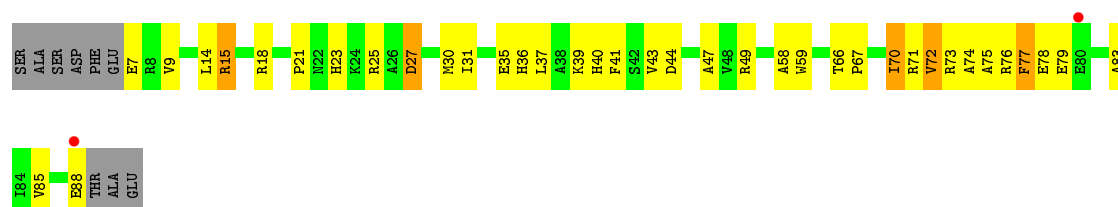
- Molecule 24: RIBOSOMAL PROTEIN L30

Chain X: 

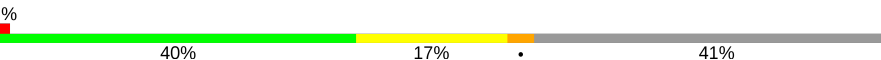


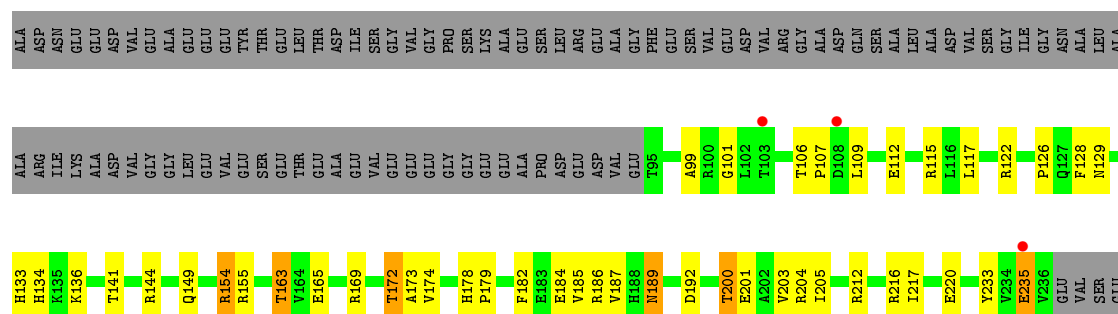
- Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y: 



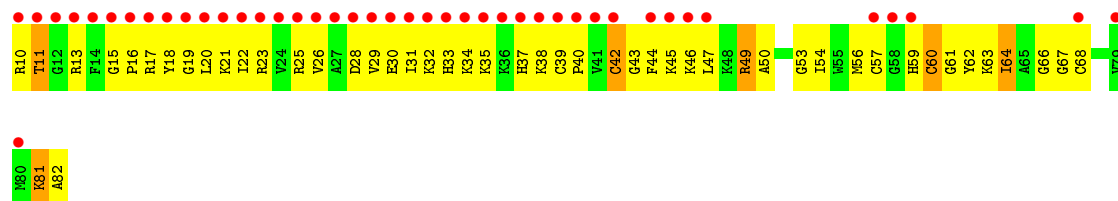
- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z: 



- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1: 



- Molecule 28: RIBOSOMAL PROTEIN L37E

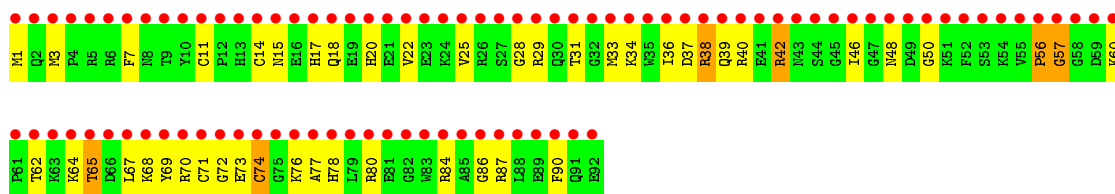
Chain 2: 



- Molecule 29: RIBOSOMAL PROTEIN L39E



- Molecule 30: RIBOSOMAL PROTEIN L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 49.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-3.00) 92.3 (49.92-2.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.262 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TYK, NA, K, CL, CD

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	0.59	13/66076 (0.0%)	0.77	38/103052 (0.0%)
2	B	0.89	17/2905 (0.6%)	0.91	16/4528 (0.4%)
3	C	0.57	3/1787 (0.2%)	0.78	1/2409 (0.0%)
4	D	0.48	0/2689	0.73	0/3652
5	E	0.51	0/1883	0.74	0/2551
6	F	0.41	0/1111	0.65	0/1498
7	G	0.44	0/1382	0.63	0/1880
8	H	0.43	0/896	0.65	0/1219
9	I	0.48	0/241	0.60	0/324
10	J	0.51	0/1246	0.80	2/1686 (0.1%)
11	K	0.49	0/1135	0.68	0/1530
12	L	0.48	0/1003	0.75	0/1351
13	M	0.46	0/1126	0.74	0/1504
14	N	0.59	0/1633	0.83	2/2180 (0.1%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.50	0/873	0.73	0/1181
17	Q	0.48	0/1143	0.64	0/1521
18	R	0.49	0/748	0.76	0/1005
19	S	0.63	1/1172 (0.1%)	0.82	2/1578 (0.1%)
20	T	0.46	0/648	0.68	1/875 (0.1%)
21	U	0.44	0/957	0.72	0/1289
22	V	0.70	0/417	0.81	1/562 (0.2%)
23	W	0.41	0/502	0.62	0/675
24	X	0.49	0/1218	0.73	0/1655
25	Y	0.48	0/664	0.68	0/895
26	Z	0.47	0/1146	0.72	0/1536
27	1	0.74	0/575	0.81	0/763
28	2	0.47	0/437	0.80	0/578
29	3	0.45	0/398	0.59	0/527
30	4	0.95	0/771	0.80	0/1024
All	All	0.58	34/98255 (0.0%)	0.76	63/147027 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	150
2	B	0	4
All	All	1	154

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2104	C	O5'-C5'	-12.61	1.22	1.42
2	B	3023	U	C2'-O2'	12.28	1.57	1.41
1	A	2103	A	C6-N1	9.66	1.42	1.35
2	B	3025	G	O3'-P	9.21	1.72	1.61
1	A	2103	A	C5-C6	8.57	1.48	1.41
1	A	2103	A	N7-C5	8.49	1.44	1.39
2	B	3025	G	C4'-O4'	8.46	1.56	1.45
2	B	3026	C	P-O5'	-8.45	1.51	1.59
2	B	3026	C	P-OP2	-8.37	1.34	1.49
1	A	2106	C	O3'-P	-8.18	1.51	1.61
2	B	3024	U	P-OP2	-7.80	1.35	1.49
2	B	3025	G	P-OP2	-7.66	1.35	1.49
2	B	3025	G	C3'-O3'	-6.95	1.32	1.42
2	B	3023	U	O5'-C5'	6.91	1.55	1.44
1	A	2103	A	C6-N6	6.88	1.39	1.33
3	C	186	TRP	CA-CB	-6.75	1.39	1.53
2	B	3025	G	N9-C4	-6.75	1.32	1.38
1	A	1206	U	P-OP2	6.34	1.59	1.49
2	B	3025	G	C2'-O2'	6.31	1.49	1.41
19	S	132	ARG	CA-CB	-5.98	1.40	1.53
3	C	186	TRP	C-O	-5.89	1.12	1.23
1	A	2105	C	O3'-P	5.88	1.68	1.61
3	C	186	TRP	N-CA	5.76	1.57	1.46
2	B	3022	G	C5'-C4'	5.67	1.58	1.51
2	B	3025	G	C2'-C1'	5.64	1.59	1.53
1	A	2433	A	C5-C6	5.64	1.46	1.41
1	A	2099	G	C3'-O3'	5.48	1.49	1.42
2	B	3024	U	N1-C2	-5.37	1.33	1.38
1	A	2106	C	N1-C2	5.20	1.45	1.40
1	A	2104	C	O3'-P	-5.15	1.54	1.61
1	A	2103	A	N3-C4	5.15	1.38	1.34
2	B	3023	U	C3'-C2'	5.14	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3024	U	O4'-C1'	5.05	1.48	1.41
2	B	3023	U	O3'-P	-5.03	1.55	1.61

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.07	63.25	105.20
1	A	1164	U	OP2-P-O3'	-17.80	66.05	105.20
1	A	1165	G	O5'-P-OP1	-13.80	93.28	105.70
1	A	2104	C	O5'-P-OP1	-13.33	93.70	105.70
1	A	2103	A	C5'-C4'-O4'	10.96	122.25	109.10
2	B	3026	C	O5'-P-OP2	-10.22	96.50	105.70
1	A	1563	G	C2'-C3'-O3'	9.62	130.66	109.50
1	A	1942	A	C5'-C4'-C3'	8.40	129.45	116.00
1	A	1165	G	O5'-P-OP2	-8.00	98.50	105.70
1	A	1942	A	C5'-C4'-O4'	7.69	118.33	109.10
2	B	3026	C	C5'-C4'-O4'	7.20	117.74	109.10
1	A	2103	A	OP2-P-O3'	7.13	120.88	105.20
2	B	3024	U	O5'-P-OP2	7.09	119.21	110.70
22	V	36	CYS	CA-CB-SG	-6.98	101.44	114.00
1	A	1979	G	C2'-C3'-O3'	6.77	124.53	113.70
2	B	3025	G	O3'-P-O5'	6.52	116.38	104.00
2	B	3026	C	O5'-P-OP1	-6.40	99.94	105.70
1	A	2313	C	C5'-C4'-O4'	6.33	116.69	109.10
1	A	2103	A	O5'-P-OP1	-6.28	100.05	105.70
19	S	130	MET	CB-CG-SD	6.26	131.17	112.40
2	B	3103	A	C5'-C4'-O4'	6.19	116.53	109.10
1	A	1165	G	OP1-P-OP2	6.19	128.89	119.60
1	A	2103	A	O4'-C1'-N9	6.13	113.10	108.20
10	J	74	ASN	N-CA-C	-6.07	94.62	111.00
2	B	3039	U	N1-C1'-C2'	6.07	121.89	114.00
2	B	3026	C	OP1-P-OP2	5.92	128.47	119.60
1	A	2099	G	OP2-P-O3'	5.90	118.19	105.20
1	A	2106	C	N1-C1'-C2'	-5.88	105.54	112.00
1	A	2419	U	N1-C1'-C2'	5.85	121.61	114.00
2	B	3024	U	C4'-C3'-O3'	5.77	124.55	113.00
2	B	3003	A	C4'-C3'-C2'	-5.76	96.84	102.60
1	A	1504	A	C1'-O4'-C4'	-5.75	105.30	109.90
1	A	1721	C	N1-C1'-C2'	5.57	121.24	114.00
1	A	324	G	N9-C1'-C2'	-5.56	105.88	112.00
14	N	139	PRO	N-CA-C	-5.53	97.72	112.10
1	A	1819	G	C5'-C4'-C3'	5.50	124.81	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	A	C2'-C3'-O3'	5.50	122.50	113.70
1	A	2103	A	N9-C1'-C2'	-5.43	106.02	112.00
1	A	2432	C	N1-C1'-C2'	5.41	121.03	114.00
1	A	1592	G	N9-C1'-C2'	5.41	121.03	114.00
1	A	2122	C	OP2-P-O3'	5.38	117.05	105.20
1	A	871	G	C5'-C4'-O4'	-5.33	102.70	109.10
1	A	1738	C	O4'-C4'-C3'	-5.33	98.67	104.00
2	B	3026	C	O3'-P-O5'	5.33	114.13	104.00
20	T	27	ALA	N-CA-C	-5.32	96.63	111.00
2	B	3023	U	P-O5'-C5'	5.30	129.38	120.90
1	A	1842	A	N9-C1'-C2'	5.28	120.87	114.00
1	A	1971	G	O4'-C1'-N9	5.27	112.41	108.20
1	A	2726	U	N1-C1'-C2'	5.25	120.83	114.00
1	A	1062	U	N1-C1'-C2'	-5.23	106.25	112.00
14	N	73	ARG	N-CA-C	-5.23	96.89	111.00
1	A	1942	A	C1'-O4'-C4'	-5.21	105.73	109.90
2	B	3025	G	C1'-C2'-O2'	-5.20	95.01	110.60
19	S	130	MET	CG-SD-CE	5.19	108.51	100.20
1	A	1121	G	N9-C1'-C2'	-5.19	106.29	112.00
2	B	3027	C	O5'-P-OP1	-5.15	101.06	105.70
3	C	186	TRP	N-CA-C	-5.11	97.20	111.00
1	A	2034	U	N1-C1'-C2'	-5.09	106.40	112.00
1	A	2315	C	C5'-C4'-C3'	-5.06	107.90	116.00
2	B	3004	G	O5'-P-OP1	-5.05	101.16	105.70
1	A	2316	G	C5'-C4'-C3'	-5.05	107.92	116.00
2	B	3025	G	C1'-O4'-C4'	-5.03	105.88	109.90
10	J	110	GLY	N-CA-C	-5.01	100.58	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (154) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	G	Sidechain
1	A	1039	G	Sidechain
1	A	1053	G	Sidechain
1	A	1072	G	Sidechain
1	A	1119	G	Sidechain
1	A	112	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1134	G	Sidechain
1	A	1140	C	Sidechain
1	A	1206	U	Sidechain
1	A	1229	C	Sidechain
1	A	1264	U	Sidechain
1	A	1309	U	Sidechain
1	A	1336	U	Sidechain
1	A	1348	A	Sidechain
1	A	1350	U	Sidechain
1	A	1376	G	Sidechain
1	A	138	U	Sidechain
1	A	1400	C	Sidechain
1	A	1408	U	Sidechain
1	A	1417	G	Sidechain
1	A	1423	C	Sidechain
1	A	1430	G	Sidechain
1	A	1433	G	Sidechain
1	A	1447	U	Sidechain
1	A	1452	G	Sidechain
1	A	1458	A	Sidechain
1	A	1470	A	Sidechain
1	A	1487	A	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1535	G	Sidechain
1	A	1595	G	Sidechain
1	A	1614	G	Sidechain
1	A	162	C	Sidechain
1	A	1647	G	Sidechain
1	A	1677	U	Sidechain
1	A	1681	G	Sidechain
1	A	1685	A	Sidechain
1	A	1688	G	Sidechain
1	A	170	U	Sidechain
1	A	171	C	Sidechain
1	A	172	U	Sidechain
1	A	1736	A	Sidechain
1	A	1747	A	Sidechain
1	A	1748	U	Sidechain
1	A	1758	U	Sidechain
1	A	176	U	Sidechain
1	A	1819	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	182	G	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1846	U	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1878	G	Sidechain
1	A	1879	U	Sidechain
1	A	1908	G	Sidechain
1	A	191	A	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	1993	C	Sidechain
1	A	2001	G	Sidechain
1	A	2035	C	Sidechain
1	A	2059	U	Sidechain
1	A	2073	G	Sidechain
1	A	2103	A	Sidechain
1	A	2106	C	Sidechain
1	A	2110	G	Sidechain
1	A	2127	U	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	2266	A	Sidechain
1	A	2294	C	Sidechain
1	A	2297	U	Sidechain
1	A	2308	U	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2364	A	Sidechain
1	A	24	G	Sidechain
1	A	2412	G	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2436	U	Sidechain
1	A	2441	U	Sidechain
1	A	2458	U	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2506	A	Sidechain
1	A	2557	U	Sidechain
1	A	2564	G	Sidechain
1	A	257	G	Sidechain
1	A	2575	C	Sidechain
1	A	2597	U	Sidechain
1	A	26	U	Sidechain
1	A	2607	U	Sidechain
1	A	2615	U	Sidechain
1	A	2630	G	Sidechain
1	A	2640	U	Sidechain
1	A	2673	U	Sidechain
1	A	2675	A	Sidechain
1	A	2730	G	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2800	A	Sidechain
1	A	2811	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	2864	U	Sidechain
1	A	333	G	Sidechain
1	A	398	U	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	471	G	Sidechain
1	A	481	U	Sidechain
1	A	486	A	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	552	A	Sidechain
1	A	589	U	Sidechain
1	A	626	U	Sidechain
1	A	669	G	Sidechain
1	A	720	G	Sidechain
1	A	722	G	Sidechain
1	A	723	G	Sidechain
1	A	757	C	Sidechain
1	A	768	U	Sidechain
1	A	773	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	781	C	Sidechain
1	A	784	A	Sidechain
1	A	791	A	Sidechain
1	A	795	G	Sidechain
1	A	815	U	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	835	U	Sidechain
1	A	840	U	Sidechain
1	A	855	U	Sidechain
1	A	869	G	Sidechain
1	A	871	G	Sidechain
1	A	877	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	898	G	Sidechain
1	A	919	U	Sidechain
1	A	954	U	Sidechain
2	B	3005	G	Sidechain
2	B	3065	A	Sidechain
2	B	3094	G	Sidechain
2	B	3120	A	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29798	1175	0
2	B	2600	0	1326	79	0
3	C	1754	0	1763	134	0
4	D	2624	0	2533	189	0
5	E	1858	0	1816	121	0
6	F	1094	0	1085	137	0
7	G	1357	0	1266	76	0
8	H	885	0	854	62	0
9	I	240	0	231	20	0
10	J	1215	0	1215	160	0
11	K	1119	0	1098	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	993	0	1027	53	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	173	0
15	O	1444	0	1401	134	0
16	P	864	0	873	38	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	24	0
19	S	1149	0	1122	57	0
20	T	641	0	605	22	0
21	U	949	0	923	56	0
22	V	410	0	368	37	0
23	W	499	0	511	31	0
24	X	1195	0	1137	98	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	76	0
28	2	430	0	426	26	0
29	3	393	0	406	26	0
30	4	755	0	732	59	0
31	A	64	0	76	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	72	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	4	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	2	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	10	0
37	2	56	0	0	4	0
37	3	43	0	0	4	0
37	4	72	0	0	4	0
37	A	5921	0	0	271	0
37	B	142	0	0	14	0
37	C	126	0	0	20	0
37	D	146	0	0	27	0
37	E	174	0	0	34	0
37	F	51	0	0	19	0
37	G	42	0	0	9	0
37	H	26	0	0	11	0
37	I	22	0	0	5	0
37	J	79	0	0	19	0
37	K	54	0	0	5	0
37	L	60	0	0	11	0
37	M	84	0	0	18	0
37	N	127	0	0	29	0
37	O	64	0	0	18	0
37	P	42	0	0	12	0
37	Q	66	0	0	5	0
37	R	53	0	0	3	0
37	S	84	0	0	7	0
37	T	34	0	0	4	0
37	U	39	0	0	4	0
37	V	26	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	W	12	0	0	1	0
37	X	70	0	0	10	0
37	Y	29	0	0	12	0
37	Z	96	0	0	17	0
All	All	98593	0	59582	3067	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 20.

All (3067) 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:1160:G:H5'	1:A:1161:A:H5'	1.25	1.15
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.30	1.13
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.13
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.14	1.10
14:N:87:MET:CG	30:4:46:ILE:HG21	1.84	1.08
6:F:25:MET:HE2	6:F:41:LEU:HG	1.36	1.07
5:E:236:THR:HG22	5:E:239:ALA:H	1.11	1.07
1:A:871:G:H8	1:A:871:G:H5'	1.17	1.07
1:A:1134:G:H4'	10:J:151:MET:HE1	1.36	1.05
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.33	1.05
14:N:164:THR:HG22	14:N:167:GLY:H	1.23	1.04
14:N:87:MET:HG2	30:4:46:ILE:CG2	1.88	1.03
4:D:62:ARG:HA	4:D:65:MET:HE3	1.40	1.03
4:D:140:LEU:HA	37:D:8577:HOH:O	1.59	1.02
1:A:871:G:C8	1:A:871:G:H5'	1.94	1.02
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.38	1.01
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.40	1.01
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.43	1.01
1:A:962:C:H1'	15:O:5:ARG:NH1	1.75	1.01
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.41	1.01
2:B:3056:A:H2'	2:B:3057:A:H5''	1.43	1.00
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.83	1.00
14:N:64:ARG:HD2	37:N:8584:HOH:O	1.59	1.00
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.27	1.00
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.44	0.99
11:K:76:ASP:HA	37:K:8563:HOH:O	1.62	0.99
1:A:2122:C:OP2	37:A:6559:HOH:O	1.80	0.99
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.43	0.99
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.45	0.98
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.44	0.98
1:A:856:G:H2'	37:A:5402:HOH:O	1.65	0.97
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.46	0.97
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.47	0.97
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.47	0.97
37:A:6752:HOH:O	15:O:4:PRO:HD2	1.65	0.97
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.63	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.47	0.97
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.78	0.96
1:A:542:A:H8	1:A:542:A:H5'	1.28	0.96
10:J:165:GLY:HA3	37:J:8399:HOH:O	1.64	0.96
1:A:541:C:H2'	1:A:542:A:H5''	1.44	0.96
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.79	0.96
1:A:2717:C:H2'	1:A:2718:C:H5''	1.47	0.96
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.45	0.96
17:Q:115:SER:H	17:Q:118:GLN:HE21	0.97	0.95
2:B:3076:G:H3'	2:B:3077:A:H5''	1.49	0.94
12:L:10:GLN:HE21	12:L:10:GLN:H	1.15	0.94
3:C:223:ARG:HG3	37:C:8605:HOH:O	1.68	0.94
4:D:86:ALA:HA	37:D:8577:HOH:O	1.67	0.94
5:E:140:VAL:HB	37:E:8456:HOH:O	1.65	0.94
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.50	0.93
6:F:105:SER:HB2	6:F:131:THR:HG23	1.50	0.93
1:A:1835:U:H5	1:A:1840:A:N7	1.65	0.93
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.48	0.93
1:A:1751:G:H2'	1:A:1752:G:H5''	1.51	0.93
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.68	0.92
16:P:7:LEU:HD22	37:P:5650:HOH:O	1.70	0.92
37:A:6854:HOH:O	14:N:178:LYS:HB2	1.70	0.92
5:E:2:GLN:HB3	37:E:8335:HOH:O	1.70	0.91
12:L:10:GLN:NE2	12:L:10:GLN:H	1.68	0.91
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.51	0.91
1:A:2121:G:OP2	37:A:3491:HOH:O	1.89	0.91
1:A:871:G:C5'	1:A:871:G:H8	1.84	0.91
13:M:68:GLU:HA	37:M:8549:HOH:O	1.70	0.90
1:A:156:C:H5''	14:N:171:ARG:HD3	1.52	0.90
24:X:88:THR:HB	37:X:6679:HOH:O	1.70	0.90
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.50	0.90
1:A:962:C:H1'	15:O:5:ARG:HH12	1.32	0.90
2:B:3023:U:H5''	2:B:3024:U:OP2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.34	0.90
1:A:1474:C:H5'	1:A:1474:C:H6	1.35	0.89
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.53	0.89
20:T:57:THR:HG22	20:T:59:ASP:H	1.37	0.89
10:J:27:LYS:H	10:J:58:HIS:HD2	1.15	0.89
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.53	0.89
13:M:133:VAL:HA	37:M:8577:HOH:O	1.72	0.89
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.53	0.88
10:J:150:LYS:HE2	37:J:8385:HOH:O	1.73	0.88
5:E:236:THR:HG21	37:E:8375:HOH:O	1.72	0.88
1:A:870:G:H2'	1:A:871:G:H5''	1.54	0.88
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.38	0.88
1:A:1116:U:HO2'	1:A:1118:A:H2	0.91	0.87
15:O:144:GLY:O	15:O:147:ILE:HG22	1.74	0.87
37:A:3656:HOH:O	14:N:79:LYS:HD3	1.73	0.87
10:J:59:ASN:H	10:J:59:ASN:HD22	1.20	0.87
1:A:2432:C:O4'	37:A:9716:HOH:O	1.93	0.87
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.38	0.87
1:A:1242:A:H5'	11:K:82:THR:HG23	1.53	0.87
4:D:321:PRO:HA	37:D:8656:HOH:O	1.72	0.86
1:A:1634:G:H3'	37:A:3866:HOH:O	1.75	0.86
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.56	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.75	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
1:A:1667:A:H8	1:A:1667:A:H5'	1.38	0.86
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.10	0.85
10:J:2:PRO:HB2	37:J:8367:HOH:O	1.74	0.85
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.58	0.85
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.76	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.04	0.85
16:P:47:ARG:HG3	16:P:47:ARG:HH11	1.41	0.85
1:A:541:C:C2'	1:A:542:A:H5''	2.06	0.85
1:A:2812:A:H2	1:A:2814:A:H62	1.25	0.85
1:A:2004:U:H4'	37:A:5282:HOH:O	1.76	0.85
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.75	0.85
14:N:87:MET:CB	30:4:46:ILE:HD13	2.07	0.85
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.76	0.85
1:A:645:U:OP2	13:M:4:LYS:HE2	1.77	0.85
13:M:79:ASP:HB3	37:M:8564:HOH:O	1.77	0.85
1:A:1118:A:H3'	1:A:1118:A:H8	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.75	0.84
29:3:41:HIS:H	29:3:45:ASN:HD22	1.24	0.84
1:A:2506:A:HO2'	1:A:2507:G:H8	0.85	0.84
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.41	0.84
24:X:88:THR:HG22	24:X:89:ASP:H	1.42	0.84
1:A:1886:A:N3	37:A:4792:HOH:O	2.10	0.84
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.60	0.84
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.59	0.84
13:M:67:ARG:O	13:M:71:GLU:HG3	1.78	0.84
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.59	0.84
1:A:1209:C:H4'	37:A:5255:HOH:O	1.78	0.83
37:A:4493:HOH:O	14:N:94:LYS:HE3	1.77	0.83
1:A:2123:A:OP2	37:A:5264:HOH:O	1.96	0.83
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.59	0.83
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.24	0.83
5:E:246:ARG:NH1	5:E:246:ARG:HB3	1.93	0.83
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.77	0.83
14:N:172:GLY:O	14:N:183:VAL:HG11	1.79	0.83
26:Z:141:THR:HG23	37:Z:8589:HOH:O	1.78	0.83
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.61	0.83
1:A:172:U:OP2	37:A:6192:HOH:O	1.97	0.82
5:E:236:THR:HG22	5:E:239:ALA:N	1.94	0.82
1:A:346:U:H4'	37:A:6824:HOH:O	1.79	0.82
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.94	0.82
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.44	0.82
30:4:73:GLU:HB3	37:4:8563:HOH:O	1.77	0.82
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.61	0.82
15:O:7:LYS:HE3	18:R:21:ARG:O	1.79	0.82
1:A:31:C:H2'	37:A:7684:HOH:O	1.78	0.82
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.60	0.82
1:A:2466:G:OP1	37:A:3621:HOH:O	1.96	0.82
1:A:2533:C:H6	1:A:2533:C:H5'	1.43	0.81
1:A:2717:C:C2'	1:A:2718:C:H5''	2.10	0.81
6:F:154:LYS:H	6:F:154:LYS:HD2	1.45	0.81
10:J:59:ASN:HD22	10:J:59:ASN:N	1.77	0.81
5:E:76:ARG:HD2	37:E:8436:HOH:O	1.80	0.81
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.78	0.81
22:V:9:CYS:HA	22:V:52:THR:HG23	1.60	0.81
1:A:544:G:H2'	1:A:545:G:H5''	1.61	0.81
8:H:96:ALA:HA	37:H:3111:HOH:O	1.80	0.81
37:A:3760:HOH:O	14:N:189:VAL:HG21	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:1:THR:HG23	23:W:2:VAL:H	1.45	0.81
1:A:1184:C:H1'	37:A:7456:HOH:O	1.81	0.81
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.10	0.81
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.61	0.81
2:B:3056:A:C2'	2:B:3057:A:H5''	2.11	0.81
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.62	0.81
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.14	0.81
1:A:545:G:H8	1:A:545:G:H5'	1.46	0.80
1:A:1118:A:C8	1:A:1118:A:H3'	2.15	0.80
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.64	0.80
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.47	0.80
1:A:797:A:H4'	27:1:10:ARG:N	1.97	0.80
14:N:87:MET:CB	30:4:46:ILE:HG21	2.11	0.80
37:A:7549:HOH:O	30:4:60:LYS:HG3	1.81	0.80
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.28	0.80
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.97	0.80
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.64	0.80
14:N:61:ILE:HG13	37:N:8621:HOH:O	1.80	0.80
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.64	0.80
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.21	0.79
1:A:797:A:C4'	27:1:10:ARG:N	2.45	0.79
27:1:54:ILE:HD12	37:1:8416:HOH:O	1.82	0.79
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.62	0.79
1:A:1120:U:H6	1:A:1120:U:H5''	1.47	0.79
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.83	0.79
1:A:1450:C:H4'	1:A:1451:C:OP2	1.82	0.79
1:A:21:G:H5'	19:S:2:ILE:HA	1.64	0.79
10:J:139:ASP:N	10:J:140:PRO:HD3	1.98	0.79
1:A:559:U:H6	1:A:559:U:H5'	1.47	0.79
26:Z:133:HIS:HD2	37:Z:8582:HOH:O	1.65	0.79
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.79
1:A:1679:C:H5'	37:A:9314:HOH:O	1.83	0.79
2:B:3014:G:H8	2:B:3014:G:H5'	1.48	0.79
4:D:62:ARG:CA	4:D:65:MET:HE3	2.13	0.79
10:J:26:LYS:HG2	10:J:28:ILE:H	1.47	0.79
1:A:1160:G:C5'	1:A:1161:A:H5'	2.10	0.78
10:J:142:VAL:HG13	37:J:8383:HOH:O	1.83	0.78
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.18	0.78
37:A:5770:HOH:O	14:N:170:CYS:SG	2.41	0.78
1:A:2506:A:O2'	1:A:2507:G:H8	1.64	0.78
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:ARG:HH11	11:K:74:ARG:HB3	1.48	0.78
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.83	0.78
1:A:289:G:H22	1:A:363:A:H2	1.32	0.78
13:M:136:ALA:HB3	37:M:8577:HOH:O	1.83	0.78
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.13	0.78
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.47	0.78
16:P:32:ARG:O	16:P:32:ARG:HD3	1.83	0.78
1:A:381:G:H5''	37:A:4290:HOH:O	1.82	0.78
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.65	0.78
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.64	0.78
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.66	0.77
6:F:20:LYS:HA	6:F:75:LEU:O	1.85	0.77
1:A:1116:U:O2'	1:A:1118:A:H2	1.68	0.77
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.77
37:A:9547:HOH:O	4:D:267:LYS:HD3	1.84	0.77
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.65	0.77
6:F:27:ILE:HG22	6:F:28:GLY:H	1.49	0.77
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.85	0.77
1:A:560:C:H42	1:A:597:A:H61	1.33	0.77
1:A:506:G:H22	1:A:509:A:C5'	1.97	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.77
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.65	0.77
1:A:1205:U:H2'	1:A:1206:U:H5'	1.66	0.77
1:A:2426:G:H1'	37:A:6072:HOH:O	1.84	0.77
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.80	0.77
3:C:192:VAL:HB	37:C:8597:HOH:O	1.85	0.77
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.99	0.77
14:N:164:THR:HG23	14:N:165:SER:N	1.99	0.77
37:A:4924:HOH:O	2:B:3103:A:H4'	1.84	0.76
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.85	0.76
1:A:288:A:H61	1:A:364:C:H42	1.33	0.76
1:A:1164:U:H3	1:A:1192:A:H2	1.31	0.76
4:D:62:ARG:HA	4:D:65:MET:CE	2.14	0.76
19:S:99:ALA:HB1	19:S:109:MET:CE	2.16	0.76
20:T:57:THR:HG22	20:T:59:ASP:N	2.00	0.76
1:A:1603:A:H5'	1:A:1605:G:O4'	1.85	0.76
4:D:41:PHE:HA	4:D:79:MET:HE2	1.68	0.76
37:A:6278:HOH:O	6:F:99:ASP:HA	1.84	0.76
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.68	0.76
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.66	0.76
8:H:91:VAL:HG12	8:H:92:GLY:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:9:CYS:SG	22:V:11:THR:HG23	2.26	0.76
24:X:88:THR:HG23	24:X:110:GLN:NE2	2.01	0.76
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.68	0.75
1:A:1474:C:H5'	1:A:1474:C:C6	2.19	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
1:A:542:A:C8	1:A:542:A:H5'	2.18	0.75
1:A:877:G:H5'	1:A:878:G:OP1	1.86	0.75
10:J:137:ASN:O	10:J:139:ASP:N	2.19	0.75
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.17	0.75
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.85	0.75
1:A:1120:U:H5''	1:A:1120:U:C6	2.22	0.75
1:A:1625:U:H4'	37:A:4639:HOH:O	1.84	0.75
4:D:238:ASN:HD22	4:D:240:GLY:H	1.35	0.75
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.68	0.75
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.86	0.75
1:A:1329:A:N1	34:A:8513:CL:CL	2.56	0.75
1:A:2054:A:N3	19:S:128:ARG:NH2	2.34	0.75
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.49	0.75
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.67	0.75
1:A:1165:G:H4'	1:A:1174:A:O2'	1.86	0.75
37:A:7413:HOH:O	21:U:9:LYS:HB2	1.86	0.75
1:A:1118:A:H62	1:A:1244:U:H3	1.34	0.75
1:A:1666:C:O2'	1:A:1667:A:H5''	1.87	0.75
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.68	0.75
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.51	0.74
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.52	0.74
1:A:1187:U:H2'	37:A:6877:HOH:O	1.87	0.74
37:A:9075:HOH:O	4:D:214:PRO:HD2	1.87	0.74
15:O:80:SER:HB2	37:O:8535:HOH:O	1.85	0.74
5:E:178:GLN:OE1	37:E:8470:HOH:O	2.05	0.74
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.84	0.74
1:A:1119:G:H22	1:A:1246:A:H2	1.31	0.74
1:A:1835:U:C5	1:A:1840:A:N7	2.53	0.74
27:1:49:ARG:HD2	37:1:8427:HOH:O	1.88	0.74
1:A:960:G:H4'	37:A:7419:HOH:O	1.87	0.74
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.28	0.74
1:A:1701:A:H5'	37:A:6266:HOH:O	1.87	0.74
10:J:140:PRO:HB3	37:J:8383:HOH:O	1.87	0.74
14:N:164:THR:HG22	14:N:167:GLY:N	2.00	0.74
37:A:4833:HOH:O	14:N:14:ARG:HG2	1.87	0.74
24:X:129:LYS:HG2	37:X:1990:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.20	0.74
13:M:148:GLU:HA	37:M:8576:HOH:O	1.87	0.74
5:E:107:ARG:HB3	5:E:107:ARG:NH1	2.03	0.73
8:H:91:VAL:HG12	8:H:92:GLY:H	1.51	0.73
37:A:9383:HOH:O	14:N:94:LYS:HE2	1.88	0.73
26:Z:216:ARG:HD3	37:Z:8569:HOH:O	1.85	0.73
9:I:12:ILE:HA	37:I:4499:HOH:O	1.88	0.73
1:A:111:C:O2'	28:2:20:ARG:HG2	1.89	0.73
1:A:1666:C:H2'	1:A:1667:A:H5'	1.69	0.73
19:S:39:THR:HB	19:S:42:GLU:HG3	1.70	0.73
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.02	0.73
37:A:7575:HOH:O	27:1:31:ILE:HG13	1.88	0.73
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.20	0.73
10:J:75:SER:O	10:J:79:ALA:HB2	1.88	0.73
30:4:65:THR:HG23	30:4:67:LEU:HG	1.71	0.73
1:A:1080:C:H4'	1:A:1081:A:OP1	1.88	0.73
3:C:53:ALA:HB3	37:C:8609:HOH:O	1.89	0.73
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.88	0.73
1:A:541:C:H2'	1:A:542:A:C5'	2.16	0.73
1:A:1834:C:H2'	1:A:1840:A:N6	2.03	0.72
11:K:93:ARG:HH11	11:K:93:ARG:HB3	1.52	0.72
18:R:23:THR:HA	37:R:4792:HOH:O	1.89	0.72
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.22	0.72
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.88	0.72
3:C:199:HIS:CD2	3:C:201:PHE:H	2.06	0.72
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.19	0.72
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.71	0.72
37:A:4641:HOH:O	20:T:23:LYS:HE2	1.89	0.72
4:D:179:LEU:O	4:D:183:GLU:HG2	1.88	0.72
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.19	0.72
8:H:46:GLU:O	8:H:73:PRO:HD2	1.89	0.72
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.71	0.72
1:A:1372:A:H3'	37:A:7173:HOH:O	1.88	0.72
1:A:2421:G:H3'	1:A:2422:U:H5''	1.70	0.72
1:A:2638:G:H1'	37:A:7756:HOH:O	1.89	0.72
37:A:7444:HOH:O	4:D:211:THR:HG21	1.89	0.72
1:A:1191:A:H3'	1:A:1192:A:H5''	1.70	0.72
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.54	0.72
1:A:1213:C:O2'	1:A:1214:G:H5'	1.89	0.72
1:A:284:C:H4'	1:A:285:A:O5'	1.89	0.72
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.20	0.72
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.88	0.72
9:I:12:ILE:N	9:I:13:PRO:HD3	2.04	0.72
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.89	0.72
1:A:1119:G:H8	11:K:52:GLN:HE22	1.36	0.72
1:A:2382:A:H5'	37:A:4714:HOH:O	1.89	0.72
10:J:162:SER:CB	10:J:163:PRO:HD3	2.17	0.72
15:O:164:ASP:CG	15:O:167:ASP:HA	2.10	0.71
24:X:154:ARG:C	37:X:4276:HOH:O	2.28	0.71
1:A:236:A:H4'	1:A:237:G:H5'	1.73	0.71
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.20	0.71
10:J:141:ASN:HA	37:J:8369:HOH:O	1.90	0.71
15:O:113:SER:HB2	37:O:8556:HOH:O	1.89	0.71
15:O:12:ARG:HD3	15:O:18:THR:OG1	1.90	0.71
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.72	0.71
1:A:1701:A:H4'	1:A:1702:U:H5''	1.71	0.71
1:A:338:C:H4'	5:E:174:ILE:CD1	2.20	0.71
1:A:2346:C:O2'	6:F:52:THR:HG21	1.91	0.71
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.73	0.71
13:M:143:THR:HG22	13:M:144:ASP:N	2.05	0.71
26:Z:220:GLU:HG2	37:Z:8551:HOH:O	1.89	0.71
1:A:870:G:C2'	1:A:871:G:H5''	2.20	0.71
1:A:1329:A:H2	37:A:4657:HOH:O	1.72	0.71
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.59	0.71
29:3:41:HIS:N	29:3:45:ASN:HD22	1.88	0.71
6:F:97:GLN:O	6:F:97:GLN:HG2	1.89	0.71
14:N:85:ARG:NE	37:N:8519:HOH:O	2.19	0.71
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.72	0.71
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.73	0.71
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.71	0.71
1:A:2420:G:O2'	1:A:2421:G:H5'	1.91	0.71
2:B:3013:A:O2'	2:B:3014:G:H5''	1.91	0.71
14:N:138:HIS:ND1	14:N:139:PRO:O	2.19	0.71
19:S:39:THR:HG23	19:S:107:GLU:O	1.90	0.71
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.90	0.71
14:N:60:ILE:C	14:N:61:ILE:HD12	2.11	0.71
23:W:39:ALA:N	23:W:40:PRO:HD2	2.06	0.71
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.53	0.71
14:N:186:SER:O	14:N:189:VAL:HG12	1.90	0.71
2:B:3029:C:H2'	2:B:3030:C:H5'	1.73	0.70
12:L:10:GLN:HE21	12:L:10:GLN:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:G:P	26:Z:204:ARG:HH22	2.14	0.70
21:U:47:THR:HB	21:U:100:ASP:HB3	1.72	0.70
27:1:30:GLU:HA	27:1:33:HIS:CB	2.21	0.70
19:S:106:GLY:HA2	19:S:109:MET:CE	2.20	0.70
1:A:2419:U:H5''	1:A:2420:G:H5'	1.73	0.70
8:H:99:THR:HA	37:H:3461:HOH:O	1.91	0.70
10:J:139:ASP:HA	37:J:8373:HOH:O	1.91	0.70
24:X:80:ASP:O	24:X:84:VAL:HG23	1.90	0.70
1:A:1353:C:P	37:A:4652:HOH:O	2.50	0.70
14:N:139:PRO:O	14:N:140:ALA:HB3	1.92	0.70
1:A:338:C:H4'	5:E:174:ILE:HD11	1.73	0.70
5:E:1:MET:HG2	5:E:2:GLN:H	1.55	0.70
7:G:11:VAL:HG12	7:G:12:ASP:N	2.07	0.70
10:J:14:TYR:H	10:J:91:HIS:CE1	2.09	0.70
3:C:121:ALA:O	3:C:124:VAL:HG22	1.92	0.70
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.56	0.70
1:A:1160:G:N3	37:A:5610:HOH:O	2.24	0.70
1:A:544:G:C2'	1:A:545:G:H5''	2.21	0.70
1:A:2768:A:H2'	1:A:2769:C:O4'	1.91	0.70
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.73	0.70
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.92	0.70
10:J:41:THR:HA	37:J:8397:HOH:O	1.91	0.70
1:A:1753:C:O2	4:D:229:ARG:NH2	2.25	0.69
1:A:2748:G:H2'	37:A:7534:HOH:O	1.92	0.69
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.73	0.69
1:A:871:G:C5'	1:A:871:G:C8	2.65	0.69
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.74	0.69
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.22	0.69
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.26	0.69
1:A:214:U:H5'	37:A:6120:HOH:O	1.91	0.69
1:A:2467:A:H2'	37:A:5431:HOH:O	1.92	0.69
19:S:9:ASP:O	19:S:13:THR:HB	1.92	0.69
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.69
1:A:1810:C:OP1	22:V:44:ARG:NE	2.18	0.69
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.22	0.69
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.25	0.69
1:A:516:A:OP2	37:A:5623:HOH:O	2.10	0.69
6:F:55:LYS:HA	37:F:6752:HOH:O	1.93	0.69
37:A:3698:HOH:O	14:N:157:LEU:HD11	1.93	0.69
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.57	0.69
30:4:48:ASN:ND2	30:4:50:GLY:H	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:A:OP2	37:A:3135:HOH:O	2.10	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
5:E:214:THR:HG21	37:E:8403:HOH:O	1.91	0.69
14:N:104:ARG:O	14:N:108:LYS:HG2	1.92	0.69
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.75	0.69
3:C:200:PRO:O	37:C:8590:HOH:O	2.10	0.69
5:E:139:VAL:HG13	37:E:8453:HOH:O	1.92	0.69
6:F:23:VAL:HG23	6:F:23:VAL:O	1.92	0.69
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.90	0.69
37:A:5197:HOH:O	12:L:39:GLY:HA2	1.93	0.69
19:S:44:VAL:O	19:S:48:GLU:HG3	1.92	0.69
1:A:1073:A:OP2	37:A:4235:HOH:O	2.11	0.69
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.58	0.69
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.75	0.69
11:K:131:THR:HG22	11:K:134:GLU:H	1.55	0.69
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.26	0.69
3:C:35:GLY:O	3:C:36:ASP:HB3	1.92	0.69
1:A:1741:U:H5'	1:A:1742:A:OP1	1.92	0.69
7:G:101:GLU:HB2	7:G:116:THR:O	1.92	0.69
14:N:152:ARG:HG3	37:N:8554:HOH:O	1.93	0.69
1:A:2468:A:H61	30:4:48:ASN:HD21	1.40	0.69
1:A:204:A:H2'	1:A:205:U:H5'	1.74	0.69
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.09	0.69
1:A:820:G:O2'	1:A:856:G:H4'	1.92	0.69
26:Z:155:ARG:NH1	37:Z:8559:HOH:O	2.24	0.69
11:K:19:MET:CE	11:K:132:LEU:HD11	2.22	0.68
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.58	0.68
1:A:2526:C:O2'	1:A:2527:U:H5'	1.93	0.68
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.93	0.68
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.75	0.68
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.75	0.68
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.06	0.68
1:A:20:G:H21	19:S:117:HIS:HD2	1.40	0.68
37:A:9116:HOH:O	14:N:82:ARG:HD2	1.93	0.68
1:A:1187:U:HO2'	1:A:1189:A:H2	1.42	0.68
1:A:1919:A:H4'	37:A:4819:HOH:O	1.92	0.68
1:A:2467:A:OP1	37:A:9040:HOH:O	2.12	0.68
10:J:27:LYS:H	10:J:58:HIS:CD2	2.06	0.68
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.68
22:V:14:GLU:O	22:V:17:THR:HB	1.93	0.68
1:A:2578:G:H8	1:A:2578:G:H5'	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.68
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.59	0.68
1:A:1667:A:H5'	1:A:1667:A:C8	2.27	0.68
11:K:19:MET:HE2	11:K:132:LEU:HD11	1.75	0.68
16:P:87:THR:O	16:P:91:GLN:HG3	1.94	0.68
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.59	0.68
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.11	0.68
1:A:1751:G:C2'	1:A:1752:G:H5''	2.24	0.68
2:B:3023:U:C5'	2:B:3024:U:OP2	2.42	0.68
1:A:2508:C:H2'	37:A:6734:HOH:O	1.94	0.67
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.94	0.67
3:C:105:VAL:HG12	3:C:106:CYS:N	2.10	0.67
10:J:49:VAL:O	10:J:157:ILE:HG23	1.94	0.67
27:1:29:VAL:O	27:1:33:HIS:HB2	1.95	0.67
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.77	0.67
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.58	0.67
6:F:95:THR:O	6:F:97:GLN:N	2.24	0.67
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.76	0.67
23:W:56:ILE:O	23:W:60:GLN:HG3	1.95	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.58	0.67
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.09	0.67
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.92	0.67
24:X:88:THR:HG22	24:X:89:ASP:N	2.10	0.67
1:A:88:G:N7	29:3:28:LYS:HD2	2.09	0.67
1:A:506:G:H22	1:A:509:A:H5'	1.59	0.67
4:D:248:ARG:HG2	37:K:8541:HOH:O	1.94	0.67
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.76	0.67
14:N:69:LYS:O	14:N:73:ARG:NH2	2.25	0.67
1:A:869:G:OP1	14:N:79:LYS:HE2	1.94	0.67
1:A:447:A:OP1	21:U:2:LYS:HG2	1.95	0.67
5:E:237:GLU:HB2	37:E:8433:HOH:O	1.94	0.67
24:X:149:LEU:HG	24:X:153:MET:HE2	1.76	0.67
1:A:2420:G:H4'	37:A:4067:HOH:O	1.95	0.67
1:A:711:G:H1'	37:A:7079:HOH:O	1.93	0.67
1:A:2646:G:H1'	31:A:9000:TYK:H221	1.76	0.67
6:F:69:ILE:O	6:F:69:ILE:HG22	1.95	0.67
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.77	0.67
22:V:6:CYS:SG	22:V:31:PHE:HA	2.35	0.67
1:A:2830:U:H3'	37:A:5204:HOH:O	1.94	0.67
10:J:71:TYR:C	10:J:73:GLN:H	1.98	0.67
1:A:450:C:OP1	5:E:184:ARG:NH2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.75	0.67
5:E:233:THR:HG22	5:E:234:VAL:N	2.09	0.67
20:T:43:GLU:HB3	37:T:8343:HOH:O	1.95	0.67
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.94	0.67
1:A:1909:A:N1	1:A:2128:G:H1'	2.10	0.66
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.77	0.66
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.60	0.66
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.66
27:1:42:CYS:SG	27:1:44:PHE:N	2.60	0.66
1:A:1766:U:O2	1:A:1778:A:H5'	1.95	0.66
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.76	0.66
1:A:21:G:C5'	19:S:2:ILE:HA	2.24	0.66
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.59	0.66
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.76	0.66
9:I:63:ARG:N	37:I:2569:HOH:O	2.28	0.66
11:K:133:GLY:O	11:K:137:GLU:HG3	1.96	0.66
37:A:9380:HOH:O	27:1:34:LYS:HD3	1.94	0.66
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.31	0.66
1:A:1130:U:H2'	1:A:1131:G:O4'	1.95	0.66
1:A:2716:G:H5''	4:D:206:THR:HG21	1.78	0.66
1:A:282:C:H1'	1:A:368:C:H42	1.60	0.66
1:A:338:C:H5''	37:E:8423:HOH:O	1.94	0.66
1:A:2862:G:H4'	4:D:336:GLN:O	1.95	0.66
27:1:10:ARG:HA	37:1:8414:HOH:O	1.94	0.66
1:A:1878:G:H1'	37:A:6101:HOH:O	1.96	0.66
37:A:4515:HOH:O	10:J:151:MET:HE2	1.95	0.66
1:A:664:U:OP1	37:A:3755:HOH:O	2.13	0.66
4:D:175:LEU:HD23	4:D:175:LEU:C	2.15	0.66
5:E:214:THR:HG23	37:E:8441:HOH:O	1.94	0.66
13:M:145:LEU:O	13:M:148:GLU:HG3	1.96	0.66
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.94	0.66
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.30	0.66
20:T:53:ASN:ND2	37:T:8322:HOH:O	2.28	0.66
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.66
1:A:2729:C:H2'	1:A:2730:G:H8	1.61	0.66
1:A:2827:A:H2'	1:A:2828:G:O4'	1.95	0.66
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.93	0.66
23:W:12:THR:HG22	23:W:15:GLU:CG	2.16	0.66
26:Z:235:GLU:CD	26:Z:235:GLU:H	1.99	0.66
1:A:603:A:H5''	1:A:604:G:OP1	1.95	0.66
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.77	0.66
14:N:30:GLU:O	14:N:34:GLU:HG3	1.96	0.66
1:A:820:G:OP1	27:1:17:ARG:NH2	2.23	0.65
1:A:845:U:OP2	37:A:9197:HOH:O	2.14	0.65
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.77	0.65
5:E:236:THR:CG2	5:E:239:ALA:H	2.01	0.65
7:G:132:THR:HB	37:G:2227:HOH:O	1.96	0.65
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.31	0.65
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.96	0.65
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.96	0.65
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
10:J:27:LYS:N	10:J:58:HIS:HD2	1.92	0.65
10:J:59:ASN:H	10:J:59:ASN:ND2	1.94	0.65
37:A:4360:HOH:O	14:N:84:LYS:HE2	1.96	0.65
1:A:506:G:H22	1:A:509:A:H5''	1.61	0.65
5:E:236:THR:H	5:E:239:ALA:HB3	1.61	0.65
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.44	0.65
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.65
37:A:9495:HOH:O	4:D:18:ARG:HD3	1.97	0.65
5:E:234:VAL:O	5:E:234:VAL:HG22	1.97	0.65
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.29	0.65
3:C:33:GLU:O	3:C:34:ASP:HB2	1.95	0.65
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.59	0.65
1:A:2329:C:O2'	1:A:2330:U:H5'	1.96	0.65
4:D:145:HIS:HD2	4:D:146:THR:O	1.79	0.65
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.10	0.65
1:A:2310:G:OP2	10:J:114:PRO:HD2	1.96	0.65
6:F:166:ILE:HD12	37:F:6326:HOH:O	1.96	0.65
14:N:52:LEU:HD21	37:N:8615:HOH:O	1.97	0.65
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.25	0.65
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.62	0.65
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.79	0.65
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.27	0.65
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.79	0.65
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.31	0.65
1:A:2421:G:H3'	1:A:2422:U:C5'	2.27	0.65
22:V:9:CYS:CA	22:V:52:THR:HG23	2.26	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.97	0.65
14:N:139:PRO:O	14:N:140:ALA:CB	2.45	0.65
14:N:172:GLY:C	14:N:183:VAL:HG11	2.18	0.65
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:258:GLY:H	4:D:260:HIS:CE1	2.14	0.64
14:N:154:ARG:NE	37:N:8639:HOH:O	2.31	0.64
24:X:130:HIS:O	24:X:136:GLY:HA3	1.97	0.64
1:A:2432:C:O2'	1:A:2433:A:H5'	1.98	0.64
1:A:2637:A:H5'	37:A:9265:HOH:O	1.97	0.64
5:E:236:THR:HA	37:E:8456:HOH:O	1.96	0.64
6:F:135:VAL:HG22	6:F:136:ARG:H	1.60	0.64
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.26	0.64
11:K:107:ASN:ND2	11:K:109:TYR:H	1.95	0.64
29:3:41:HIS:H	29:3:45:ASN:ND2	1.95	0.64
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.64
14:N:104:ARG:O	14:N:108:LYS:HE2	1.97	0.64
1:A:962:C:C1'	15:O:5:ARG:NH1	2.59	0.64
37:A:6951:HOH:O	23:W:4:HIS:HB3	1.97	0.64
1:A:1700:C:OP2	37:A:6013:HOH:O	2.14	0.64
1:A:272:A:H3'	37:A:7522:HOH:O	1.97	0.64
1:A:31:C:H4'	37:A:7413:HOH:O	1.97	0.64
1:A:1185:U:H2'	1:A:1186:C:C6	2.32	0.64
1:A:1123:A:C6	1:A:1238:C:H5'	2.33	0.64
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.31	0.64
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.12	0.64
11:K:99:GLU:HA	37:K:8573:HOH:O	1.97	0.64
1:A:2359:G:N7	37:A:3675:HOH:O	2.29	0.64
3:C:175:LYS:HE2	37:C:8578:HOH:O	1.98	0.64
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.30	0.64
14:N:154:ARG:CZ	37:N:8639:HOH:O	2.45	0.64
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.63	0.64
4:D:305:ASP:O	4:D:306:LYS:HB2	1.98	0.64
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.96	0.64
1:A:1329:A:C2	37:A:4657:HOH:O	2.49	0.64
3:C:94:LEU:HD23	3:C:94:LEU:N	2.12	0.64
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.80	0.64
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.33	0.64
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.96	0.64
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.98	0.64
1:A:2912:C:OP2	37:A:5528:HOH:O	2.15	0.63
2:B:3020:G:O2'	2:B:3021:G:H5'	1.98	0.63
1:A:188:C:H5''	14:N:163:LEU:HD21	1.80	0.63
27:1:46:LYS:O	27:1:57:CYS:HA	1.98	0.63
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.80	0.63
28:2:10:LYS:HG3	37:2:2979:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.81	0.63
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.63	0.63
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.79	0.63
1:A:157:G:OP2	37:A:9466:HOH:O	2.15	0.63
1:A:263:U:O4'	8:H:59:ILE:HD13	1.98	0.63
1:A:282:C:O2'	1:A:283:U:H5'	1.99	0.63
4:D:162:MET:CE	4:D:308:LEU:HD21	2.27	0.63
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.62	0.63
10:J:139:ASP:H	10:J:140:PRO:HD3	1.64	0.63
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.80	0.63
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.80	0.63
1:A:1159:G:P	37:A:4264:HOH:O	2.56	0.63
1:A:272:A:H5'	1:A:273:G:OP2	1.99	0.63
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.13	0.63
6:F:25:MET:CE	6:F:37:ALA:HB1	2.28	0.63
15:O:58:LEU:HD12	15:O:58:LEU:N	2.14	0.63
24:X:4:LEU:O	24:X:32:CYS:HA	1.99	0.63
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.64	0.63
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.28	0.63
1:A:2281:C:C2'	1:A:2282:U:H5'	2.29	0.63
2:B:3039:U:H1'	2:B:3044:A:H61	1.62	0.63
1:A:251:C:O2'	1:A:252:C:H5'	1.99	0.63
16:P:47:ARG:NH1	16:P:47:ARG:HG3	2.12	0.63
23:W:39:ALA:C	23:W:41:GLU:H	2.02	0.63
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.80	0.63
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.79	0.63
1:A:941:G:O2'	1:A:942:U:H5'	1.98	0.63
6:F:95:THR:C	6:F:97:GLN:H	2.02	0.63
14:N:39:ARG:NH2	37:N:8621:HOH:O	2.31	0.63
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.80	0.63
12:L:115:ARG:HG3	12:L:116:GLU:N	2.14	0.62
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.81	0.62
1:A:656:G:OP2	16:P:37:ARG:HD2	1.98	0.62
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.29	0.62
1:A:2094:G:H4'	4:D:245:SER:HB3	1.81	0.62
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.28	0.62
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.80	0.62
10:J:127:GLY:O	10:J:128:ALA:HB3	1.99	0.62
24:X:38:THR:HG22	37:X:3580:HOH:O	1.99	0.62
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.81	0.62
6:F:19:GLU:O	6:F:20:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.80	0.62
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.15	0.62
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.81	0.62
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.34	0.62
1:A:2005:G:O2'	1:A:2008:U:OP2	2.16	0.62
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.40	0.62
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.62	0.62
5:E:12:THR:HB	37:E:8446:HOH:O	1.98	0.62
10:J:166:ASN:N	10:J:166:ASN:HD22	1.97	0.62
14:N:154:ARG:HG3	37:N:8612:HOH:O	1.99	0.62
24:X:13:MET:CE	24:X:17:ILE:HG22	2.29	0.62
6:F:99:ASP:CB	6:F:103:ASN:H	2.13	0.62
7:G:23:GLU:HG2	7:G:28:SER:CB	2.30	0.62
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.29	0.62
1:A:2064:U:H5'	1:A:2652:U:H4'	1.82	0.62
6:F:101:THR:HG22	37:F:7400:HOH:O	1.99	0.62
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.15	0.62
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.00	0.62
1:A:299:U:H5'	37:A:7324:HOH:O	1.99	0.62
1:A:885:G:OP2	37:A:9389:HOH:O	2.16	0.62
1:A:1119:G:H8	11:K:52:GLN:NE2	1.97	0.62
1:A:902:G:N7	13:M:18:HIS:HD2	1.97	0.62
21:U:19:ARG:HD3	21:U:67:LEU:O	2.00	0.62
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.27	0.62
27:1:31:ILE:O	27:1:35:LYS:HG3	1.98	0.62
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.38	0.62
1:A:2291:A:C8	1:A:2309:C:H5'	2.34	0.62
1:A:2878:U:H2'	1:A:2879:A:O4'	2.00	0.62
3:C:199:HIS:HD2	3:C:201:PHE:H	1.46	0.62
1:A:1187:U:O2'	1:A:1189:A:H2	1.82	0.62
1:A:1735:C:O2'	1:A:1736:A:H5'	1.99	0.62
1:A:2346:C:H6	1:A:2346:C:O5'	1.83	0.62
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.82	0.62
23:W:58:THR:O	23:W:62:GLU:HG3	2.00	0.62
1:A:960:G:N3	1:A:960:G:H2'	2.15	0.62
3:C:11:ARG:HD3	37:C:8517:HOH:O	1.99	0.62
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.81	0.62
1:A:1377:C:H5'	1:A:1377:C:H6	1.65	0.61
37:A:4806:HOH:O	11:K:47:THR:HB	1.99	0.61
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.65	0.61
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:61:GLY:HA3	37:1:8425:HOH:O	1.99	0.61
1:A:2408:A:H2	37:A:3073:HOH:O	1.83	0.61
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.34	0.61
8:H:110:GLU:HG2	37:H:6926:HOH:O	2.00	0.61
15:O:154:LEU:O	15:O:155:GLU:HB3	2.00	0.61
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.83	0.61
1:A:2769:C:H2'	1:A:2770:G:O4'	2.00	0.61
3:C:131:HIS:O	3:C:132:ASP:HB2	1.98	0.61
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.14	0.61
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.35	0.61
1:A:821:U:H2'	1:A:822:C:H6	1.64	0.61
1:A:155:C:OP2	14:N:188:ARG:NH1	2.28	0.61
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.83	0.61
5:E:133:ARG:HD2	37:E:8411:HOH:O	2.01	0.61
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.81	0.61
14:N:164:THR:CG2	14:N:165:SER:N	2.62	0.61
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.81	0.61
37:A:4162:HOH:O	26:Z:186:ARG:HD2	2.00	0.61
1:A:119:A:H2'	1:A:120:A:H5''	1.83	0.61
1:A:558:C:C2'	1:A:559:U:H5''	2.31	0.61
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.31	0.61
5:E:132:ASP:HB3	37:E:8365:HOH:O	2.01	0.61
37:A:6229:HOH:O	22:V:56:ARG:HB3	2.00	0.61
24:X:110:GLN:HA	24:X:110:GLN:HE21	1.62	0.61
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.97	0.61
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.99	0.61
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.82	0.61
25:Y:41:PHE:O	25:Y:43:VAL:HG23	2.01	0.61
27:1:53:GLY:HA2	27:1:67:GLY:O	2.00	0.61
1:A:396:U:OP2	30:4:38:ARG:NH1	2.34	0.61
37:A:6017:HOH:O	30:4:62:THR:HB	2.00	0.61
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.00	0.61
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.81	0.61
1:A:625:U:H5''	1:A:1044:C:N4	2.15	0.61
2:B:3107:C:H5	37:B:3167:HOH:O	1.84	0.61
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.83	0.61
10:J:46:VAL:O	10:J:146:TRP:HH2	1.84	0.61
30:4:57:GLY:HA2	37:4:8529:HOH:O	2.00	0.60
1:A:2324:G:H4'	1:A:2418:G:O2'	2.01	0.60
1:A:2649:A:H8	1:A:2649:A:H5'	1.66	0.60
2:B:3049:G:H5''	37:B:4707:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.27	0.60
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.31	0.60
27:1:42:CYS:SG	27:1:43:GLY:N	2.74	0.60
1:A:121:U:OP2	29:3:10:ARG:NH2	2.34	0.60
6:F:25:MET:CE	6:F:41:LEU:HG	2.23	0.60
12:L:55:VAL:HG12	12:L:56:SER:N	2.16	0.60
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.66	0.60
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.13	0.60
29:3:18:ASN:HD21	29:3:40:ARG:H	1.49	0.60
1:A:661:G:C5	1:A:686:A:C2	2.89	0.60
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.81	0.60
5:E:78:ARG:NH1	5:E:78:ARG:HG3	2.12	0.60
13:M:26:HIS:HB2	37:M:8512:HOH:O	2.00	0.60
14:N:48:ARG:NH2	37:N:8561:HOH:O	2.32	0.60
15:O:169:PRO:O	15:O:172:PHE:HB3	2.01	0.60
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.82	0.60
1:A:2780:C:H2'	1:A:2781:U:C6	2.37	0.60
1:A:775:G:OP1	28:2:16:HIS:HE1	1.85	0.60
3:C:191:GLY:HA2	3:C:194:MET:HE3	1.83	0.60
7:G:69:ILE:HA	7:G:72:MET:CE	2.32	0.60
14:N:133:LEU:O	14:N:134:ILE:HD13	2.01	0.60
15:O:141:ARG:HB3	37:O:8566:HOH:O	2.02	0.60
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.82	0.60
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.83	0.60
1:A:204:A:C2'	1:A:205:U:H5'	2.30	0.60
1:A:2533:C:C6	1:A:2533:C:H5'	2.32	0.60
5:E:115:LEU:O	5:E:118:THR:HB	2.01	0.60
5:E:16:VAL:HG12	5:E:17:ASP:N	2.16	0.60
37:A:4540:HOH:O	5:E:50:GLU:HG2	2.00	0.60
9:I:12:ILE:N	9:I:13:PRO:CD	2.65	0.60
7:G:81:GLU:HG2	7:G:134:SER:CB	2.32	0.60
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.82	0.60
1:A:283:U:H5''	1:A:284:C:P	2.42	0.60
1:A:474:C:O3'	5:E:73:LEU:HD21	2.01	0.60
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.83	0.60
6:F:37:ALA:O	6:F:40:ILE:HG12	2.02	0.60
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.82	0.60
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.42	0.60
1:A:212:A:O4'	1:A:214:U:C6	2.55	0.60
1:A:2361:A:H2'	1:A:2362:A:C8	2.35	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:C:H5'	37:A:5233:HOH:O	2.02	0.60
4:D:36:PRO:HA	4:D:168:GLY:CA	2.31	0.60
6:F:136:ARG:HD2	6:F:155:HIS:O	2.01	0.60
1:A:280:C:H2'	1:A:281:U:O4'	2.02	0.60
1:A:2429:A:H2'	1:A:2430:A:C8	2.37	0.60
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.31	0.60
1:A:1422:U:H2'	1:A:1423:C:C6	2.36	0.59
1:A:2748:G:H5'	37:A:7534:HOH:O	2.02	0.59
1:A:2088:C:H1'	1:A:2841:A:N1	2.17	0.59
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.02	0.59
34:K:8501:CL:CL	37:K:8547:HOH:O	2.53	0.59
19:S:119:VAL:HG12	19:S:119:VAL:O	2.01	0.59
1:A:151:A:C2	1:A:442:A:C8	2.90	0.59
15:O:163:PHE:HA	37:O:8520:HOH:O	2.02	0.59
19:S:39:THR:HB	19:S:42:GLU:CG	2.31	0.59
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.59
4:D:79:MET:HE1	37:D:8623:HOH:O	2.02	0.59
5:E:118:THR:O	5:E:136:VAL:HG13	2.02	0.59
6:F:135:VAL:HG22	6:F:136:ARG:N	2.16	0.59
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.83	0.59
23:W:44:GLY:O	23:W:48:GLU:HG2	2.01	0.59
1:A:739:G:C5	37:A:7536:HOH:O	2.51	0.59
37:A:9111:HOH:O	5:E:103:ASN:HB3	2.01	0.59
1:A:2505:G:O2'	1:A:2506:A:H5'	2.02	0.59
1:A:951:A:C2'	1:A:952:G:H5'	2.33	0.59
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.84	0.59
37:A:3960:HOH:O	21:U:82:THR:HA	2.02	0.59
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.59
1:A:2284:G:H1'	37:A:9555:HOH:O	2.00	0.59
1:A:514:G:OP1	1:A:514:G:H2'	2.03	0.59
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.32	0.59
10:J:136:VAL:HG22	10:J:137:ASN:O	2.02	0.59
14:N:74:ARG:NH2	37:N:8629:HOH:O	2.32	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	0.59
1:A:1819:G:H2'	1:A:1820:G:H4'	1.84	0.59
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.84	0.59
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.84	0.59
1:A:820:G:H5'	1:A:821:U:H5'	1.84	0.59
2:B:3003:A:N6	2:B:3022:G:H1'	2.18	0.59
10:J:136:VAL:HG23	37:J:8345:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:H4'	14:N:157:LEU:HD13	1.83	0.59
1:A:2635:A:O2'	1:A:2636:C:H5'	2.03	0.59
1:A:485:A:N3	1:A:487:G:H5''	2.17	0.59
1:A:2690:U:O2'	7:G:111:LYS:HE3	2.03	0.59
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.32	0.59
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.18	0.59
30:4:40:ARG:HD2	37:4:8553:HOH:O	2.02	0.59
1:A:57:C:H5''	37:A:6739:HOH:O	2.02	0.59
3:C:188:ASN:OD1	37:C:8559:HOH:O	2.16	0.59
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.02	0.59
10:J:144:GLU:HA	10:J:144:GLU:OE1	2.03	0.59
2:B:3042:C:H2'	37:B:6700:HOH:O	2.02	0.58
4:D:254:GLN:HG2	4:D:255:GLY:N	2.18	0.58
4:D:7:ARG:HD3	4:D:9:GLY:O	2.02	0.58
6:F:105:SER:CB	6:F:131:THR:HG23	2.30	0.58
7:G:32:ARG:O	7:G:33:LEU:HD23	2.03	0.58
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.84	0.58
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.01	0.58
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.33	0.58
1:A:485:A:O2'	1:A:487:G:H5'	2.03	0.58
1:A:559:U:C6	1:A:559:U:H5'	2.36	0.58
9:I:64:ASN:HD22	9:I:64:ASN:N	2.01	0.58
10:J:44:ALA:HA	10:J:163:PRO:O	2.04	0.58
19:S:33:ARG:NH1	37:S:8544:HOH:O	2.36	0.58
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.04	0.58
2:B:3055:U:H4'	2:B:3056:A:C8	2.38	0.58
3:C:37:VAL:HG22	37:C:8601:HOH:O	2.03	0.58
4:D:168:GLY:N	4:D:174:ARG:HD3	2.18	0.58
6:F:50:VAL:O	6:F:71:ALA:HA	2.03	0.58
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.33	0.58
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.15	0.58
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.43	0.58
1:A:1615:A:H4'	37:A:5863:HOH:O	2.02	0.58
1:A:542:A:H2'	1:A:543:G:O4'	2.03	0.58
2:B:3001:U:O3'	2:B:3003:A:H5''	2.03	0.58
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.18	0.58
1:A:391:U:OP2	14:N:84:LYS:NZ	2.36	0.58
37:A:3731:HOH:O	21:U:9:LYS:CD	2.51	0.58
1:A:2064:U:OP1	37:A:3324:HOH:O	2.17	0.58
1:A:2241:C:O2'	1:A:2242:U:H5'	2.02	0.58
5:E:219:ASN:O	5:E:222:ASP:OD1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.84	0.58
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.86	0.58
8:H:58:GLU:HA	8:H:61:MET:HG3	1.86	0.58
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.66	0.58
14:N:68:ARG:HD3	14:N:68:ARG:O	2.04	0.58
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.86	0.58
24:X:41:TYR:O	24:X:45:VAL:HG13	2.04	0.58
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.33	0.58
1:A:157:G:H4'	14:N:95:LYS:HE3	1.85	0.58
1:A:2394:A:OP1	37:A:7078:HOH:O	2.17	0.58
1:A:2502:C:C2'	1:A:2503:A:H5'	2.33	0.58
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.58
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.84	0.58
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.38	0.58
1:A:1127:C:H2'	1:A:1128:U:H5'	1.85	0.58
1:A:1200:A:H4'	37:A:7328:HOH:O	2.02	0.58
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.58
1:A:2415:A:C2	15:O:25:ARG:HB3	2.39	0.58
1:A:2443:C:H3'	37:A:3453:HOH:O	2.03	0.58
1:A:2456:A:H5'	37:A:5671:HOH:O	2.02	0.58
1:A:2897:C:H2'	1:A:2898:G:H8	1.68	0.58
1:A:797:A:O4'	27:1:10:ARG:N	2.36	0.58
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.03	0.58
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.34	0.58
13:M:73:VAL:HG23	13:M:74:THR:H	1.67	0.58
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.85	0.58
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.36	0.58
1:A:281:U:O2'	1:A:282:C:H5'	2.04	0.58
3:C:211:LYS:NZ	37:C:8575:HOH:O	2.37	0.58
1:A:1118:A:C8	1:A:1118:A:C3'	2.81	0.58
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.85	0.58
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.84	0.58
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.50	0.58
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.04	0.58
26:Z:212:ARG:HD2	37:Z:8601:HOH:O	2.03	0.58
1:A:2587:U:H2'	1:A:2589:U:H5''	1.85	0.58
1:A:2783:A:H3'	37:A:5208:HOH:O	2.03	0.58
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.03	0.58
5:E:84:VAL:O	5:E:85:LYS:HB2	2.04	0.58
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.86	0.58
11:K:74:ARG:O	11:K:78:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:C:H4'	14:N:146:GLN:NE2	2.19	0.58
23:W:39:ALA:N	23:W:40:PRO:CD	2.66	0.58
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.17	0.58
1:A:1825:U:O4'	1:A:1999:C:H5''	2.04	0.57
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.52	0.57
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.36	0.57
10:J:75:SER:C	10:J:79:ALA:HB2	2.24	0.57
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.39	0.57
1:A:289:G:N2	1:A:363:A:H2	1.99	0.57
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.04	0.57
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.87	0.57
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.04	0.57
22:V:52:THR:CG2	22:V:54:THR:HB	2.34	0.57
1:A:1641:A:H2'	1:A:1642:A:H5'	1.85	0.57
4:D:14:GLY:HA2	4:D:15:PRO:C	2.25	0.57
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.66	0.57
19:S:132:ARG:CZ	37:S:8583:HOH:O	2.52	0.57
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.67	0.57
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.07	0.57
1:A:182:G:H5'	37:A:5132:HOH:O	2.04	0.57
1:A:1923:G:H4'	30:4:31:THR:O	2.05	0.57
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.86	0.57
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.57
19:S:39:THR:HG22	19:S:42:GLU:H	1.69	0.57
23:W:64:GLY:O	23:W:65:ASP:CB	2.52	0.57
24:X:26:ILE:CG1	24:X:26:ILE:O	2.52	0.57
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.05	0.57
1:A:1200:A:C4'	37:A:7328:HOH:O	2.52	0.57
1:A:1972:U:H2'	1:A:1973:A:H5'	1.87	0.57
1:A:513:A:N3	37:A:3635:HOH:O	2.33	0.57
4:D:2:GLN:CD	37:D:8618:HOH:O	2.42	0.57
6:F:27:ILE:HG22	6:F:28:GLY:N	2.20	0.57
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.20	0.57
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.86	0.57
27:1:25:ARG:O	27:1:29:VAL:HG23	2.05	0.57
1:A:1773:G:C8	27:1:16:PRO:HA	2.40	0.57
1:A:184:G:H5''	14:N:153:THR:HG22	1.87	0.57
2:B:3039:U:H1'	2:B:3044:A:N6	2.19	0.57
8:H:107:VAL:O	8:H:111:ILE:HG13	2.04	0.57
14:N:72:SER:OG	14:N:74:ARG:HB2	2.04	0.57
6:F:86:THR:O	6:F:90:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:GLN:HG2	7:G:19:ASP:O	2.05	0.57
7:G:6:GLU:HA	7:G:46:THR:HG22	1.87	0.57
16:P:39:THR:O	16:P:115:ARG:NH2	2.38	0.57
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.57
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.57
1:A:1827:G:H2'	1:A:1828:G:C8	2.40	0.57
1:A:2729:C:O2'	1:A:2730:G:H5'	2.05	0.57
4:D:275:GLY:O	4:D:291:ASP:HA	2.05	0.57
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.70	0.57
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.40	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.20	0.57
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.39	0.57
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.86	0.57
15:O:64:SER:C	15:O:66:LEU:H	2.08	0.57
1:A:2484:U:C2	37:A:9601:HOH:O	2.52	0.57
1:A:681:G:N3	1:A:681:G:H5'	2.20	0.57
3:C:36:ASP:OD2	3:C:85:ASP:HB2	2.04	0.57
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.68	0.57
6:F:25:MET:HE1	6:F:37:ALA:O	2.05	0.57
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.05	0.57
8:H:99:THR:O	8:H:99:THR:HG23	2.04	0.57
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.35	0.57
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.88	0.57
37:L:1387:HOH:O	22:V:20:MET:HE3	2.04	0.57
24:X:149:LEU:HG	24:X:153:MET:CE	2.35	0.57
28:2:25:LYS:HG2	28:2:25:LYS:O	2.04	0.56
1:A:183:A:H5'	14:N:157:LEU:HD12	1.87	0.56
1:A:1855:G:H8	3:C:144:GLU:OE2	1.88	0.56
1:A:2466:G:H5'	37:A:3621:HOH:O	2.05	0.56
1:A:545:G:C8	1:A:545:G:H5'	2.35	0.56
2:B:3014:G:H5'	2:B:3014:G:C8	2.34	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.18	0.56
4:D:280:VAL:CG1	4:D:334:SER:HA	2.35	0.56
13:M:143:THR:HG22	13:M:144:ASP:H	1.70	0.56
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.34	0.56
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.86	0.56
30:4:3:MET:O	30:4:90:PHE:HA	2.04	0.56
1:A:2414:A:H2'	1:A:2415:A:C8	2.40	0.56
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.40	0.56
4:D:125:GLU:O	4:D:129:ARG:HG3	2.05	0.56
7:G:137:ASP:O	7:G:141:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:MET:O	14:N:28:MET:HG3	2.05	0.56
15:O:110:THR:HB	15:O:113:SER:OG	2.04	0.56
37:A:3731:HOH:O	21:U:9:LYS:HD2	2.04	0.56
1:A:470:U:O2'	28:2:16:HIS:HD2	1.87	0.56
1:A:1947:G:N2	1:A:1966:U:C2	2.73	0.56
1:A:816:G:H5'	1:A:1598:A:H4'	1.86	0.56
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.06	0.56
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.87	0.56
8:H:2:VAL:HG22	8:H:57:GLU:OE1	2.04	0.56
37:A:5504:HOH:O	14:N:58:GLN:HG3	2.03	0.56
19:S:132:ARG:HG2	19:S:133:ALA:N	2.20	0.56
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.87	0.56
26:Z:185:VAL:HG12	37:Z:8570:HOH:O	2.04	0.56
28:2:28:HIS:HD2	28:2:31:LYS:H	1.52	0.56
1:A:1523:G:H2'	1:A:1524:U:C6	2.40	0.56
1:A:2010:A:H2'	37:A:5935:HOH:O	2.05	0.56
15:O:37:ARG:NE	37:O:8533:HOH:O	2.38	0.56
16:P:25:VAL:HG23	16:P:26:TRP:N	2.21	0.56
22:V:52:THR:HG22	22:V:54:THR:HB	1.88	0.56
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.03	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.36	0.56
2:B:3002:U:H4'	2:B:3002:U:OP2	2.05	0.56
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.69	0.56
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.20	0.56
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.86	0.56
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.39	0.56
1:A:2710:U:H1'	37:A:7618:HOH:O	2.06	0.56
1:A:558:C:O2'	1:A:559:U:H5''	2.06	0.56
1:A:88:G:H5'	1:A:88:G:H8	1.70	0.56
10:J:28:ILE:HA	10:J:62:GLU:OE1	2.06	0.56
14:N:38:VAL:O	14:N:63:VAL:HG13	2.06	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.20	0.56
1:A:1162:G:H2'	37:A:6565:HOH:O	2.05	0.56
1:A:1205:U:H2'	1:A:1206:U:C5'	2.34	0.56
1:A:1308:A:H5'	37:A:6916:HOH:O	2.06	0.56
1:A:1636:G:O2'	1:A:1637:A:H5'	2.05	0.56
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.06	0.56
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.88	0.56
8:H:110:GLU:O	8:H:114:LYS:HG3	2.06	0.56
8:H:19:ALA:O	8:H:22:VAL:HG22	2.06	0.56
11:K:52:GLN:HG3	11:K:53:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:37:GLN:OE1	21:U:118:SER:HA	2.05	0.56
1:A:1025:C:H5'	24:X:23:MET:O	2.06	0.56
1:A:1423:C:O2'	1:A:1424:A:H5'	2.06	0.56
1:A:2472:C:O2'	1:A:2634:G:H4'	2.05	0.56
1:A:283:U:H5''	1:A:284:C:OP2	2.06	0.56
1:A:536:A:H3'	37:A:5022:HOH:O	2.05	0.56
37:A:5494:HOH:O	4:D:298:LYS:HD3	2.04	0.56
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.88	0.56
14:N:149:TRP:O	14:N:152:ARG:HG2	2.06	0.56
14:N:154:ARG:HD3	37:N:8639:HOH:O	2.03	0.56
17:Q:143:ALA:HA	37:Q:2178:HOH:O	2.06	0.56
1:A:1086:A:C6	24:X:11:VAL:HG11	2.40	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:1918:U:OP2	37:A:3996:HOH:O	2.18	0.56
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.87	0.56
28:2:1:THR:HB	37:2:6858:HOH:O	2.06	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
1:A:2362:A:H2'	1:A:2363:G:C8	2.40	0.56
2:B:3028:U:H2'	2:B:3029:C:C6	2.41	0.56
8:H:28:ALA:HB3	8:H:99:THR:O	2.05	0.56
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.17	0.56
37:A:6687:HOH:O	26:Z:165:GLU:HB3	2.05	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
1:A:660:A:H4'	1:A:661:G:O5'	2.06	0.55
1:A:926:A:O2'	13:M:41:HIS:HD2	1.88	0.55
15:O:155:GLU:O	15:O:156:GLU:HG3	2.06	0.55
26:Z:144:ARG:CZ	37:Z:8612:HOH:O	2.53	0.55
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.32	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.22	0.55
14:N:35:PRO:O	37:N:8537:HOH:O	2.18	0.55
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.41	0.55
2:B:3055:U:H4'	2:B:3056:A:H8	1.70	0.55
14:N:154:ARG:CD	37:N:8639:HOH:O	2.55	0.55
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.88	0.55
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.03	0.55
1:A:1044:C:H5''	37:A:9022:HOH:O	2.07	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.20	0.55
1:A:1249:U:H2'	1:A:1250:C:C6	2.41	0.55
10:J:57:ARG:O	10:J:61:LEU:HD22	2.06	0.55
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.36	0.55
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
1:A:2301:A:H5''	1:A:2302:A:H5'	1.88	0.55
5:E:37:ALA:O	5:E:41:ASN:ND2	2.39	0.55
7:G:79:GLY:HA3	37:G:7046:HOH:O	2.06	0.55
9:I:12:ILE:HG22	9:I:12:ILE:O	2.06	0.55
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.51	0.55
10:J:59:ASN:ND2	10:J:59:ASN:N	2.50	0.55
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.42	0.55
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.27	0.55
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.87	0.55
1:A:447:A:O2'	1:A:448:G:H5'	2.07	0.55
3:C:211:LYS:NZ	37:C:8622:HOH:O	2.39	0.55
24:X:119:HIS:HD2	24:X:120:PRO:O	1.89	0.55
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.42	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.22	0.55
5:E:107:ARG:HH11	5:E:107:ARG:CB	2.19	0.55
8:H:91:VAL:CG1	8:H:92:GLY:N	2.70	0.55
10:J:149:ALA:C	10:J:151:MET:H	2.10	0.55
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.55
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.06	0.55
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.89	0.55
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.07	0.55
1:A:1116:U:O2'	1:A:1118:A:C2	2.51	0.55
1:A:2649:A:C8	1:A:2649:A:H5'	2.42	0.55
1:A:564:G:H1'	37:A:6293:HOH:O	2.07	0.55
6:F:99:ASP:HB3	6:F:103:ASN:H	1.71	0.55
37:A:4432:HOH:O	14:N:146:GLN:HG2	2.06	0.55
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.22	0.55
21:U:19:ARG:NH1	21:U:68:ASP:O	2.40	0.55
24:X:88:THR:O	37:X:2374:HOH:O	2.18	0.55
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.07	0.55
1:A:1456:C:H2'	1:A:1457:U:C6	2.42	0.55
1:A:158:A:O2'	1:A:159:G:H5'	2.07	0.55
1:A:2115:U:H2'	1:A:2116:U:C6	2.42	0.55
5:E:168:ARG:NH2	5:E:190:ALA:O	2.40	0.55
1:A:1311:G:C2	1:A:1312:G:C8	2.95	0.55
1:A:2082:G:O2'	1:A:2083:A:H5'	2.06	0.55
1:A:625:U:H5'	37:A:3162:HOH:O	2.05	0.55
4:D:248:ARG:O	4:D:251:VAL:CG1	2.55	0.55
4:D:305:ASP:O	4:D:306:LYS:CB	2.55	0.55
4:D:75:GLU:C	4:D:77:PRO:HD3	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:38:VAL:C	14:N:63:VAL:HG13	2.28	0.55
15:O:73:ALA:N	37:O:8563:HOH:O	2.40	0.55
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.42	0.55
37:L:408:HOH:O	22:V:37:GLU:HB3	2.06	0.55
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.36	0.54
1:A:2316:G:H8	37:A:5631:HOH:O	1.90	0.54
1:A:2787:C:H5	37:A:4605:HOH:O	1.88	0.54
1:A:371:U:H2'	1:A:372:A:H8	1.72	0.54
1:A:669:G:O2'	1:A:670:G:H5'	2.07	0.54
1:A:671:A:O2'	1:A:672:G:H2'	2.08	0.54
4:D:7:ARG:CD	4:D:9:GLY:O	2.54	0.54
8:H:58:GLU:HA	8:H:61:MET:HE2	1.88	0.54
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.20	0.54
13:M:104:ASP:HB3	37:M:8569:HOH:O	2.07	0.54
13:M:114:VAL:HG11	37:M:8577:HOH:O	2.08	0.54
15:O:152:GLU:C	15:O:154:LEU:H	2.09	0.54
27:1:22:ILE:O	27:1:26:VAL:HG23	2.08	0.54
1:A:1393:A:H2'	1:A:1394:C:C6	2.43	0.54
1:A:1477:C:O2'	1:A:1478:U:H5'	2.06	0.54
1:A:1741:U:O2'	1:A:2723:G:H4'	2.07	0.54
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.54
1:A:567:U:H5''	37:X:5817:HOH:O	2.07	0.54
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.89	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
1:A:710:G:OP1	16:P:24:ALA:HB3	2.07	0.54
16:P:26:TRP:N	37:P:3062:HOH:O	2.39	0.54
18:R:32:GLU:HA	18:R:71:TYR:OH	2.07	0.54
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.07	0.54
22:V:9:CYS:HA	22:V:52:THR:CG2	2.35	0.54
1:A:134:U:C2	1:A:145:A:C2	2.95	0.54
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.90	0.54
6:F:10:PHE:CG	6:F:11:HIS:N	2.75	0.54
1:A:2779:G:H21	7:G:143:GLN:NE2	2.05	0.54
8:H:104:ALA:HA	37:H:6617:HOH:O	2.08	0.54
10:J:154:THR:HB	10:J:155:PRO:HD3	1.89	0.54
10:J:31:PHE:HE2	10:J:87:LYS:O	1.89	0.54
19:S:29:LYS:HB3	37:S:8533:HOH:O	2.07	0.54
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.28	0.54
1:A:1527:A:H1'	1:A:1528:A:C8	2.42	0.54
1:A:2383:G:N3	37:A:6686:HOH:O	2.33	0.54
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:A:H2'	1:A:591:A:H5'	1.90	0.54
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.89	0.54
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.42	0.54
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.54
13:M:143:THR:HG22	13:M:145:LEU:H	1.71	0.54
1:A:1165:G:OP1	1:A:1165:G:H3'	2.08	0.54
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.39	0.54
1:A:2325:C:H1'	37:A:4122:HOH:O	2.08	0.54
1:A:2494:G:H4'	10:J:5:MET:SD	2.47	0.54
6:F:140:ARG:O	6:F:144:ARG:HG2	2.08	0.54
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.08	0.54
12:L:30:LYS:O	12:L:55:VAL:HG13	2.07	0.54
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.35	0.54
37:A:4330:HOH:O	16:P:37:ARG:HG3	2.07	0.54
24:X:90:TYR:N	24:X:90:TYR:CD1	2.75	0.54
26:Z:133:HIS:CD2	37:Z:8582:HOH:O	2.50	0.54
1:A:1118:A:H8	1:A:1119:G:H5''	1.72	0.54
1:A:2672:C:H1'	37:D:8634:HOH:O	2.08	0.54
1:A:305:A:C5	1:A:329:A:C2	2.96	0.54
4:D:43:GLY:O	4:D:308:LEU:HD12	2.07	0.54
5:E:76:ARG:HD3	37:E:8368:HOH:O	2.07	0.54
6:F:59:GLY:C	6:F:61:PHE:H	2.11	0.54
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.22	0.54
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.23	0.54
1:A:221:G:H2'	1:A:222:A:C8	2.42	0.54
1:A:2502:C:H2'	1:A:2503:A:H5'	1.89	0.54
1:A:349:U:O2'	1:A:350:C:H5'	2.08	0.54
2:B:3054:A:O2'	2:B:3055:U:H5'	2.08	0.54
4:D:146:THR:O	4:D:159:PRO:HB3	2.07	0.54
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.32	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.08	0.54
5:E:104:ASP:O	5:E:108:GLN:HG3	2.08	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.07	0.54
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.08	0.54
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.72	0.54
1:A:431:G:P	14:N:48:ARG:HH12	2.31	0.54
24:X:139:GLY:O	24:X:141:HIS:HD2	1.90	0.54
1:A:138:U:H5''	1:A:139:C:OP2	2.08	0.54
14:N:79:LYS:HD2	37:N:8555:HOH:O	2.08	0.54
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.22	0.54
27:1:34:LYS:HE2	37:1:8424:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.07	0.54
1:A:2906:A:H5'	1:A:2907:C:O4'	2.07	0.54
4:D:72:THR:HB	37:D:8603:HOH:O	2.07	0.54
4:D:82:VAL:O	4:D:82:VAL:HG12	2.07	0.54
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.06	0.54
8:H:58:GLU:HG3	8:H:61:MET:HE1	1.89	0.54
10:J:71:TYR:C	10:J:73:GLN:N	2.59	0.54
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.23	0.54
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.55	0.54
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.43	0.54
27:1:19:GLY:O	27:1:23:ARG:HG2	2.07	0.54
1:A:1293:U:O2'	26:Z:149:GLN:NE2	2.28	0.54
1:A:2507:G:H2'	1:A:2510:C:H42	1.73	0.54
1:A:316:A:H5'	21:U:54:ASP:OD2	2.07	0.54
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.38	0.54
9:I:16:LYS:O	9:I:20:VAL:HG23	2.08	0.54
14:N:79:LYS:NZ	37:N:8565:HOH:O	2.41	0.54
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.53
1:A:1559:A:H1'	37:A:5842:HOH:O	2.07	0.53
1:A:1711:A:O2'	1:A:1712:A:H5'	2.08	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.90	0.53
1:A:2769:C:C2'	1:A:2770:G:H5'	2.38	0.53
1:A:926:A:O2'	13:M:41:HIS:CD2	2.61	0.53
4:D:119:HIS:O	4:D:121:PRO:HD3	2.07	0.53
4:D:204:GLY:HA3	37:D:8652:HOH:O	2.07	0.53
5:E:107:ARG:CB	5:E:107:ARG:NH1	2.70	0.53
7:G:15:GLN:NE2	7:G:40:VAL:O	2.41	0.53
10:J:69:ASN:O	10:J:72:VAL:HG12	2.08	0.53
13:M:73:VAL:HG23	13:M:74:THR:N	2.23	0.53
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.73	0.53
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.08	0.53
1:A:1182:C:H1'	1:A:1192:A:H8	1.73	0.53
1:A:1422:U:H2'	1:A:1423:C:H6	1.72	0.53
1:A:2011:A:H4'	1:A:2012:U:O5'	2.09	0.53
6:F:57:THR:HG23	6:F:63:ILE:CB	2.38	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.90	0.53
10:J:139:ASP:N	10:J:140:PRO:CD	2.70	0.53
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.43	0.53
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.09	0.53
1:A:1733:A:H4'	4:D:212:GLN:HA	1.88	0.53
1:A:2276:U:H2'	1:A:2277:U:C6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:U:O2'	1:A:822:C:H5'	2.09	0.53
3:C:179:MET:HG2	3:C:186:TRP:CB	2.39	0.53
10:J:109:ASP:HB2	37:J:8348:HOH:O	2.08	0.53
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.90	0.53
1:A:56:G:H5''	23:W:50:ARG:NH1	2.23	0.53
1:A:631:A:N3	1:A:2073:G:O2'	2.38	0.53
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.34	0.53
6:F:35:ALA:N	37:F:5576:HOH:O	2.41	0.53
7:G:22:VAL:O	7:G:28:SER:HA	2.08	0.53
10:J:118:PRO:HD2	37:J:8341:HOH:O	2.09	0.53
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.90	0.53
13:M:143:THR:CG2	13:M:144:ASP:N	2.70	0.53
14:N:186:SER:OG	14:N:189:VAL:HG12	2.09	0.53
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.53
1:A:1299:G:O6	13:M:6:ARG:HD3	2.08	0.53
1:A:2433:A:H2'	1:A:2434:A:C8	2.43	0.53
1:A:2860:G:H1'	37:A:6782:HOH:O	2.09	0.53
4:D:51:VAL:HG21	4:D:327:VAL:HG13	1.90	0.53
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.54	0.53
8:H:46:GLU:N	37:H:3461:HOH:O	2.41	0.53
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.24	0.53
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.72	0.53
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.09	0.53
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.24	0.53
22:V:52:THR:HG22	22:V:54:THR:H	1.74	0.53
1:A:1172:G:H1'	37:A:4947:HOH:O	2.08	0.53
1:A:2256:G:H2'	1:A:2257:G:C5'	2.38	0.53
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.34	0.53
1:A:489:A:C8	21:U:82:THR:HG22	2.44	0.53
4:D:88:GLU:O	4:D:88:GLU:HG3	2.08	0.53
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.24	0.53
13:M:57:VAL:HG12	13:M:57:VAL:O	2.09	0.53
19:S:82:GLU:HG3	19:S:83:LYS:N	2.23	0.53
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.09	0.53
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.21	0.53
1:A:1189:A:H1'	1:A:1209:C:H1'	1.91	0.53
1:A:1441:G:O2'	1:A:1442:A:H5'	2.09	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.09	0.53
1:A:1778:A:H2'	1:A:1779:A:H5'	1.90	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.09	0.53
1:A:2001:G:O2'	1:A:2002:C:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:A:N6	1:A:2247:C:H1'	2.24	0.53
1:A:45:A:N6	1:A:147:G:C4	2.77	0.53
1:A:51:G:O2'	1:A:52:A:H5'	2.08	0.53
2:B:3096:C:H2'	2:B:3097:U:C6	2.44	0.53
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.08	0.53
14:N:87:MET:SD	37:N:8530:HOH:O	2.59	0.53
15:O:37:ARG:HD3	34:O:8507:CL:CL	2.46	0.53
22:V:33:SER:O	22:V:37:GLU:HG3	2.08	0.53
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.08	0.53
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.90	0.53
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.09	0.53
37:A:7662:HOH:O	26:Z:172:THR:HB	2.08	0.53
1:A:2321:A:O2'	1:A:2322:U:H3'	2.09	0.53
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.07	0.53
26:Z:144:ARG:NE	37:Z:8612:HOH:O	2.41	0.53
27:1:28:ASP:O	27:1:31:ILE:HG22	2.09	0.53
1:A:113:A:OP2	1:A:114:A:H5''	2.09	0.53
1:A:1209:C:C2	1:A:1210:G:C8	2.97	0.53
2:B:3041:C:C6	6:F:50:VAL:HG21	2.44	0.53
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.91	0.53
6:F:86:THR:HG23	37:F:7477:HOH:O	2.09	0.53
10:J:163:PRO:O	10:J:164:ALA:HB2	2.09	0.53
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.39	0.53
23:W:11:MET:HB3	23:W:15:GLU:HB2	1.90	0.53
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.41	0.53
1:A:2089:A:O2'	1:A:2090:G:H5'	2.09	0.53
1:A:256:C:H2'	1:A:257:G:O4'	2.08	0.53
1:A:516:A:P	37:A:5623:HOH:O	2.67	0.53
3:C:18:ALA:O	3:C:20:SER:N	2.38	0.53
7:G:93:MET:HE1	7:G:165:GLY:N	2.24	0.53
14:N:76:ARG:HG2	14:N:76:ARG:HH11	1.73	0.53
1:A:21:G:H4'	19:S:2:ILE:HG22	1.90	0.53
29:3:48:ASP:O	29:3:49:GLU:HB2	2.10	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.52
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.73	0.52
1:A:2478:U:O2'	1:A:2479:A:H5'	2.09	0.52
1:A:512:G:O3'	1:A:513:A:H8	1.92	0.52
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.90	0.52
13:M:149:ARG:O	13:M:150:GLN:HB2	2.09	0.52
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.24	0.52
2:B:3006:C:P	15:O:37:ARG:NH1	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:89:GLY:O	15:O:92:ALA:HB3	2.09	0.52
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.73	0.52
1:A:1675:C:H5''	29:3:5:LYS:HD2	1.91	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.56	0.52
1:A:1268:C:O2'	26:Z:169:ARG:HB2	2.08	0.52
1:A:1353:C:O5'	37:A:4652:HOH:O	2.19	0.52
1:A:2015:A:H2'	1:A:2016:U:O4'	2.09	0.52
1:A:2911:C:H3'	37:A:5528:HOH:O	2.09	0.52
1:A:415:A:O2'	1:A:416:G:H5'	2.09	0.52
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.75	0.52
4:D:74:ILE:HG13	37:D:8603:HOH:O	2.08	0.52
6:F:64:ARG:O	6:F:67:ASP:OD2	2.26	0.52
37:A:3818:HOH:O	10:J:11:LYS:HE2	2.08	0.52
16:P:21:SER:OG	16:P:106:PRO:HB2	2.09	0.52
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.91	0.52
26:Z:144:ARG:NH2	37:Z:8612:HOH:O	2.42	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.52
1:A:1192:A:H3'	1:A:1193:A:H5'	1.90	0.52
9:I:63:ARG:O	9:I:67:LEU:HG	2.09	0.52
37:A:9312:HOH:O	27:1:16:PRO:HG3	2.10	0.52
1:A:1535:G:H2'	1:A:1536:C:C6	2.44	0.52
1:A:2004:U:H5''	1:A:2005:G:C8	2.45	0.52
1:A:2604:A:H5'	37:A:5768:HOH:O	2.10	0.52
1:A:2780:C:H2'	1:A:2781:U:H6	1.73	0.52
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.91	0.52
5:E:242:GLU:HG3	37:E:8383:HOH:O	2.09	0.52
37:A:6303:HOH:O	6:F:55:LYS:HB2	2.10	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.72	0.52
7:G:69:ILE:HA	7:G:72:MET:HE3	1.91	0.52
15:O:119:GLN:O	15:O:123:ILE:HG13	2.09	0.52
20:T:81:ILE:HG23	37:T:8335:HOH:O	2.09	0.52
1:A:1058:A:H2'	1:A:1060:C:H5''	1.90	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.57	0.52
1:A:1666:C:C2'	1:A:1667:A:C5'	2.88	0.52
1:A:1829:A:H2'	1:A:1830:C:H5'	1.92	0.52
1:A:2833:C:C2	1:A:2848:G:N2	2.78	0.52
1:A:834:G:H5''	1:A:835:U:O5'	2.10	0.52
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.52
4:D:297:VAL:HB	37:D:8603:HOH:O	2.10	0.52
4:D:76:THR:N	4:D:77:PRO:HD3	2.25	0.52
6:F:11:HIS:O	6:F:12:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:163:VAL:HA	37:F:6326:HOH:O	2.09	0.52
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.39	0.52
11:K:45:VAL:HG23	11:K:130:VAL:O	2.08	0.52
17:Q:115:SER:O	17:Q:117:SER:N	2.43	0.52
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.57	0.52
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.10	0.52
1:A:160:A:C4	1:A:177:A:C2	2.98	0.52
1:A:2638:G:H5'	37:A:4902:HOH:O	2.09	0.52
1:A:285:A:H2'	1:A:286:U:O4'	2.09	0.52
1:A:92:G:H4'	23:W:44:GLY:HA3	1.91	0.52
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.43	0.52
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.45	0.52
1:A:1003:U:O2	10:J:90:PHE:CZ	2.62	0.52
1:A:1119:G:C8	11:K:52:GLN:NE2	2.78	0.52
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.10	0.52
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.40	0.52
1:A:1269:G:H2'	1:A:1270:U:C6	2.45	0.52
1:A:2795:C:O2'	1:A:2796:U:H5'	2.09	0.52
1:A:344:C:H2'	1:A:345:G:O4'	2.09	0.52
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.10	0.52
3:C:191:GLY:HA2	3:C:194:MET:CE	2.40	0.52
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.43	0.52
4:D:87:TYR:O	4:D:138:GLY:N	2.36	0.52
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.56	0.52
6:F:94:ALA:O	6:F:95:THR:O	2.28	0.52
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.27	0.52
16:P:25:VAL:HG23	16:P:26:TRP:H	1.74	0.52
19:S:39:THR:HB	19:S:42:GLU:CD	2.29	0.52
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.91	0.52
1:A:1015:C:H2'	1:A:1016:U:H6	1.74	0.52
1:A:2819:C:H2'	1:A:2820:A:C8	2.44	0.52
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.52
1:A:920:C:H5'	1:A:921:G:C4	2.45	0.52
37:A:5053:HOH:O	4:D:216:LYS:HA	2.09	0.52
8:H:2:VAL:HG11	14:N:23:LEU:HD23	1.91	0.52
10:J:5:MET:HG3	37:J:8367:HOH:O	2.09	0.52
11:K:19:MET:HE1	11:K:79:PHE:HA	1.91	0.52
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.74	0.52
1:A:1752:G:H2'	37:A:7541:HOH:O	2.10	0.52
1:A:283:U:H5	1:A:284:C:N4	2.07	0.52
1:A:394:G:H1	14:N:181:GLU:CD	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:U:O4	37:A:9155:HOH:O	2.19	0.52
2:B:3107:C:C5	37:B:3167:HOH:O	2.54	0.52
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.91	0.52
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.91	0.52
7:G:21:THR:HG23	7:G:30:THR:OG1	2.10	0.52
37:B:5071:HOH:O	15:O:20:TYR:CE2	2.54	0.52
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.90	0.52
1:A:1139:U:H2'	1:A:1140:C:C6	2.45	0.52
1:A:1119:G:N2	1:A:1246:A:H2	2.04	0.52
1:A:1666:C:C2'	1:A:1667:A:H5'	2.38	0.52
1:A:2256:G:C2'	1:A:2257:G:H5'	2.40	0.52
3:C:105:VAL:CG1	3:C:106:CYS:N	2.72	0.52
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.09	0.52
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.55	0.52
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.45	0.52
14:N:164:THR:HB	37:N:8520:HOH:O	2.10	0.52
27:1:13:ARG:NH1	37:1:8420:HOH:O	2.37	0.51
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.51
1:A:1056:U:H2'	1:A:1057:A:O4'	2.10	0.51
1:A:1555:G:H4'	1:A:1630:A:H2	1.75	0.51
1:A:2536:C:OP1	37:A:3089:HOH:O	2.19	0.51
1:A:2760:C:H5''	37:A:5303:HOH:O	2.10	0.51
2:B:3029:C:C2'	2:B:3030:C:H5'	2.40	0.51
7:G:68:HIS:O	7:G:72:MET:HG3	2.10	0.51
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.40	0.51
13:M:21:ARG:N	37:M:8536:HOH:O	2.43	0.51
37:A:7212:HOH:O	14:N:13:LYS:HE2	2.10	0.51
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.39	0.51
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.45	0.51
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.92	0.51
1:A:1209:C:O2	1:A:1210:G:C8	2.63	0.51
1:A:1701:A:H4'	1:A:1702:U:C5'	2.40	0.51
1:A:952:G:H4'	37:A:4002:HOH:O	2.11	0.51
37:A:7009:HOH:O	3:C:211:LYS:HG2	2.09	0.51
7:G:77:THR:OG1	7:G:78:GLU:N	2.41	0.51
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.09	0.51
19:S:132:ARG:NH2	37:S:8583:HOH:O	2.41	0.51
20:T:23:LYS:HD3	20:T:65:VAL:HG12	1.91	0.51
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.51
1:A:1189:A:H1'	1:A:1209:C:O4'	2.11	0.51
1:A:189:A:OP1	14:N:171:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2010:A:C2'	37:A:5935:HOH:O	2.58	0.51
2:B:3092:G:H2'	2:B:3093:A:C8	2.45	0.51
3:C:192:VAL:CG1	3:C:192:VAL:O	2.58	0.51
10:J:150:LYS:HE2	37:J:8381:HOH:O	2.10	0.51
10:J:4:ALA:HB3	37:J:8367:HOH:O	2.11	0.51
10:J:71:TYR:O	10:J:73:GLN:N	2.43	0.51
15:O:157:PRO:HA	37:O:8527:HOH:O	2.09	0.51
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.75	0.51
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.55	0.51
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.25	0.51
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.44	0.51
1:A:113:A:OP2	1:A:114:A:H2'	2.10	0.51
1:A:629:A:C2	1:A:2074:A:C2	2.99	0.51
1:A:2768:A:H3'	37:A:4392:HOH:O	2.11	0.51
1:A:440:C:H2'	1:A:441:A:C8	2.45	0.51
1:A:558:C:H2'	1:A:559:U:H5''	1.92	0.51
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.10	0.51
13:M:148:GLU:HB2	37:M:8592:HOH:O	2.09	0.51
13:M:77:ALA:HB3	37:M:8535:HOH:O	2.09	0.51
14:N:137:ASP:HA	14:N:142:LYS:HE3	1.92	0.51
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.40	0.51
23:W:4:HIS:O	23:W:8:ILE:HG13	2.11	0.51
26:Z:115:ARG:NE	37:Z:8557:HOH:O	2.43	0.51
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.38	0.51
1:A:1667:A:H2'	1:A:1668:U:C6	2.46	0.51
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.51
1:A:2812:A:H1'	37:A:5767:HOH:O	2.09	0.51
1:A:661:G:C4	1:A:686:A:C2	2.99	0.51
5:E:16:VAL:HG12	5:E:17:ASP:H	1.74	0.51
5:E:233:THR:CG2	5:E:234:VAL:N	2.74	0.51
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.39	0.51
10:J:157:ILE:CG2	10:J:158:ASN:N	2.73	0.51
10:J:166:ASN:ND2	10:J:166:ASN:N	2.58	0.51
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.44	0.51
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.75	0.51
1:A:51:G:N2	1:A:111:C:C2	2.78	0.51
1:A:657:G:OP1	5:E:27:ARG:NH2	2.40	0.51
1:A:920:C:H5''	1:A:921:G:O5'	2.10	0.51
1:A:963:C:H6	1:A:963:C:O5'	1.93	0.51
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.11	0.51
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:57:GLU:O	8:H:61:MET:HG3	2.09	0.51
10:J:127:GLY:O	10:J:128:ALA:CB	2.58	0.51
10:J:162:SER:CB	10:J:163:PRO:CD	2.79	0.51
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.09	0.51
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.51
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.92	0.51
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.75	0.51
1:A:1827:G:C6	1:A:1828:G:C6	2.99	0.51
4:D:175:LEU:HD23	4:D:175:LEU:O	2.10	0.51
5:E:1:MET:HG2	5:E:2:GLN:N	2.24	0.51
1:A:1134:G:C4'	10:J:151:MET:HE1	2.26	0.51
11:K:131:THR:HG22	11:K:133:GLY:N	2.26	0.51
11:K:142:ASN:O	11:K:144:THR:N	2.44	0.51
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.93	0.51
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.26	0.51
24:X:38:THR:HG22	24:X:39:ASP:H	1.76	0.51
1:A:1625:U:H5''	37:A:5999:HOH:O	2.11	0.51
1:A:2314:G:C2'	1:A:2315:C:H5'	2.40	0.51
1:A:2487:C:H5	37:A:4859:HOH:O	1.94	0.51
1:A:2506:A:O2'	1:A:2507:G:O5'	2.29	0.51
1:A:2613:G:O2'	1:A:2614:C:H5'	2.11	0.51
10:J:65:ARG:HB3	37:J:8387:HOH:O	2.10	0.51
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.92	0.51
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.40	0.51
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.37	0.51
29:3:18:ASN:ND2	29:3:40:ARG:H	2.09	0.51
1:A:1862:C:C2'	1:A:1863:G:H5'	2.41	0.51
1:A:1942:A:H3'	37:A:7334:HOH:O	2.10	0.51
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.11	0.51
1:A:694:A:H2'	1:A:695:C:H5'	1.92	0.51
1:A:795:G:N3	1:A:817:G:C2	2.79	0.51
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.41	0.51
8:H:59:ILE:O	8:H:59:ILE:HG22	2.10	0.51
1:A:21:G:H5''	19:S:1:GLY:O	2.11	0.51
1:A:317:A:H5''	21:U:52:ARG:HD2	1.93	0.51
27:1:10:ARG:HG3	27:1:11:THR:N	2.26	0.51
28:2:15:THR:O	28:2:29:THR:HG22	2.11	0.51
30:4:1:MET:N	30:4:87:ARG:O	2.41	0.51
1:A:1118:A:C8	1:A:1119:G:H5''	2.45	0.51
1:A:2326:U:H4'	1:A:2412:G:C4'	2.41	0.51
3:C:173:GLY:O	3:C:176:HIS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:205:VAL:O	4:D:307:ARG:NE	2.44	0.51
4:D:162:MET:CE	4:D:310:ARG:HD3	2.41	0.51
6:F:23:VAL:CG2	6:F:23:VAL:O	2.59	0.51
7:G:7:ILE:HD11	7:G:11:VAL:O	2.11	0.51
8:H:100:ASP:O	8:H:101:ALA:O	2.29	0.51
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.11	0.51
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
1:A:2730:G:O2'	1:A:2731:G:H5'	2.12	0.50
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.58	0.50
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.76	0.50
10:J:35:ASN:ND2	10:J:79:ALA:O	2.44	0.50
15:O:182:GLY:O	15:O:183:ASP:O	2.29	0.50
22:V:20:MET:CG	22:V:28:THR:HG23	2.41	0.50
1:A:1819:G:H5'	37:A:4684:HOH:O	2.12	0.50
1:A:2679:G:H2'	1:A:2681:A:OP2	2.11	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
10:J:129:ASN:HD22	10:J:129:ASN:N	2.09	0.50
11:K:45:VAL:HG22	11:K:46:ILE:N	2.25	0.50
6:F:146:LYS:HZ1	15:O:107:ASN:HD21	1.57	0.50
16:P:25:VAL:O	16:P:29:VAL:HG23	2.10	0.50
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.41	0.50
1:A:1015:C:H2'	1:A:1016:U:C6	2.46	0.50
1:A:306:A:P	21:U:38:ARG:HH21	2.34	0.50
1:A:922:A:N7	1:A:2281:C:H5'	2.25	0.50
5:E:133:ARG:NH2	37:E:8428:HOH:O	2.43	0.50
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.11	0.50
13:M:30:ARG:NH2	37:M:8525:HOH:O	2.33	0.50
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.73	0.50
14:N:78:ASN:ND2	37:N:8642:HOH:O	2.37	0.50
1:A:952:G:OP1	18:R:42:LYS:HE2	2.11	0.50
19:S:34:GLU:HG2	19:S:46:TYR:OH	2.11	0.50
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.46	0.50
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.92	0.50
27:1:59:HIS:HA	37:1:8440:HOH:O	2.11	0.50
1:A:2121:G:O2'	1:A:2122:C:H5'	2.12	0.50
1:A:257:G:O2'	1:A:258:G:H5'	2.10	0.50
1:A:539:G:H2'	1:A:540:A:C8	2.46	0.50
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.75	0.50
4:D:138:GLY:O	4:D:139:ASP:O	2.29	0.50
8:H:28:ALA:CB	8:H:99:THR:HG23	2.41	0.50
2:B:3008:G:O6	15:O:11:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:32:PRO:HD2	15:O:99:GLU:O	2.12	0.50
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.59	0.50
23:W:49:LEU:O	23:W:53:ILE:HG13	2.11	0.50
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.54	0.50
1:A:522:U:O2'	1:A:1366:C:H5'	2.12	0.50
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.47	0.50
1:A:816:G:C6	1:A:817:G:N1	2.79	0.50
37:A:4036:HOH:O	4:D:27:ASN:HB2	2.12	0.50
11:K:22:VAL:O	11:K:26:VAL:HG23	2.12	0.50
14:N:61:ILE:N	14:N:61:ILE:HD12	2.26	0.50
15:O:163:PHE:HA	37:O:8564:HOH:O	2.09	0.50
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.17	0.50
16:P:44:ASN:HA	16:P:65:LEU:O	2.11	0.50
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.12	0.50
26:Z:122:ARG:NH2	37:Z:8536:HOH:O	2.45	0.50
1:A:1681:G:H5''	1:A:1682:A:H5'	1.93	0.50
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.76	0.50
1:A:2433:A:H2'	1:A:2434:A:H8	1.76	0.50
1:A:2713:G:O2'	1:A:2714:U:H5'	2.12	0.50
1:A:653:C:H2'	1:A:654:A:C8	2.45	0.50
3:C:132:ASP:OD1	3:C:133:ARG:N	2.42	0.50
6:F:36:ASN:HA	37:F:7500:HOH:O	2.12	0.50
10:J:53:PRO:HG3	10:J:127:GLY:H	1.77	0.50
15:O:149:GLU:O	15:O:152:GLU:HB2	2.12	0.50
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.77	0.50
22:V:34:SER:O	22:V:38:ASN:ND2	2.45	0.50
24:X:76:ASP:O	24:X:77:ALA:C	2.50	0.50
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.11	0.50
28:2:28:HIS:CD2	28:2:31:LYS:H	2.30	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50
1:A:514:G:H8	1:A:514:G:O5'	1.95	0.50
1:A:820:G:C5	3:C:171:LYS:HB2	2.47	0.50
3:C:192:VAL:O	3:C:207:GLN:HG2	2.11	0.50
3:C:8:ARG:NH1	37:C:8553:HOH:O	2.32	0.50
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.09	0.50
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.93	0.50
10:J:26:LYS:CD	10:J:28:ILE:HB	2.42	0.50
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.59	0.50
19:S:40:ALA:O	19:S:44:VAL:HG23	2.11	0.50
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.26	0.50
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:C:O5'	1:A:40:C:H6	1.95	0.50
1:A:703:G:O2'	1:A:704:C:H5'	2.11	0.50
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.94	0.50
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.94	0.50
6:F:10:PHE:CD1	6:F:11:HIS:N	2.80	0.50
9:I:23:ILE:O	9:I:27:ILE:HG13	2.11	0.50
29:3:39:ARG:NH1	37:3:6391:HOH:O	2.45	0.50
1:A:1669:A:H2'	1:A:1670:G:C8	2.47	0.50
1:A:1783:A:O2'	1:A:1784:U:H5'	2.11	0.50
1:A:2073:G:OP2	1:A:2490:A:H5'	2.12	0.50
1:A:590:A:C2'	1:A:591:A:H5'	2.42	0.50
3:C:192:VAL:HG12	3:C:192:VAL:O	2.11	0.50
4:D:280:VAL:HG13	4:D:334:SER:HA	1.94	0.50
37:A:9870:HOH:O	11:K:46:ILE:HA	2.12	0.50
15:O:170:GLU:O	15:O:174:GLU:HG3	2.12	0.50
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.46	0.50
24:X:38:THR:HG22	24:X:39:ASP:N	2.27	0.50
24:X:5:VAL:O	24:X:52:VAL:HG22	2.11	0.50
24:X:88:THR:CG2	24:X:89:ASP:H	2.20	0.50
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
1:A:1434:A:H2'	1:A:1436:C:C5	2.46	0.49
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
1:A:949:U:O2'	18:R:40:HIS:HE1	1.95	0.49
2:B:3009:C:OP2	37:B:466:HOH:O	2.19	0.49
4:D:2:GLN:HA	37:D:8618:HOH:O	2.12	0.49
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.25	0.49
5:E:236:THR:O	5:E:237:GLU:C	2.49	0.49
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.92	0.49
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.46	0.49
14:N:14:ARG:HB3	14:N:17:GLU:HG3	1.94	0.49
1:A:1250:C:O2'	1:A:1251:C:H5'	2.11	0.49
1:A:2769:C:O2'	1:A:2770:G:H5'	2.12	0.49
1:A:316:A:N3	1:A:336:G:O2'	2.43	0.49
1:A:603:A:H4'	1:A:604:G:O5'	2.12	0.49
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.26	0.49
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.47	0.49
5:E:43:LYS:NZ	37:E:8390:HOH:O	2.37	0.49
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.94	0.49
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.12	0.49
1:A:1850:U:H2'	1:A:1851:G:H8	1.76	0.49
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:A:H2'	1:A:640:G:C8	2.46	0.49
1:A:714:U:H3'	37:A:6924:HOH:O	2.12	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.12	0.49
6:F:99:ASP:HB2	6:F:103:ASN:H	1.77	0.49
1:A:1450:C:O2'	1:A:1494:A:H5'	2.13	0.49
1:A:664:U:O4	1:A:681:G:H5''	2.12	0.49
6:F:58:VAL:HG12	6:F:59:GLY:N	2.27	0.49
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.49
37:B:7568:HOH:O	15:O:107:ASN:HB3	2.10	0.49
15:O:58:LEU:CD1	15:O:58:LEU:N	2.75	0.49
15:O:71:TRP:N	37:O:8538:HOH:O	2.44	0.49
1:A:1500:U:P	17:Q:41:ARG:HH22	2.35	0.49
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.94	0.49
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.95	0.49
1:A:1209:C:H2'	1:A:1210:G:C8	2.44	0.49
1:A:2251:G:H2'	1:A:2252:A:C8	2.48	0.49
1:A:2359:G:H3'	37:A:5667:HOH:O	2.12	0.49
1:A:2756:U:H3	1:A:2896:A:H2	1.58	0.49
1:A:400:C:O3'	37:A:5770:HOH:O	2.20	0.49
2:B:3023:U:C4'	2:B:3024:U:OP2	2.56	0.49
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.42	0.49
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.37	0.49
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.94	0.49
1:A:2064:U:H5'	1:A:2652:U:O3'	2.13	0.49
1:A:2265:U:H2'	1:A:2266:A:C8	2.48	0.49
1:A:2502:C:C4'	10:J:151:MET:HG2	2.43	0.49
3:C:55:VAL:HG22	3:C:68:ILE:O	2.12	0.49
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.47	0.49
1:A:449:A:N7	5:E:43:LYS:HG2	2.27	0.49
8:H:37:THR:O	8:H:41:GLU:HG3	2.12	0.49
13:M:134:GLU:HA	13:M:138:GLY:O	2.13	0.49
1:A:1174:A:C5	1:A:1201:C:H4'	2.47	0.49
1:A:1268:C:O2'	1:A:1269:G:H5'	2.12	0.49
1:A:154:C:H2'	1:A:155:C:H6	1.77	0.49
1:A:195:C:H2'	1:A:196:G:H5'	1.94	0.49
1:A:2271:G:P	37:A:9418:HOH:O	2.70	0.49
1:A:2346:C:O3'	6:F:52:THR:HG23	2.11	0.49
1:A:2459:G:P	30:4:64:LYS:HB2	2.52	0.49
1:A:960:G:N3	1:A:960:G:C2'	2.75	0.49
1:A:820:G:C6	3:C:171:LYS:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:ALA:O	5:E:78:ARG:HG3	2.12	0.49
8:H:91:VAL:CG1	8:H:92:GLY:H	2.20	0.49
10:J:53:PRO:HA	10:J:125:VAL:O	2.13	0.49
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.12	0.49
20:T:80:ARG:NH1	37:T:8344:HOH:O	2.45	0.49
25:Y:30:MET:HE3	25:Y:59:TRP:HE1	1.77	0.49
1:A:1657:A:H2'	1:A:1658:A:C8	2.47	0.49
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.49
1:A:2488:A:H61	1:A:2534:C:H42	1.61	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.11	0.49
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.43	0.49
4:D:177:HIS:O	4:D:181:ILE:HG13	2.13	0.49
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.49
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.43	0.49
10:J:33:MET:SD	10:J:65:ARG:HD2	2.53	0.49
14:N:77:PHE:HD2	37:N:8527:HOH:O	1.94	0.49
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	0.49
1:A:1218:U:H2'	1:A:1219:U:C6	2.47	0.49
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.49
1:A:1723:G:H2'	37:A:9608:HOH:O	2.13	0.49
1:A:1890:U:H4'	1:A:2010:A:C6	2.48	0.49
1:A:2011:A:P	37:A:5935:HOH:O	2.71	0.49
1:A:2083:A:C8	37:A:7572:HOH:O	2.54	0.49
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.93	0.49
1:A:470:U:O2'	28:2:16:HIS:CD2	2.65	0.49
1:A:95:A:H5''	1:A:97:G:O4'	2.13	0.49
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.12	0.49
6:F:102:GLY:O	6:F:134:LEU:HD12	2.13	0.49
7:G:7:ILE:HG22	7:G:45:ASP:O	2.13	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.95	0.49
18:R:28:ARG:HG2	37:R:4350:HOH:O	2.13	0.49
30:4:31:THR:HB	30:4:33:MET:CE	2.42	0.49
1:A:1213:C:C2'	1:A:1214:G:H5'	2.43	0.49
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.95	0.49
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.42	0.49
5:E:7:ASP:OD1	5:E:11:ASN:O	2.31	0.49
7:G:118:ILE:HG23	7:G:144:THR:HG21	1.95	0.49
14:N:77:PHE:O	14:N:77:PHE:CD1	2.65	0.49
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.95	0.49
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.48	0.49
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:52:THR:HG22	22:V:54:THR:N	2.28	0.49
1:A:1829:A:N6	27:1:18:TYR:HA	2.28	0.48
1:A:1594:C:O2'	1:A:1607:A:H4'	2.13	0.48
1:A:2894:C:O2'	1:A:2895:C:H5'	2.13	0.48
1:A:432:G:O2'	1:A:433:C:H5'	2.13	0.48
1:A:739:G:N7	37:A:7536:HOH:O	2.44	0.48
1:A:812:A:H2'	1:A:813:C:C6	2.48	0.48
4:D:140:LEU:HD23	37:D:8577:HOH:O	2.13	0.48
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.94	0.48
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.95	0.48
1:A:97:G:C2	21:U:107:LYS:HD2	2.47	0.48
25:Y:36:HIS:CE1	25:Y:40:HIS:CD2	3.01	0.48
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.42	0.48
1:A:1189:A:O2'	1:A:1208:C:H2'	2.13	0.48
1:A:1197:G:N2	37:A:6214:HOH:O	2.46	0.48
1:A:187:A:H3'	1:A:188:C:H6	1.77	0.48
1:A:201:G:N2	1:A:202:U:C2	2.81	0.48
1:A:2269:C:C2'	1:A:2270:G:H5'	2.43	0.48
1:A:2459:G:OP1	30:4:64:LYS:N	2.25	0.48
1:A:428:G:OP1	37:A:6202:HOH:O	2.19	0.48
1:A:542:A:H1'	37:A:4650:HOH:O	2.13	0.48
2:B:3049:G:H2'	2:B:3050:G:O4'	2.13	0.48
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.42	0.48
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.60	0.48
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.94	0.48
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.26	0.48
37:A:6017:HOH:O	30:4:84:ARG:HB3	2.13	0.48
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.76	0.48
1:A:1205:U:C2'	1:A:1206:U:C5'	2.90	0.48
1:A:790:A:H1'	1:A:1710:A:H2'	1.95	0.48
1:A:2464:C:H5''	1:A:2465:A:OP1	2.13	0.48
1:A:2630:G:O6	3:C:206:ARG:NH2	2.46	0.48
4:D:301:VAL:HG13	4:D:302:PRO:HD2	1.95	0.48
4:D:85:ARG:NH1	37:D:8634:HOH:O	2.46	0.48
6:F:59:GLY:O	6:F:61:PHE:N	2.36	0.48
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.96	0.48
14:N:36:ALA:HB1	37:N:8549:HOH:O	2.13	0.48
1:A:2365:G:H4'	18:R:45:PRO:O	2.13	0.48
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.13	0.48
37:L:7438:HOH:O	22:V:20:MET:HE1	2.12	0.48
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:G:H5'	37:A:5905:HOH:O	2.12	0.48
1:A:120:A:H2'	1:A:120:A:N3	2.27	0.48
1:A:1593:C:OP1	17:Q:117:SER:CB	2.62	0.48
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.94	0.48
1:A:2432:C:H4'	30:4:36:ILE:HG12	1.95	0.48
1:A:2524:G:H21	1:A:2526:C:N4	2.11	0.48
1:A:2598:U:O2	1:A:2600:A:H8	1.96	0.48
31:A:9000:TYK:H7A2	31:A:9000:TYK:O2A	2.13	0.48
4:D:4:SER:O	4:D:5:ARG:HB2	2.14	0.48
19:S:33:ARG:NH2	37:S:8533:HOH:O	2.37	0.48
24:X:48:VAL:O	24:X:48:VAL:CG1	2.59	0.48
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.13	0.48
1:A:1444:G:O2'	1:A:1445:G:H5'	2.13	0.48
1:A:1589:G:N2	1:A:1605:G:H1'	2.28	0.48
1:A:1862:C:H1'	37:A:7204:HOH:O	2.14	0.48
1:A:1909:A:H2'	1:A:1910:A:C8	2.48	0.48
1:A:553:G:P	26:Z:204:ARG:NH2	2.86	0.48
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.43	0.48
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.42	0.48
4:D:274:GLU:HA	4:D:292:GLY:O	2.13	0.48
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.43	0.48
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.13	0.48
24:X:26:ILE:HG13	24:X:26:ILE:O	2.11	0.48
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.49	0.48
1:A:1699:C:H4'	37:A:6425:HOH:O	2.13	0.48
1:A:182:G:O2'	1:A:183:A:H5'	2.14	0.48
1:A:1840:A:OP1	37:A:9595:HOH:O	2.20	0.48
1:A:281:U:H3'	37:A:7191:HOH:O	2.14	0.48
2:B:3042:C:O2	6:F:76:ARG:NH1	2.47	0.48
3:C:51:ARG:NH2	37:C:8609:HOH:O	2.47	0.48
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.95	0.48
12:L:101:ASN:O	12:L:102:GLU:HB2	2.13	0.48
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.44	0.48
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.14	0.48
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.42	0.48
1:A:1883:U:OP1	37:A:7834:HOH:O	2.20	0.48
1:A:1995:G:O2'	1:A:1997:A:N7	2.46	0.48
1:A:2501:G:H1'	37:A:4515:HOH:O	2.13	0.48
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.14	0.48
1:A:2815:G:OP2	11:K:99:GLU:HG2	2.14	0.48
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:123:ASP:OD1	14:N:123:ASP:C	2.52	0.48
14:N:12:TRP:CZ2	14:N:20:ILE:HD11	2.48	0.48
16:P:54:GLU:HG2	16:P:73:ASP:O	2.14	0.48
1:A:2133:U:H4'	1:A:2134:G:H5'	1.96	0.48
1:A:241:A:C2	1:A:378:A:H4'	2.49	0.48
1:A:716:G:H2'	1:A:717:C:O5'	2.14	0.48
3:C:105:VAL:HG12	3:C:106:CYS:H	1.79	0.48
4:D:54:VAL:O	4:D:55:ASN:C	2.51	0.48
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.43	0.48
11:K:93:ARG:HH11	11:K:93:ARG:CB	2.22	0.48
13:M:133:VAL:HB	37:M:8563:HOH:O	2.13	0.48
13:M:143:THR:CG2	13:M:144:ASP:H	2.26	0.48
37:B:4707:HOH:O	15:O:147:ILE:HB	2.14	0.48
24:X:122:ARG:NH1	24:X:122:ARG:CG	2.74	0.48
1:A:1183:C:N4	37:A:4370:HOH:O	2.42	0.48
1:A:1328:A:N7	1:A:1329:A:C5	2.82	0.48
1:A:1976:G:O2'	1:A:1977:U:H5'	2.13	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.43	0.48
1:A:2361:A:H5''	37:A:9001:HOH:O	2.14	0.48
8:H:34:ASN:O	8:H:38:LYS:HG3	2.14	0.48
10:J:39:GLY:O	10:J:41:THR:N	2.47	0.48
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.95	0.48
20:T:57:THR:C	20:T:59:ASP:H	2.17	0.48
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.79	0.48
1:A:1191:A:C3'	1:A:1192:A:H5''	2.39	0.48
1:A:1132:A:N6	1:A:1229:C:H2'	2.29	0.48
1:A:1925:G:OP1	30:4:29:ARG:NH2	2.47	0.48
1:A:2326:U:H4'	1:A:2412:G:H4'	1.96	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
1:A:602:A:O2'	1:A:605:C:H4'	2.14	0.48
8:H:117:GLU:C	8:H:119:ARG:H	2.17	0.48
1:A:2502:C:H4'	10:J:151:MET:HG2	1.96	0.48
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.96	0.48
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.94	0.48
15:O:171:HIS:CE1	37:O:8563:HOH:O	2.67	0.48
27:I:37:HIS:O	27:I:45:LYS:HA	2.13	0.47
1:A:2050:G:H5''	19:S:80:TYR:O	2.14	0.47
1:A:1562:C:H42	1:A:2738:G:H1	1.62	0.47
1:A:371:U:H2'	1:A:372:A:C8	2.47	0.47
1:A:450:C:H4'	5:E:46:TYR:CE1	2.49	0.47
1:A:731:U:O2'	1:A:732:C:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H2'	1:A:738:G:O4'	2.14	0.47
1:A:918:G:C2	1:A:926:A:C2	3.02	0.47
6:F:174:VAL:CG1	37:F:6555:HOH:O	2.61	0.47
6:F:84:LEU:C	6:F:86:THR:H	2.17	0.47
23:W:27:LEU:O	23:W:30:ALA:N	2.47	0.47
24:X:13:MET:HE1	24:X:18:GLN:HA	1.94	0.47
24:X:142:ASP:HB3	24:X:145:GLY:H	1.78	0.47
24:X:76:ASP:O	24:X:77:ALA:O	2.32	0.47
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.49	0.47
1:A:407:A:H5'	37:A:6003:HOH:O	2.13	0.47
5:E:180:SER:HB2	37:E:8450:HOH:O	2.14	0.47
37:A:7447:HOH:O	5:E:188:ARG:HD3	2.14	0.47
10:J:65:ARG:CZ	37:J:8387:HOH:O	2.62	0.47
11:K:130:VAL:HG12	11:K:131:THR:N	2.29	0.47
27:I:47:LEU:HD23	27:I:57:CYS:CB	2.44	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.49	0.47
1:A:1477:C:H5'	1:A:1868:G:C5'	2.45	0.47
1:A:2284:G:H5'	37:A:9440:HOH:O	2.13	0.47
1:A:457:U:H5	1:A:460:A:OP2	1.97	0.47
1:A:951:A:H2'	1:A:952:G:H5'	1.95	0.47
3:C:93:THR:C	3:C:94:LEU:HD23	2.34	0.47
4:D:248:ARG:O	4:D:251:VAL:HG12	2.14	0.47
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.90	0.47
12:L:40:THR:O	12:L:41:LYS:C	2.52	0.47
37:A:9583:HOH:O	14:N:165:SER:HB3	2.14	0.47
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.96	0.47
14:N:80:GLY:O	14:N:81:ARG:HD3	2.14	0.47
14:N:87:MET:CE	37:N:8530:HOH:O	2.63	0.47
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.49	0.47
24:X:40:ALA:O	24:X:44:MET:HG3	2.14	0.47
1:A:1773:G:H2'	1:A:1774:G:H5'	1.96	0.47
1:A:2724:U:H2'	1:A:2725:G:O4'	2.14	0.47
1:A:716:G:C2'	1:A:717:C:O5'	2.63	0.47
3:C:36:ASP:O	3:C:38:ILE:N	2.48	0.47
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.96	0.47
37:A:7447:HOH:O	5:E:188:ARG:CD	2.62	0.47
7:G:69:ILE:HA	7:G:72:MET:HE2	1.95	0.47
10:J:132:PHE:O	10:J:133:ILE:HD13	2.15	0.47
11:K:103:VAL:HG12	37:K:8563:HOH:O	2.15	0.47
15:O:141:ARG:N	37:O:8566:HOH:O	2.47	0.47
1:A:710:G:P	16:P:24:ALA:HB3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.12	0.47
18:R:75:ILE:HD11	18:R:84:ILE:HD11	1.96	0.47
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.47
1:A:130:C:H5'	37:A:5189:HOH:O	2.13	0.47
1:A:2000:G:O2'	1:A:2001:G:H5'	2.15	0.47
1:A:2353:A:H4'	1:A:2354:A:O5'	2.14	0.47
1:A:445:U:H1'	37:A:7324:HOH:O	2.14	0.47
4:D:279:THR:CG2	4:D:280:VAL:N	2.77	0.47
24:X:137:GLN:HG3	24:X:137:GLN:O	2.15	0.47
1:A:1850:U:H2'	1:A:1851:G:C8	2.48	0.47
1:A:1820:G:C6	1:A:2030:A:C2	3.03	0.47
1:A:2896:A:N3	1:A:2896:A:H2'	2.30	0.47
1:A:764:C:H2'	1:A:765:G:O4'	2.15	0.47
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.49	0.47
4:D:55:ASN:HB3	4:D:64:GLY:H	1.79	0.47
5:E:165:ASP:O	5:E:168:ARG:HB3	2.15	0.47
5:E:20:ASP:O	5:E:23:GLU:HB2	2.15	0.47
10:J:113:ALA:N	10:J:114:PRO:CD	2.78	0.47
10:J:163:PRO:HG2	37:J:8340:HOH:O	2.14	0.47
11:K:77:GLY:O	11:K:78:ILE:C	2.53	0.47
13:M:146:GLY:C	13:M:148:GLU:H	2.18	0.47
14:N:61:ILE:HA	37:N:8621:HOH:O	2.15	0.47
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.44	0.47
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.97	0.47
22:V:44:ARG:CB	37:V:3805:HOH:O	2.61	0.47
30:4:74:CYS:SG	30:4:76:LYS:CB	3.03	0.47
1:A:101:C:H2'	1:A:102:A:H8	1.80	0.47
1:A:1116:U:H3	1:A:1246:A:N6	2.03	0.47
1:A:125:U:H2'	37:A:3740:HOH:O	2.15	0.47
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.44	0.47
5:E:238:SER:HB3	37:E:8383:HOH:O	2.13	0.47
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.83	0.47
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.44	0.47
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.50	0.47
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.30	0.47
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.50	0.47
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.49	0.47
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.15	0.47
1:A:1380:U:H5'	37:A:9211:HOH:O	2.14	0.47
1:A:2466:G:H8	37:A:9516:HOH:O	1.98	0.47
1:A:2718:C:H6	1:A:2718:C:H5'	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.96	0.47
12:L:101:ASN:O	12:L:102:GLU:CB	2.63	0.47
37:A:7413:HOH:O	21:U:9:LYS:HD2	2.14	0.47
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.14	0.47
30:4:17:HIS:O	30:4:18:GLN:HG3	2.15	0.47
1:A:1167:G:O2'	1:A:1168:C:H5'	2.15	0.47
1:A:1029:U:O2'	1:A:1273:C:OP1	2.30	0.47
1:A:222:A:H2'	1:A:223:G:O4'	2.14	0.47
1:A:2791:U:H1'	1:A:2792:A:H5''	1.96	0.47
3:C:88:ILE:O	3:C:88:ILE:HG22	2.14	0.47
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.14	0.47
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.97	0.47
28:2:5:THR:HB	28:2:6:PRO:CD	2.45	0.47
1:A:1333:U:H2'	1:A:1334:C:H6	1.78	0.47
1:A:1942:A:O2'	1:A:1943:C:H5'	2.15	0.47
1:A:2269:C:H2'	1:A:2270:G:H5'	1.96	0.47
1:A:2667:G:H1'	1:A:2914:A:N3	2.29	0.47
2:B:3064:C:C2'	2:B:3065:A:H5'	2.45	0.47
37:A:5383:HOH:O	3:C:164:ARG:NE	2.47	0.47
3:C:2:ARG:NH1	37:C:8513:HOH:O	2.29	0.47
3:C:55:VAL:HG13	3:C:67:LEU:HD22	1.97	0.47
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.15	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.80	0.47
21:U:41:ARG:NH1	21:U:42:VAL:O	2.48	0.47
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.13	0.47
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.29	0.47
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.14	0.47
1:A:2106:C:H2'	1:A:2107:U:C6	2.50	0.47
1:A:778:C:C4	1:A:779:U:C4	3.03	0.47
4:D:175:LEU:C	4:D:175:LEU:CD2	2.82	0.47
6:F:92:GLU:O	6:F:93:LEU:O	2.33	0.47
7:G:84:MET:HB2	7:G:131:LEU:HB2	1.96	0.47
1:A:1003:U:O2	10:J:90:PHE:HZ	1.98	0.47
12:L:20:CYS:HB3	12:L:26:ALA:O	2.15	0.47
15:O:82:TYR:C	15:O:82:TYR:CD2	2.88	0.47
24:X:122:ARG:HH22	24:X:154:ARG:C	2.19	0.47
25:Y:73:ARG:O	25:Y:85:VAL:HG13	2.14	0.47
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.45	0.47
1:A:1114:A:H2'	1:A:1115:U:H6	1.79	0.46
1:A:1592:G:O2'	1:A:1593:C:O5'	2.33	0.46
1:A:1743:G:H1'	37:A:4863:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1829:A:H61	27:1:18:TYR:HA	1.80	0.46
1:A:2533:C:H5'	37:A:6882:HOH:O	2.15	0.46
1:A:2064:U:H4'	1:A:2653:A:OP1	2.15	0.46
2:B:3008:G:C6	2:B:3009:C:C4	3.03	0.46
2:B:3057:A:C8	6:F:141:VAL:HG21	2.50	0.46
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.97	0.46
5:E:246:ARG:NE	37:E:8426:HOH:O	2.48	0.46
1:A:675:U:O2'	5:E:42:ARG:NH1	2.48	0.46
1:A:2453:G:H4'	13:M:50:GLY:C	2.35	0.46
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.97	0.46
18:R:93:ARG:NH1	18:R:93:ARG:HG3	2.31	0.46
21:U:27:LEU:HD23	21:U:98:VAL:HB	1.97	0.46
26:Z:134:HIS:H	26:Z:134:HIS:CD2	2.33	0.46
30:4:69:TYR:O	30:4:77:ALA:HA	2.15	0.46
1:A:1269:G:H2'	1:A:1270:U:H6	1.79	0.46
1:A:128:A:H3'	1:A:128:A:C8	2.50	0.46
1:A:1594:C:C2	1:A:1601:G:C2	3.03	0.46
1:A:1996:U:O2'	1:A:1997:A:H5'	2.15	0.46
1:A:818:A:O2'	27:1:13:ARG:HD3	2.15	0.46
1:A:1352:A:N1	5:E:48:SER:HB3	2.31	0.46
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.46	0.46
13:M:148:GLU:HG2	37:M:8558:HOH:O	2.14	0.46
14:N:87:MET:HB3	30:4:46:ILE:CD1	2.32	0.46
14:N:89:ASN:HA	37:N:8551:HOH:O	2.14	0.46
16:P:105:ASN:HD21	16:P:109:SER:H	1.64	0.46
21:U:38:ARG:NH1	37:U:6217:HOH:O	2.47	0.46
25:Y:79:GLU:OE2	37:Y:5564:HOH:O	2.21	0.46
28:2:29:THR:O	28:2:32:LYS:HE2	2.16	0.46
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.46
1:A:1191:A:N1	1:A:1206:U:O4	2.48	0.46
1:A:1562:C:O2	1:A:1562:C:H2'	2.15	0.46
3:C:58:VAL:O	3:C:65:ARG:HD2	2.16	0.46
5:E:84:VAL:O	5:E:85:LYS:CB	2.63	0.46
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.45	0.46
13:M:107:LYS:HE3	13:M:124:ASP:OD2	2.15	0.46
13:M:14:GLY:N	37:M:8519:HOH:O	2.15	0.46
15:O:34:LEU:HA	15:O:47:LEU:CD2	2.45	0.46
28:2:28:HIS:O	28:2:32:LYS:N	2.43	0.46
30:4:38:ARG:O	30:4:42:ARG:HB2	2.16	0.46
30:4:74:CYS:SG	30:4:76:LYS:CG	3.03	0.46
1:A:1079:A:N1	1:A:2068:G:O2'	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:G:H2'	1:A:175:G:N2	2.31	0.46
1:A:567:U:O2'	1:A:568:G:H5'	2.14	0.46
6:F:154:LYS:H	6:F:154:LYS:CD	2.22	0.46
7:G:34:TRP:O	11:K:127:ILE:HD11	2.14	0.46
15:O:120:GLU:HG3	15:O:136:LEU:HD13	1.97	0.46
15:O:37:ARG:HA	15:O:37:ARG:HD3	1.78	0.46
26:Z:109:LEU:HA	37:Z:8571:HOH:O	2.14	0.46
1:A:1044:C:C5'	37:A:9022:HOH:O	2.61	0.46
1:A:2594:C:O2'	1:A:2595:U:H5'	2.16	0.46
1:A:401:C:P	37:A:5770:HOH:O	2.74	0.46
2:B:3014:G:H2'	2:B:3015:C:H5'	1.98	0.46
2:B:3088:G:OP1	24:X:130:HIS:NE2	2.46	0.46
3:C:109:GLU:HG2	3:C:116:GLY:H	1.81	0.46
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.79	0.46
4:D:146:THR:C	4:D:148:PRO:HD3	2.35	0.46
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.45	0.46
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.16	0.46
8:H:72:VAL:HA	8:H:73:PRO:HD3	1.84	0.46
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.16	0.46
15:O:154:LEU:HG	15:O:155:GLU:N	2.29	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.14	0.46
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.96	0.46
1:A:1086:A:N6	24:X:11:VAL:HG11	2.31	0.46
1:A:1375:A:O2'	1:A:1376:G:H5'	2.16	0.46
1:A:383:A:H4'	37:A:5304:HOH:O	2.16	0.46
1:A:665:A:H2'	1:A:666:A:C8	2.50	0.46
5:E:111:VAL:HB	37:E:8321:HOH:O	2.15	0.46
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.51	0.46
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.44	0.46
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.97	0.46
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.45	0.46
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.55	0.46
1:A:1391:G:H2'	1:A:1392:A:H5'	1.98	0.46
1:A:1398:G:H2'	1:A:1399:A:C8	2.51	0.46
1:A:1615:A:H5'	37:A:4155:HOH:O	2.14	0.46
1:A:1989:G:O2'	1:A:1990:C:H5'	2.15	0.46
1:A:1815:A:H4'	1:A:2751:C:O4'	2.16	0.46
1:A:278:A:H2'	1:A:279:C:O4'	2.16	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.51	0.46
7:G:64:THR:HG22	7:G:68:HIS:CD2	2.51	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.98	0.46
10:J:81:TYR:C	10:J:81:TYR:CD1	2.88	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.97	0.46
15:O:154:LEU:O	15:O:155:GLU:CB	2.64	0.46
15:O:182:GLY:N	37:O:8567:HOH:O	2.49	0.46
27:1:21:LYS:O	27:1:25:ARG:HG3	2.15	0.46
1:A:175:G:H2'	14:N:192:ALA:HB3	1.96	0.46
1:A:2506:A:H1'	37:A:6034:HOH:O	2.16	0.46
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.30	0.46
4:D:238:ASN:HD22	4:D:240:GLY:N	2.08	0.46
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.98	0.46
5:E:13:ASP:N	37:E:8446:HOH:O	2.49	0.46
6:F:101:THR:O	6:F:101:THR:HG22	2.16	0.46
6:F:169:THR:O	6:F:170:TYR:HB2	2.16	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46
11:K:126:ASN:O	11:K:129:PHE:HE2	1.99	0.46
13:M:72:ASN:HB2	37:M:8585:HOH:O	2.15	0.46
14:N:63:VAL:O	14:N:130:GLU:HA	2.16	0.46
14:N:87:MET:SD	37:N:8532:HOH:O	2.61	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.30	0.46
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.51	0.46
1:A:1185:U:H5'	37:A:7456:HOH:O	2.16	0.46
1:A:13:G:H2'	1:A:14:C:H6	1.80	0.46
1:A:1474:C:C5'	1:A:1474:C:H6	2.18	0.46
1:A:1730:G:H5'	1:A:1731:C:C5	2.51	0.46
1:A:1754:A:N7	37:A:7857:HOH:O	2.36	0.46
1:A:1894:C:C2	1:A:1939:U:C4	3.03	0.46
1:A:2087:C:O2'	1:A:2088:C:H5'	2.15	0.46
1:A:2488:A:H2	37:A:7264:HOH:O	1.98	0.46
1:A:2564:G:OP2	1:A:2565:C:H5''	2.16	0.46
1:A:259:G:H21	14:N:58:GLN:NE2	2.14	0.46
1:A:402:U:H2'	1:A:403:C:C6	2.50	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.41	0.46
1:A:677:C:H4'	5:E:246:ARG:NH2	2.31	0.46
2:B:3031:C:O2'	2:B:3032:G:H5'	2.15	0.46
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.46	0.46
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.98	0.46
4:D:51:VAL:HG23	4:D:329:TYR:O	2.16	0.46
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.98	0.46
8:H:58:GLU:HG3	8:H:61:MET:CE	2.45	0.46
11:K:54:VAL:HG11	11:K:138:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:87:ARG:NH1	37:L:4066:HOH:O	2.48	0.46
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.49	0.46
15:O:50:LEU:HB2	37:O:8524:HOH:O	2.16	0.46
25:Y:14:LEU:HD12	25:Y:67:PRO:O	2.16	0.46
1:A:2121:G:H5'	37:A:3491:HOH:O	2.16	0.46
4:D:168:GLY:O	4:D:169:GLY:O	2.34	0.46
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.98	0.46
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.16	0.46
12:L:14:LYS:NZ	12:L:32:ILE:O	2.46	0.46
14:N:155:HIS:O	14:N:158:ARG:HG2	2.15	0.46
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.97	0.46
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.77	0.46
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.15	0.46
1:A:1398:G:O2'	1:A:1399:A:H5'	2.16	0.45
1:A:303:C:H2'	1:A:304:G:O4'	2.16	0.45
1:A:308:U:C4	1:A:342:C:H1'	2.50	0.45
1:A:553:G:H5'	37:A:3479:HOH:O	2.15	0.45
1:A:646:G:H2'	1:A:647:U:C6	2.51	0.45
3:C:109:GLU:HG2	3:C:116:GLY:N	2.31	0.45
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.45
6:F:86:THR:CG2	37:F:7477:HOH:O	2.64	0.45
7:G:11:VAL:HG11	7:G:22:VAL:HG13	1.97	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.98	0.45
9:I:64:ASN:O	9:I:68:GLU:HG3	2.15	0.45
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.97	0.45
1:A:2435:U:P	30:4:28:GLY:HA3	2.56	0.45
1:A:1114:A:H2'	1:A:1115:U:C6	2.52	0.45
1:A:1407:A:O2'	1:A:1408:U:H3'	2.17	0.45
1:A:1441:G:H1'	37:A:7762:HOH:O	2.16	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.17	0.45
14:N:98:GLN:NE2	14:N:117:SER:O	2.49	0.45
16:P:96:VAL:HA	37:P:4258:HOH:O	2.16	0.45
24:X:139:GLY:O	24:X:141:HIS:CD2	2.68	0.45
26:Z:115:ARG:CZ	37:Z:8557:HOH:O	2.64	0.45
1:A:517:U:H2'	1:A:518:G:H5'	1.97	0.45
1:A:657:G:H2'	1:A:658:C:C6	2.52	0.45
4:D:215:VAL:HA	4:D:220:VAL:HG22	1.97	0.45
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.98	0.45
4:D:316:ARG:N	4:D:317:PRO:HD3	2.32	0.45
1:A:2719:A:C2	4:D:70:PRO:HG3	2.51	0.45
6:F:53:LYS:HA	6:F:67:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:LEU:HG	37:F:3862:HOH:O	2.16	0.45
10:J:157:ILE:HG22	10:J:158:ASN:N	2.31	0.45
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.52	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
12:L:125:ALA:C	12:L:127:ALA:H	2.19	0.45
14:N:57:LYS:HE2	14:N:140:ALA:O	2.16	0.45
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.45
28:2:52:SER:HA	37:2:4248:HOH:O	2.15	0.45
1:A:2112:A:H2'	1:A:2113:G:C8	2.52	0.45
1:A:2314:G:H2'	1:A:2315:C:H5'	1.98	0.45
1:A:2421:G:H4'	37:A:4751:HOH:O	2.17	0.45
1:A:2445:U:H2'	1:A:2446:G:C8	2.51	0.45
1:A:319:A:H4'	1:A:338:C:C5	2.51	0.45
1:A:683:G:O2'	1:A:684:G:H5'	2.16	0.45
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.45
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.82	0.45
4:D:198:GLU:HB3	37:D:8593:HOH:O	2.16	0.45
4:D:1:PRO:O	4:D:2:GLN:HB2	2.17	0.45
5:E:236:THR:C	37:E:8453:HOH:O	2.55	0.45
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.31	0.45
1:A:926:A:H1'	13:M:38:HIS:O	2.16	0.45
37:A:9401:HOH:O	14:N:52:LEU:HD23	2.17	0.45
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.97	0.45
24:X:88:THR:CG2	24:X:89:ASP:N	2.79	0.45
25:Y:71:ARG:HD2	37:Y:7542:HOH:O	2.16	0.45
1:A:1292:G:HO2'	1:A:1293:U:H6	1.62	0.45
1:A:1375:A:C2'	1:A:1376:G:H5'	2.46	0.45
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.16	0.45
1:A:2271:G:N3	1:A:2271:G:H2'	2.32	0.45
1:A:2403:C:H3'	37:A:5187:HOH:O	2.16	0.45
1:A:2406:U:C4	1:A:2407:G:N7	2.84	0.45
1:A:2577:A:H5'	37:A:7748:HOH:O	2.15	0.45
1:A:2776:A:H2'	1:A:2777:G:O4'	2.16	0.45
5:E:85:LYS:NZ	37:E:8325:HOH:O	2.42	0.45
37:A:4700:HOH:O	15:O:21:HIS:HD2	2.00	0.45
19:S:82:GLU:HG3	19:S:83:LYS:H	1.82	0.45
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.30	0.45
37:A:6492:HOH:O	29:3:1:GLY:HA3	2.15	0.45
1:A:1391:G:C5	1:A:1435:U:C4	3.04	0.45
1:A:1420:C:C2	1:A:1445:G:N2	2.84	0.45
1:A:1883:U:O2'	1:A:1884:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2505:G:H8	37:A:5616:HOH:O	2.00	0.45
1:A:2777:G:O2'	1:A:2778:A:H5'	2.16	0.45
1:A:35:U:O2'	1:A:36:C:H5'	2.17	0.45
1:A:558:C:C2	1:A:600:G:N2	2.84	0.45
1:A:746:A:C6	16:P:65:LEU:HD13	2.52	0.45
1:A:2272:G:H5'	3:C:223:ARG:HB2	1.99	0.45
4:D:280:VAL:CG1	4:D:281:ASP:N	2.80	0.45
6:F:40:ILE:HG23	37:F:5583:HOH:O	2.15	0.45
14:N:134:ILE:O	14:N:136:PRO:HD3	2.17	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.31	0.45
19:S:79:ARG:C	19:S:81:PRO:HD3	2.37	0.45
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.49	0.45
24:X:63:GLU:HG2	24:X:93:ILE:HG22	1.98	0.45
1:A:797:A:H5'	27:1:10:ARG:HG2	1.99	0.45
1:A:1161:A:H8	1:A:1161:A:O5'	2.00	0.45
1:A:1299:G:N2	37:A:4657:HOH:O	2.49	0.45
1:A:164:G:H3'	37:A:3620:HOH:O	2.17	0.45
1:A:2456:A:H2'	1:A:2457:U:C6	2.52	0.45
1:A:327:A:H2'	5:E:150:THR:OG1	2.16	0.45
1:A:424:C:H2'	1:A:425:U:C6	2.51	0.45
2:B:3093:A:C5	2:B:3094:G:H1'	2.52	0.45
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.15	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.45	0.45
9:I:12:ILE:HB	37:I:4714:HOH:O	2.16	0.45
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.16	0.45
37:A:9538:HOH:O	24:X:119:HIS:HE1	2.00	0.45
1:A:105:G:O2'	1:A:106:A:H5'	2.17	0.45
1:A:12:U:H2'	1:A:13:G:H5'	1.98	0.45
1:A:1592:G:C5	1:A:1593:C:C4	3.04	0.45
1:A:1878:G:O2'	1:A:1879:U:C6	2.68	0.45
1:A:2001:G:C2'	1:A:2002:C:H5'	2.47	0.45
1:A:2073:G:C6	1:A:2489:G:H4'	2.52	0.45
1:A:2356:A:H2'	1:A:2357:G:O4'	2.17	0.45
1:A:2456:A:H2'	1:A:2457:U:H6	1.82	0.45
1:A:2761:A:C4	1:A:2763:G:C8	3.04	0.45
1:A:324:G:O2'	1:A:325:U:H5'	2.16	0.45
1:A:426:G:H2'	1:A:427:C:O4'	2.15	0.45
1:A:69:A:H5'	1:A:69:A:C8	2.51	0.45
1:A:738:G:H3'	37:A:7031:HOH:O	2.16	0.45
1:A:766:A:H5'	37:A:4624:HOH:O	2.17	0.45
2:B:3035:C:H5''	37:B:4078:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:VAL:CG1	3:C:106:CYS:H	2.30	0.45
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.46	0.45
1:A:1687:C:O2	28:2:9:GLY:HA2	2.17	0.45
1:A:1834:C:H2'	1:A:1840:A:H62	1.78	0.45
1:A:2032:U:O2'	1:A:2033:G:H5''	2.17	0.45
1:A:2896:A:H5''	37:A:6079:HOH:O	2.16	0.45
1:A:565:A:OP2	1:A:592:G:N1	2.43	0.45
1:A:929:A:O5'	1:A:929:A:H8	2.00	0.45
2:B:3056:A:C3'	2:B:3057:A:H5''	2.47	0.45
4:D:132:HIS:HB2	4:D:137:LEU:HD22	1.99	0.45
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.00	0.45
4:D:243:ASN:HA	4:D:244:PRO:C	2.36	0.45
5:E:246:ARG:CB	5:E:246:ARG:HH11	2.24	0.45
7:G:11:VAL:HG12	7:G:12:ASP:H	1.82	0.45
7:G:43:ASP:HA	37:G:5864:HOH:O	2.16	0.45
10:J:84:ARG:CZ	10:J:135:TRP:CH2	3.00	0.45
14:N:84:LYS:O	14:N:87:MET:CG	2.65	0.45
1:A:1010:C:H4'	15:O:4:PRO:HB2	1.99	0.45
37:A:3749:HOH:O	22:V:17:THR:CG2	2.64	0.45
24:X:48:VAL:HG12	24:X:48:VAL:O	2.15	0.45
27:1:46:LYS:NZ	37:1:8440:HOH:O	2.49	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
1:A:333:G:O2'	1:A:334:G:H5'	2.17	0.45
1:A:558:C:H2'	1:A:559:U:H5'	1.99	0.45
1:A:584:U:H3'	37:A:6075:HOH:O	2.15	0.45
1:A:679:G:OP2	37:A:4408:HOH:O	2.20	0.45
4:D:2:GLN:NE2	37:D:8618:HOH:O	2.50	0.45
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.85	0.45
9:I:12:ILE:HD12	37:I:692:HOH:O	2.16	0.45
10:J:117:LYS:O	10:J:119:VAL:HG13	2.17	0.45
10:J:26:LYS:HG2	10:J:28:ILE:N	2.24	0.45
1:A:251:C:H1'	14:N:58:GLN:HE22	1.81	0.45
24:X:122:ARG:CG	24:X:152:ALA:O	2.65	0.45
24:X:14:HIS:HB2	24:X:17:ILE:HG13	1.99	0.45
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.51	0.45
1:A:1669:A:H2	37:A:3678:HOH:O	2.00	0.44
1:A:1829:A:C2'	1:A:1830:C:H5'	2.46	0.44
1:A:2559:C:H4'	37:A:7243:HOH:O	2.17	0.44
1:A:328:U:O4'	5:E:202:THR:HG22	2.17	0.44
1:A:883:U:H2'	1:A:883:U:O2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3020:G:H3'	37:B:2984:HOH:O	2.17	0.44
2:B:3092:G:C6	2:B:3093:A:C6	3.06	0.44
5:E:187:ARG:HG3	5:E:187:ARG:O	2.16	0.44
7:G:95:VAL:O	7:G:126:ILE:HD13	2.17	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.47	0.44
10:J:150:LYS:NZ	37:J:8381:HOH:O	2.49	0.44
23:W:42:ASN:O	23:W:44:GLY:N	2.50	0.44
1:A:1004:C:O2'	1:A:1005:A:H5'	2.17	0.44
1:A:1139:U:H2'	1:A:1140:C:H6	1.82	0.44
1:A:1242:A:H5'	11:K:82:THR:CG2	2.38	0.44
1:A:2546:U:OP1	37:A:3821:HOH:O	2.21	0.44
1:A:2607:U:O5'	1:A:2609:G:H4'	2.16	0.44
1:A:2697:A:H2'	1:A:2698:G:O4'	2.16	0.44
1:A:558:C:C2'	1:A:559:U:C5'	2.95	0.44
1:A:84:G:O2'	1:A:85:C:H5'	2.17	0.44
2:B:3038:A:H2	2:B:3043:G:H5''	1.83	0.44
3:C:95:PRO:HA	3:C:153:ARG:HA	2.00	0.44
4:D:212:GLN:HB2	4:D:257:THR:CG2	2.41	0.44
5:E:218:VAL:HG12	37:E:8426:HOH:O	2.17	0.44
12:L:118:ALA:C	12:L:120:ARG:H	2.21	0.44
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.32	0.44
23:W:39:ALA:C	23:W:41:GLU:N	2.70	0.44
24:X:26:ILE:HB	37:X:5420:HOH:O	2.16	0.44
1:A:88:G:C8	29:3:28:LYS:HB2	2.52	0.44
37:N:8532:HOH:O	30:4:46:ILE:HB	2.17	0.44
1:A:1066:U:H2'	1:A:1067:A:C8	2.52	0.44
1:A:1412:U:O4	1:A:1681:G:H2'	2.18	0.44
1:A:2563:U:H2'	1:A:2565:C:O5'	2.17	0.44
1:A:282:C:H2'	1:A:283:U:O4'	2.16	0.44
1:A:883:U:C2'	1:A:883:U:O2	2.65	0.44
2:B:3014:G:C2'	2:B:3015:C:H5'	2.47	0.44
3:C:36:ASP:HB2	3:C:83:GLY:HA3	2.00	0.44
5:E:79:ARG:O	5:E:87:ARG:HG2	2.18	0.44
6:F:59:GLY:C	6:F:61:PHE:N	2.71	0.44
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.46	0.44
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.66	0.44
14:N:108:LYS:N	14:N:108:LYS:HD3	2.32	0.44
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.17	0.44
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.99	0.44
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.80	0.44
27:1:57:CYS:O	27:1:61:GLY:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.82	0.44
1:A:10:U:O4	1:A:532:A:OP2	2.35	0.44
1:A:1236:A:H2'	1:A:1237:U:O4'	2.16	0.44
1:A:2045:G:H2'	1:A:2046:G:O4'	2.17	0.44
1:A:2135:A:O2'	1:A:2136:G:H5'	2.18	0.44
1:A:2346:C:H4'	6:F:52:THR:CG2	2.46	0.44
1:A:492:C:O2'	1:A:493:U:H5'	2.17	0.44
1:A:68:U:O2'	1:A:69:A:H5''	2.17	0.44
1:A:873:G:H2'	1:A:875:A:N7	2.32	0.44
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.47	0.44
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.47	0.44
7:G:162:PHE:N	7:G:162:PHE:CD1	2.85	0.44
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.99	0.44
24:X:42:ARG:O	24:X:45:VAL:HG22	2.18	0.44
1:A:2334:C:O2'	1:A:2335:C:H5'	2.18	0.44
1:A:2338:G:H1'	6:F:105:SER:OG	2.17	0.44
1:A:245:C:C2'	1:A:246:G:H5'	2.48	0.44
1:A:67:A:H5''	1:A:69:A:C8	2.53	0.44
1:A:694:A:C2'	1:A:695:C:H5'	2.47	0.44
1:A:902:G:N7	13:M:18:HIS:CD2	2.84	0.44
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.48	0.44
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.00	0.44
10:J:114:PRO:O	10:J:115:PHE:C	2.55	0.44
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.44
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.29	0.44
26:Z:106:THR:HG22	26:Z:107:PRO:O	2.17	0.44
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.53	0.44
1:A:1081:A:C6	1:A:1082:A:N1	2.85	0.44
1:A:245:C:H2'	1:A:246:G:H5'	1.98	0.44
2:B:3107:C:H2'	2:B:3108:C:C6	2.52	0.44
4:D:240:GLY:HA3	37:D:8654:HOH:O	2.17	0.44
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.77	0.44
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.30	0.44
17:Q:27:ARG:O	17:Q:31:ILE:HG13	2.18	0.44
21:U:75:GLU:O	21:U:76:ASP:HB2	2.18	0.44
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.44
24:X:126:ASP:HB3	24:X:135:GLY:O	2.18	0.44
25:Y:27:ASP:N	25:Y:27:ASP:OD2	2.51	0.44
1:A:1127:C:C2'	1:A:1128:U:H5'	2.48	0.44
1:A:1409:G:H5'	37:A:3700:HOH:O	2.17	0.44
1:A:1515:A:H2'	1:A:1516:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:A:N7	1:A:1970:G:C6	2.85	0.44
1:A:204:A:H2'	1:A:205:U:C5'	2.45	0.44
1:A:2289:G:H21	1:A:2291:A:H2	1.63	0.44
1:A:2727:A:H2'	1:A:2728:C:H5'	1.99	0.44
5:E:235:PHE:CE2	5:E:243:VAL:HG21	2.48	0.44
5:E:25:PRO:HD2	37:E:8431:HOH:O	2.15	0.44
1:A:449:A:C8	5:E:43:LYS:HG2	2.52	0.44
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.01	0.44
12:L:55:VAL:CG1	12:L:56:SER:N	2.80	0.44
16:P:99:GLU:CG	37:P:6044:HOH:O	2.66	0.44
24:X:65:VAL:HA	24:X:68:THR:CG2	2.47	0.44
1:A:1690:C:C5	1:A:1692:C:C4	3.06	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.18	0.44
1:A:1925:G:O2'	1:A:1926:G:H5'	2.18	0.44
1:A:2506:A:C1'	37:A:6034:HOH:O	2.65	0.44
1:A:259:G:O2'	1:A:260:C:H5'	2.18	0.44
1:A:538:C:H5''	1:A:539:G:C8	2.53	0.44
1:A:853:C:H2'	1:A:854:G:O4'	2.17	0.44
6:F:103:ASN:ND2	6:F:134:LEU:H	2.16	0.44
10:J:31:PHE:CD2	10:J:85:ILE:HG23	2.53	0.44
11:K:107:ASN:HD22	11:K:109:TYR:H	1.62	0.44
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.53	0.44
19:S:132:ARG:NH1	37:S:8559:HOH:O	2.51	0.44
1:A:2055:A:H5'	19:S:134:SER:HB2	2.00	0.44
1:A:2050:G:OP1	19:S:79:ARG:HB3	2.18	0.44
21:U:26:THR:HA	21:U:39:ASN:HB3	1.99	0.44
1:A:2090:G:H2'	1:A:2091:G:C8	2.52	0.44
1:A:2134:G:C6	1:A:2258:A:C8	3.06	0.44
1:A:2482:G:O2'	1:A:2535:U:OP2	2.29	0.44
1:A:435:A:O2'	1:A:436:A:H5'	2.18	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
1:A:875:A:C2	3:C:194:MET:SD	3.11	0.44
10:J:31:PHE:HD2	10:J:85:ILE:O	2.01	0.44
14:N:84:LYS:O	14:N:87:MET:HG2	2.18	0.44
15:O:154:LEU:HD12	15:O:156:GLU:O	2.18	0.44
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.18	0.44
1:A:1169:U:C5	1:A:1170:U:C4	3.06	0.43
1:A:1666:C:H2'	1:A:1667:A:H8	1.83	0.43
1:A:2408:A:H4'	30:4:15:ASN:O	2.17	0.43
1:A:244:C:O5'	1:A:244:C:H6	2.00	0.43
1:A:2724:U:O4	1:A:2725:G:N1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:U:C1'	37:A:7324:HOH:O	2.66	0.43
1:A:51:G:C2	1:A:111:C:C2	3.06	0.43
1:A:870:G:C3'	1:A:871:G:H5''	2.48	0.43
6:F:58:VAL:CG1	6:F:59:GLY:N	2.80	0.43
10:J:46:VAL:O	10:J:146:TRP:CH2	2.68	0.43
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.47	0.43
13:M:65:ASP:HA	13:M:109:LEU:O	2.17	0.43
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.88	0.43
14:N:184:ARG:NH1	14:N:184:ARG:HB2	2.33	0.43
14:N:57:LYS:HB3	14:N:60:ILE:HD12	2.00	0.43
16:P:41:ALA:HA	37:P:5104:HOH:O	2.18	0.43
17:Q:27:ARG:HA	37:Q:3969:HOH:O	2.18	0.43
1:A:892:G:H5''	28:2:54:ALA:HB2	2.00	0.43
1:A:1096:U:H5''	1:A:1258:G:O6	2.18	0.43
1:A:1173:A:H4'	1:A:1174:A:C8	2.53	0.43
1:A:1419:U:O2	1:A:1419:U:H3'	2.18	0.43
1:A:13:G:H2'	1:A:14:C:C6	2.53	0.43
1:A:2265:U:H2'	1:A:2266:A:H8	1.84	0.43
1:A:69:A:H5'	1:A:69:A:H8	1.83	0.43
1:A:912:A:C4	1:A:1294:A:C2	3.06	0.43
5:E:162:VAL:O	5:E:162:VAL:HG12	2.18	0.43
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.46	0.43
6:F:95:THR:C	6:F:97:GLN:N	2.67	0.43
1:A:244:C:OP2	8:H:38:LYS:HE3	2.18	0.43
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.49	0.43
8:H:99:THR:O	8:H:100:ASP:HB2	2.17	0.43
13:M:98:GLU:O	13:M:99:GLU:CB	2.66	0.43
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.47	0.43
17:Q:115:SER:C	17:Q:117:SER:H	2.21	0.43
20:T:57:THR:CG2	20:T:58:MET:N	2.81	0.43
37:A:6175:HOH:O	29:3:44:ARG:HG2	2.18	0.43
1:A:1215:A:O3'	1:A:1216:G:C4'	2.66	0.43
1:A:2119:C:O2'	1:A:2120:U:H5'	2.18	0.43
4:D:103:ASP:HB2	37:D:8590:HOH:O	2.17	0.43
4:D:144:THR:HG22	4:D:145:HIS:N	2.33	0.43
4:D:190:MET:CE	4:D:194:PHE:CD1	2.94	0.43
10:J:57:ARG:C	10:J:59:ASN:N	2.70	0.43
14:N:76:ARG:HG2	14:N:76:ARG:NH1	2.34	0.43
15:O:37:ARG:CD	34:O:8507:CL:CL	3.03	0.43
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.17	0.43
1:A:1097:A:H5''	24:X:125:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:43:VAL:HG12	25:Y:47:ALA:HB3	2.00	0.43
1:A:1205:U:C2'	1:A:1206:U:H5'	2.42	0.43
1:A:2004:U:O2	1:A:2004:U:H2'	2.17	0.43
1:A:2092:G:H2'	1:A:2613:G:OP1	2.18	0.43
1:A:329:A:OP2	5:E:206:ASN:HB2	2.18	0.43
1:A:580:A:N1	1:A:1253:C:O2'	2.47	0.43
2:B:3047:A:C2	2:B:3048:C:C2	3.06	0.43
11:K:6:PHE:O	11:K:8:ALA:N	2.51	0.43
14:N:169:ARG:NH1	37:N:8572:HOH:O	2.52	0.43
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.18	0.43
19:S:39:THR:CB	19:S:42:GLU:HG3	2.42	0.43
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.00	0.43
37:A:7395:HOH:O	21:U:2:LYS:HE2	2.17	0.43
21:U:48:VAL:HG22	21:U:97:ARG:O	2.19	0.43
1:A:538:C:OP2	26:Z:134:HIS:HE1	2.01	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:1257:C:H2'	1:A:1258:G:O4'	2.18	0.43
1:A:1609:C:H2'	1:A:1610:G:H8	1.82	0.43
1:A:1666:C:O2'	1:A:1667:A:C5'	2.62	0.43
1:A:1783:A:C2'	1:A:1784:U:H5'	2.48	0.43
1:A:2095:A:C2	1:A:2651:C:C2	3.06	0.43
1:A:2468:A:N6	30:4:50:GLY:O	2.52	0.43
1:A:566:A:H2'	1:A:567:U:O4'	2.18	0.43
1:A:65:C:O2'	1:A:66:G:H5'	2.18	0.43
2:B:3104:A:O2'	2:B:3105:A:H5'	2.19	0.43
3:C:211:LYS:CB	3:C:212:PRO:HD2	2.36	0.43
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.18	0.43
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.19	0.43
13:M:101:ASP:C	13:M:103:ALA:H	2.21	0.43
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.01	0.43
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.36	0.43
15:O:116:PHE:HB2	37:O:8556:HOH:O	2.19	0.43
15:O:184:ILE:HG22	15:O:185:GLU:N	2.33	0.43
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.67	0.43
15:O:67:ALA:HA	15:O:71:TRP:H	1.83	0.43
15:O:91:ARG:HG3	15:O:186:LEU:HD23	2.01	0.43
17:Q:13:VAL:CG2	17:Q:41:ARG:HG2	2.46	0.43
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.65	0.43
3:C:170:VAL:HG13	27:1:22:ILE:CG2	2.48	0.43
1:A:1164:U:O4'	1:A:1165:G:OP1	2.35	0.43
1:A:2036:C:OP1	37:A:6682:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:C:H4'	6:F:52:THR:HG22	2.01	0.43
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.43
1:A:2900:G:H2'	1:A:2901:C:O4'	2.19	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
1:A:396:U:H1'	37:A:7626:HOH:O	2.17	0.43
1:A:563:C:H2'	1:A:564:G:O4'	2.19	0.43
1:A:643:A:N1	1:A:902:G:O2'	2.45	0.43
1:A:734:U:O2'	1:A:737:A:N6	2.51	0.43
2:B:3092:G:H22	10:J:52:LYS:NZ	2.16	0.43
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.34	0.43
5:E:114:ALA:HB1	5:E:223:LEU:HB3	2.01	0.43
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.49	0.43
14:N:191:GLY:O	14:N:192:ALA:HB3	2.17	0.43
14:N:35:PRO:HD2	14:N:38:VAL:HG21	2.01	0.43
14:N:49:ALA:C	14:N:54:TYR:HB3	2.38	0.43
15:O:114:LYS:O	15:O:118:ILE:HG13	2.18	0.43
1:A:2054:A:H2	19:S:128:ARG:HH22	1.62	0.43
20:T:73:ASP:O	20:T:77:VAL:HG23	2.19	0.43
24:X:110:GLN:CA	24:X:110:GLN:HE21	2.27	0.43
27:1:46:LYS:HB3	37:1:8438:HOH:O	2.17	0.43
27:1:50:ALA:HB3	27:1:54:ILE:HG22	2.00	0.43
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.53	0.43
1:A:1332:C:O2'	1:A:1333:U:H5'	2.19	0.43
1:A:2300:A:H4'	1:A:2301:A:O5'	2.19	0.43
1:A:2898:G:O2'	1:A:2899:A:H5'	2.18	0.43
1:A:820:G:H5'	1:A:821:U:C5'	2.49	0.43
1:A:929:A:C8	1:A:930:C:C5	3.07	0.43
3:C:8:ARG:HG2	37:C:8553:HOH:O	2.17	0.43
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.33	0.43
5:E:129:HIS:CE1	5:E:232:LEU:H	2.37	0.43
5:E:39:GLN:O	5:E:43:LYS:HD3	2.19	0.43
13:M:35:ARG:O	13:M:40:PHE:HA	2.18	0.43
13:M:91:VAL:O	13:M:91:VAL:HG13	2.18	0.43
14:N:138:HIS:C	14:N:139:PRO:O	2.50	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.79	0.43
15:O:67:ALA:C	15:O:69:TYR:H	2.22	0.43
18:R:53:HIS:O	18:R:55:ARG:N	2.52	0.43
1:A:2055:A:H4'	19:S:132:ARG:NH2	2.33	0.43
26:Z:187:VAL:CG1	26:Z:205:ILE:HA	2.47	0.43
1:A:1992:U:H2'	1:A:1994:A:OP2	2.19	0.43
1:A:2416:G:H2'	1:A:2417:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2837:U:H2'	37:A:6820:HOH:O	2.19	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.01	0.43
1:A:489:A:C8	21:U:82:THR:CG2	3.02	0.43
1:A:757:C:H2'	1:A:758:A:C8	2.54	0.43
2:B:3078:G:N2	2:B:3103:A:OP2	2.48	0.43
3:C:169:PHE:O	3:C:170:VAL:HB	2.18	0.43
3:C:211:LYS:HD3	37:C:8613:HOH:O	2.18	0.43
3:C:94:LEU:CD2	3:C:94:LEU:N	2.82	0.43
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.19	0.43
7:G:49:ILE:HD11	7:G:69:ILE:HD12	2.00	0.43
7:G:7:ILE:HA	7:G:8:PRO:HD3	1.82	0.43
10:J:15:THR:HG22	10:J:91:HIS:HA	1.99	0.43
12:L:118:ALA:O	12:L:120:ARG:N	2.52	0.43
15:O:161:GLY:O	15:O:162:ASP:C	2.56	0.43
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.81	0.43
17:Q:2:ASP:C	17:Q:2:ASP:OD1	2.56	0.43
20:T:58:MET:SD	29:3:8:LYS:HE3	2.59	0.43
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.29	0.43
1:A:1176:C:H1'	37:A:3901:HOH:O	2.18	0.43
1:A:1301:C:O2'	1:A:1331:A:H4'	2.19	0.43
1:A:1921:A:C6	1:A:1922:A:C2	3.07	0.43
1:A:2626:C:H2'	1:A:2627:G:C8	2.54	0.43
1:A:2681:A:N6	1:A:2714:U:H4'	2.33	0.43
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.43
1:A:321:A:H1'	37:A:7016:HOH:O	2.19	0.43
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.19	0.43
1:A:69:A:H2'	1:A:70:A:OP2	2.18	0.43
5:E:115:LEU:HD12	5:E:115:LEU:HA	1.83	0.43
8:H:80:GLN:HB3	37:H:2563:HOH:O	2.19	0.43
10:J:50:VAL:HA	10:J:157:ILE:HG12	2.00	0.43
1:A:221:G:OP2	13:M:46:LEU:HB3	2.19	0.43
14:N:37:VAL:HG21	14:N:108:LYS:HG3	2.01	0.43
15:O:113:SER:C	37:O:8556:HOH:O	2.58	0.43
15:O:129:ILE:HA	15:O:130:PRO:HD3	1.93	0.43
15:O:66:LEU:HA	15:O:66:LEU:HD12	1.92	0.43
15:O:71:TRP:CE3	15:O:175:LEU:CD2	2.97	0.43
37:E:8360:HOH:O	16:P:3:THR:HG21	2.19	0.43
27:1:30:GLU:O	27:1:33:HIS:HB3	2.18	0.43
1:A:1021:G:O2'	1:A:1022:A:H5'	2.18	0.43
1:A:1023:C:H2'	1:A:1024:G:O4'	2.19	0.43
1:A:1543:G:N1	1:A:1641:A:OP2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:A:N6	1:A:194:A:C2	2.87	0.43
1:A:542:A:C8	1:A:542:A:C5'	2.98	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	2.00	0.43
2:B:3057:A:N3	2:B:3057:A:H5'	2.33	0.43
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.34	0.43
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.30	0.43
3:C:223:ARG:NH1	37:C:8518:HOH:O	2.50	0.43
4:D:11:LEU:HA	37:D:8614:HOH:O	2.18	0.43
4:D:279:THR:HG22	4:D:280:VAL:N	2.33	0.43
4:D:41:PHE:N	37:D:8647:HOH:O	2.52	0.43
8:H:113:ASP:O	8:H:117:GLU:HG3	2.19	0.43
10:J:95:GLU:HB3	10:J:119:VAL:HG11	2.01	0.43
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.49	0.43
13:M:30:ARG:NH1	37:M:8511:HOH:O	2.42	0.43
14:N:47:ASP:CG	14:N:48:ARG:N	2.73	0.43
18:R:77:ASP:N	18:R:80:LYS:O	2.52	0.43
1:A:818:A:C2	27:1:13:ARG:HA	2.54	0.42
1:A:1137:G:H1'	37:A:3851:HOH:O	2.19	0.42
1:A:1513:C:O2'	1:A:1514:C:H5'	2.18	0.42
1:A:2656:G:C2'	1:A:2657:G:H5'	2.48	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.77	0.42
5:E:14:GLY:N	37:E:8446:HOH:O	2.52	0.42
6:F:17:ARG:NH2	37:F:3723:HOH:O	2.40	0.42
10:J:136:VAL:HG22	10:J:137:ASN:N	2.34	0.42
14:N:77:PHE:CE2	14:N:86:MET:HG2	2.53	0.42
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.49	0.42
1:A:100:C:H4'	21:U:16:LEU:HB2	2.01	0.42
22:V:49:LEU:O	22:V:55:ALA:CB	2.67	0.42
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.18	0.42
24:X:6:GLN:HA	24:X:52:VAL:HG23	2.00	0.42
24:X:90:TYR:N	37:X:6679:HOH:O	2.52	0.42
30:4:31:THR:HB	30:4:33:MET:HE2	2.00	0.42
1:A:164:G:C6	1:A:165:A:C5	3.06	0.42
1:A:1717:A:H5''	17:Q:54:LYS:HB2	2.01	0.42
1:A:1746:A:N3	1:A:1748:U:C4	2.87	0.42
1:A:1947:G:N2	1:A:1966:U:O2	2.51	0.42
2:B:3006:C:P	15:O:37:ARG:HH11	2.42	0.42
3:C:55:VAL:CG1	3:C:67:LEU:HD22	2.49	0.42
4:D:129:ARG:NH2	4:D:176:ASP:OD1	2.51	0.42
4:D:254:GLN:HG2	4:D:255:GLY:H	1.83	0.42
5:E:98:ARG:NH1	37:E:8358:HOH:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:107:ASN:HD22	11:K:107:ASN:C	2.22	0.42
11:K:88:PRO:HA	34:K:8502:CL:CL	2.55	0.42
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.97	0.42
23:W:12:THR:O	23:W:15:GLU:N	2.51	0.42
1:A:1123:A:C2	1:A:1129:C:H4'	2.54	0.42
1:A:1532:G:C6	1:A:1533:A:C6	3.08	0.42
1:A:1701:A:H5''	1:A:1702:U:H3'	2.01	0.42
1:A:1733:A:C6	1:A:1734:C:C2	3.07	0.42
1:A:1773:G:C2'	1:A:1774:G:H5'	2.49	0.42
1:A:2113:G:C6	1:A:2114:C:C4	3.07	0.42
1:A:2481:G:C3'	1:A:2482:G:H5''	2.49	0.42
1:A:2833:C:O2	1:A:2848:G:C2	2.72	0.42
1:A:29:C:O2'	1:A:30:U:H5'	2.19	0.42
1:A:407:A:C2	1:A:408:A:C4	3.07	0.42
2:B:3003:A:H2'	37:B:2430:HOH:O	2.19	0.42
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.81	0.42
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.81	0.42
4:D:84:LEU:HD13	4:D:84:LEU:O	2.19	0.42
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.49	0.42
7:G:20:ILE:O	7:G:30:THR:HA	2.19	0.42
14:N:137:ASP:C	14:N:142:LYS:HE3	2.40	0.42
14:N:18:GLY:O	14:N:21:ALA:HB3	2.20	0.42
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.48	0.42
24:X:122:ARG:HG3	24:X:152:ALA:O	2.20	0.42
28:2:19:CYS:SG	28:2:21:ARG:N	2.93	0.42
1:A:1573:A:H2'	1:A:1574:C:O4'	2.19	0.42
1:A:1804:A:H2'	1:A:1805:G:H8	1.84	0.42
1:A:1862:C:O2'	1:A:1863:G:H5'	2.20	0.42
1:A:23:G:C6	1:A:24:G:N1	2.88	0.42
1:A:2405:C:H5'	37:A:6578:HOH:O	2.18	0.42
1:A:2432:C:C4'	37:A:9716:HOH:O	2.60	0.42
1:A:2637:A:C4'	37:A:4335:HOH:O	2.67	0.42
1:A:2656:G:O2'	1:A:2657:G:H5'	2.18	0.42
1:A:585:C:H6	37:A:6075:HOH:O	2.01	0.42
3:C:170:VAL:HG13	27:1:22:ILE:HG21	2.01	0.42
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.55	0.42
7:G:137:ASP:OD1	7:G:139:GLU:HB2	2.19	0.42
10:J:150:LYS:HA	10:J:153:VAL:CG2	2.49	0.42
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.42
17:Q:115:SER:C	17:Q:117:SER:N	2.73	0.42
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.47	0.42
1:A:1215:A:O3'	1:A:1216:G:H4'	2.19	0.42
1:A:1253:C:H5'	37:A:7728:HOH:O	2.19	0.42
1:A:1459:A:OP2	37:A:9229:HOH:O	2.22	0.42
1:A:1506:U:H6	1:A:1506:U:H5'	1.85	0.42
1:A:1751:G:C3'	1:A:1752:G:H5''	2.49	0.42
1:A:1863:G:OP2	37:A:3122:HOH:O	2.22	0.42
1:A:2121:G:C2'	1:A:2122:C:H5'	2.50	0.42
1:A:2769:C:H2'	1:A:2770:G:C5'	2.49	0.42
1:A:661:G:C6	1:A:686:A:C2	3.08	0.42
1:A:80:A:H3'	21:U:43:ASN:OD1	2.18	0.42
1:A:911:G:H5'	1:A:932:U:OP1	2.19	0.42
4:D:307:ARG:HH11	4:D:307:ARG:HG3	1.83	0.42
1:A:380:A:OP2	14:N:9:ARG:HD2	2.20	0.42
15:O:47:LEU:HA	15:O:47:LEU:HD23	1.79	0.42
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.82	0.42
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.49	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:168:C:C2'	1:A:169:A:H5'	2.49	0.42
1:A:2079:G:C6	1:A:2080:G:C5	3.08	0.42
1:A:2387:U:H2'	1:A:2388:C:C6	2.54	0.42
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.53	0.42
1:A:2812:A:C2	1:A:2814:A:N6	2.75	0.42
1:A:370:G:O2'	1:A:371:U:H5'	2.20	0.42
1:A:492:C:C2'	1:A:493:U:H5'	2.49	0.42
1:A:666:A:H2'	1:A:667:C:O4'	2.20	0.42
1:A:69:A:C2'	1:A:70:A:OP2	2.68	0.42
1:A:736:A:H2'	1:A:737:A:O4'	2.19	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.42
4:D:16:ARG:NE	37:D:8553:HOH:O	2.19	0.42
4:D:168:GLY:H	4:D:174:ARG:HD3	1.83	0.42
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.50	0.42
6:F:64:ARG:HD3	6:F:67:ASP:HB3	2.02	0.42
10:J:47:GLU:HG2	10:J:133:ILE:HD12	2.00	0.42
15:O:38:LYS:HB2	15:O:38:LYS:HE3	1.71	0.42
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.67	0.42
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.52	0.42
30:4:7:PHE:CE2	30:4:22:VAL:CG2	3.00	0.42
1:A:1123:A:N6	1:A:1238:C:H5'	2.33	0.42
1:A:1211:G:O2'	1:A:1212:C:H5'	2.19	0.42
1:A:2833:C:C2	1:A:2848:G:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2909:G:H2'	1:A:2910:A:H8	1.84	0.42
1:A:581:G:H5'	37:A:7679:HOH:O	2.20	0.42
1:A:710:G:N2	1:A:719:C:C2	2.88	0.42
4:D:277:GLU:N	4:D:278:PRO:HD2	2.34	0.42
7:G:11:VAL:HG13	7:G:23:GLU:O	2.18	0.42
10:J:55:GLN:HE21	10:J:124:ARG:NE	2.08	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.55	0.42
14:N:186:SER:OG	14:N:189:VAL:CG1	2.67	0.42
15:O:86:LEU:O	15:O:90:LEU:HG	2.18	0.42
19:S:39:THR:O	19:S:40:ALA:C	2.58	0.42
26:Z:101:GLY:HA3	37:Z:8561:HOH:O	2.20	0.42
29:3:19:SER:O	29:3:36:ASN:ND2	2.53	0.42
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.34	0.42
1:A:1163:G:H3'	1:A:1164:U:H2'	2.02	0.42
1:A:1191:A:C2	1:A:1207:A:C2	3.08	0.42
1:A:177:A:C8	1:A:178:U:C5	3.07	0.42
1:A:1886:A:H4'	37:1:8405:HOH:O	2.19	0.42
1:A:1934:A:C8	1:A:1935:C:C5	3.07	0.42
1:A:2432:C:C2'	1:A:2433:A:H5'	2.50	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
1:A:394:G:HO2'	1:A:395:A:H8	1.63	0.42
1:A:752:G:O6	37:A:4299:HOH:O	2.22	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.31	0.42
2:B:3078:G:N2	2:B:3102:G:H2'	2.34	0.42
3:C:123:GLY:HA3	3:C:162:GLY:HA2	2.01	0.42
4:D:101:TRP:HB2	4:D:119:HIS:CD2	2.55	0.42
5:E:107:ARG:HB3	5:E:107:ARG:CZ	2.48	0.42
5:E:141:SER:HA	37:E:8381:HOH:O	2.19	0.42
6:F:10:PHE:CE1	6:F:11:HIS:HB3	2.54	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.35	0.42
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.55	0.42
37:A:4546:HOH:O	14:N:83:SER:HA	2.19	0.42
17:Q:120:ARG:NH2	17:Q:123:TYR:HD2	2.12	0.42
24:X:88:THR:HG23	24:X:110:GLN:HB3	2.02	0.42
1:A:1185:U:O4'	37:A:7456:HOH:O	2.21	0.42
1:A:1400:C:O2'	1:A:1401:G:H5'	2.20	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:1692:C:H1'	37:A:9450:HOH:O	2.19	0.42
1:A:2012:U:H2'	1:A:2013:G:OP1	2.19	0.42
1:A:218:C:P	30:4:39:GLN:HE21	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2531:U:O2'	1:A:2532:A:H5'	2.19	0.42
1:A:25:A:C2'	1:A:26:U:H5'	2.50	0.42
1:A:2897:C:O2'	1:A:2898:G:H5'	2.20	0.42
1:A:724:G:O2'	1:A:725:C:H5'	2.20	0.42
2:B:3030:C:OP1	6:F:137:PRO:O	2.37	0.42
3:C:69:LEU:CD2	3:C:120:ARG:HB3	2.44	0.42
4:D:16:ARG:NH1	37:D:8614:HOH:O	2.53	0.42
4:D:215:VAL:HB	4:D:234:ARG:NH1	2.34	0.42
4:D:248:ARG:NH2	37:D:8522:HOH:O	2.52	0.42
5:E:27:ARG:CG	5:E:29:ASP:OD1	2.63	0.42
2:B:3040:C:N4	6:F:51:ARG:HB2	2.34	0.42
12:L:14:LYS:CB	12:L:45:PRO:HG2	2.45	0.42
13:M:145:LEU:O	13:M:145:LEU:HD23	2.20	0.42
1:A:1299:G:N7	13:M:6:ARG:NH1	2.67	0.42
37:A:3731:HOH:O	21:U:9:LYS:HD3	2.18	0.42
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.68	0.42
27:1:47:LEU:HA	27:1:56:MET:O	2.20	0.42
30:4:62:THR:HG23	30:4:86:GLY:HA2	2.02	0.42
1:A:1773:G:O2'	27:1:15:GLY:HA2	2.20	0.42
1:A:2415:A:C2	15:O:25:ARG:CB	3.03	0.42
1:A:818:A:H5''	37:A:6570:HOH:O	2.20	0.42
1:A:827:A:H2'	1:A:828:G:O4'	2.19	0.42
1:A:889:C:H2'	1:A:890:C:C6	2.55	0.42
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.42
3:C:111:SER:O	3:C:112:PRO:C	2.58	0.42
7:G:81:GLU:HA	7:G:133:VAL:O	2.19	0.42
7:G:23:GLU:HG2	7:G:28:SER:HB2	2.01	0.42
7:G:5:LEU:HD21	7:G:66:GLN:HG3	2.02	0.42
8:H:33:THR:HG21	8:H:59:ILE:O	2.19	0.42
9:I:64:ASN:N	9:I:64:ASN:ND2	2.67	0.42
10:J:111:MET:O	10:J:114:PRO:HD3	2.20	0.42
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.01	0.42
12:L:118:ALA:HA	12:L:125:ALA:HB2	2.02	0.42
12:L:9:THR:O	12:L:10:GLN:C	2.56	0.42
15:O:39:SER:HB3	15:O:42:HIS:H	1.85	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.48	0.42
1:A:841:A:OP2	19:S:128:ARG:HD2	2.20	0.42
37:A:7050:HOH:O	19:S:33:ARG:HD3	2.20	0.42
30:4:87:ARG:HD2	37:4:8528:HOH:O	2.21	0.41
1:A:1098:A:H2'	1:A:1099:G:O4'	2.20	0.41
1:A:1469:C:N3	1:A:1472:C:OP2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:G:N1	1:A:202:U:C4	2.88	0.41
1:A:2044:G:OP1	25:Y:23:HIS:CE1	2.69	0.41
1:A:2379:G:N7	1:A:2408:A:N1	2.67	0.41
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.20	0.41
1:A:2869:G:H2'	1:A:2870:C:C6	2.55	0.41
1:A:825:U:H5''	1:A:826:U:OP1	2.20	0.41
2:B:3039:U:HO2'	2:B:3042:C:H5	1.58	0.41
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.39	0.41
3:C:51:ARG:HB2	37:C:8609:HOH:O	2.19	0.41
4:D:17:LYS:O	4:D:260:HIS:HD2	2.03	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.85	0.41
13:M:148:GLU:CG	37:M:8558:HOH:O	2.67	0.41
13:M:54:PRO:HG2	13:M:57:VAL:HG21	2.01	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.20	0.41
14:N:98:GLN:O	14:N:101:ALA:HB3	2.19	0.41
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.34	0.41
24:X:38:THR:O	24:X:42:ARG:HB2	2.20	0.41
1:A:315:G:C6	1:A:316:A:C6	3.08	0.41
1:A:593:A:N7	37:A:4369:HOH:O	2.52	0.41
3:C:186:TRP:CG	3:C:187:PRO:HA	2.55	0.41
4:D:307:ARG:HG3	4:D:307:ARG:NH1	2.35	0.41
5:E:102:LEU:HD12	37:E:8315:HOH:O	2.20	0.41
6:F:23:VAL:HG12	6:F:130:VAL:HG22	2.01	0.41
7:G:138:ILE:HG22	37:G:5404:HOH:O	2.19	0.41
37:A:5662:HOH:O	15:O:21:HIS:HE1	2.04	0.41
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.74	0.41
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	2.01	0.41
29:3:40:ARG:HG2	29:3:40:ARG:NH1	2.35	0.41
1:A:99:A:H3'	1:A:100:C:C6	2.56	0.41
1:A:1014:A:H2'	1:A:1015:C:H5'	2.02	0.41
1:A:2470:A:O2'	37:A:6532:HOH:O	2.20	0.41
1:A:517:U:C2'	1:A:518:G:H5'	2.50	0.41
1:A:637:C:OP1	26:Z:136:LYS:NZ	2.43	0.41
4:D:150:ALA:O	4:D:152:PRO:HD3	2.20	0.41
4:D:41:PHE:HB3	4:D:190:MET:HE1	2.02	0.41
7:G:84:MET:HE1	7:G:148:ILE:HD12	2.01	0.41
10:J:56:ILE:HG21	10:J:61:LEU:HD13	2.02	0.41
12:L:98:VAL:HG13	12:L:99:ASP:O	2.21	0.41
13:M:64:ILE:O	13:M:64:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:132:ASN:O	15:O:135:VAL:HG12	2.20	0.41
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.50	0.41
16:P:113:VAL:O	16:P:114:ILE:HD13	2.20	0.41
16:P:39:THR:HB	37:P:3360:HOH:O	2.19	0.41
19:S:104:PHE:HB2	19:S:109:MET:HE1	2.01	0.41
19:S:99:ALA:CB	19:S:109:MET:HE1	2.25	0.41
19:S:149:GLU:HA	19:S:150:PRO:HD3	1.92	0.41
21:U:96:VAL:HG13	21:U:97:ARG:N	2.36	0.41
23:W:38:GLY:C	23:W:40:PRO:HD2	2.41	0.41
24:X:13:MET:O	24:X:14:HIS:C	2.58	0.41
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.50	0.41
1:A:159:G:H2'	1:A:175:G:H22	1.85	0.41
1:A:1846:U:H2'	1:A:1847:A:C4	2.56	0.41
1:A:1943:C:O4'	3:C:212:PRO:HA	2.19	0.41
1:A:377:C:H5	37:A:3286:HOH:O	2.03	0.41
1:A:380:A:H5''	14:N:48:ARG:NH2	2.35	0.41
1:A:454:U:C2	37:A:9027:HOH:O	2.57	0.41
1:A:492:C:C2	1:A:501:G:N2	2.88	0.41
1:A:711:G:C2	1:A:718:C:C2	3.08	0.41
3:C:135:VAL:N	37:C:8600:HOH:O	2.52	0.41
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.55	0.41
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.52	0.41
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.50	0.41
10:J:26:LYS:HE3	10:J:28:ILE:HB	2.02	0.41
37:A:4806:HOH:O	11:K:47:THR:CB	2.64	0.41
12:L:4:LEU:HD22	12:L:116:GLU:HB3	2.02	0.41
14:N:173:LEU:HA	14:N:183:VAL:HG11	2.03	0.41
19:S:61:GLN:NE2	37:S:8540:HOH:O	2.54	0.41
21:U:48:VAL:HG22	21:U:97:ARG:C	2.40	0.41
22:V:38:ASN:O	22:V:42:LEU:HG	2.20	0.41
23:W:12:THR:HG23	23:W:14:ALA:N	2.36	0.41
1:A:1132:A:H2'	1:A:1133:A:C8	2.55	0.41
1:A:123:U:H2'	1:A:124:C:C6	2.56	0.41
1:A:1305:C:O2'	1:A:1306:U:H5'	2.19	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:1969:A:O2'	1:A:1970:G:H5'	2.20	0.41
1:A:1992:U:C2	1:A:1994:A:OP2	2.74	0.41
1:A:2488:A:H1'	37:A:9092:HOH:O	2.20	0.41
1:A:2836:G:C6	1:A:2838:A:C2	3.08	0.41
1:A:654:A:OP2	16:P:38:ARG:HD3	2.20	0.41
1:A:695:C:H2'	1:A:696:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:H22	1:A:97:G:H1'	1.85	0.41
2:B:3057:A:H8	6:F:141:VAL:HG21	1.85	0.41
1:A:2767:C:OP1	4:D:318:ASN:ND2	2.53	0.41
5:E:154:VAL:O	5:E:158:GLU:HG3	2.20	0.41
10:J:112:ARG:O	10:J:113:ALA:C	2.58	0.41
10:J:84:ARG:NH2	10:J:135:TRP:CH2	2.82	0.41
10:J:86:ARG:HG2	10:J:86:ARG:H	1.63	0.41
17:Q:13:VAL:HG11	17:Q:40:VAL:HG12	2.03	0.41
21:U:113:GLU:O	21:U:114:SER:C	2.58	0.41
23:W:42:ASN:N	23:W:43:PRO:HD3	2.35	0.41
24:X:110:GLN:CA	24:X:110:GLN:NE2	2.69	0.41
25:Y:9:VAL:HG22	25:Y:88:GLU:OE2	2.20	0.41
1:A:107:U:H2'	1:A:108:U:H5'	2.02	0.41
1:A:168:C:H6	1:A:168:C:O5'	2.03	0.41
1:A:2251:G:H4'	37:A:7398:HOH:O	2.21	0.41
1:A:2252:A:C5	1:A:2253:G:H1'	2.55	0.41
1:A:2435:U:H1'	37:A:5404:HOH:O	2.19	0.41
1:A:2505:G:C2'	1:A:2506:A:H5'	2.50	0.41
1:A:2570:G:H5''	37:A:4885:HOH:O	2.20	0.41
1:A:644:G:H5'	1:A:644:G:N3	2.35	0.41
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.41
1:A:790:A:H1'	1:A:1710:A:O2'	2.21	0.41
3:C:51:ARG:CZ	37:C:8609:HOH:O	2.68	0.41
4:D:105:PHE:CD1	4:D:115:VAL:HG11	2.56	0.41
37:A:9678:HOH:O	4:D:254:GLN:HG3	2.19	0.41
4:D:7:ARG:CG	4:D:7:ARG:HH11	2.25	0.41
4:D:7:ARG:NH1	4:D:7:ARG:CG	2.81	0.41
5:E:196:THR:HG23	37:E:8400:HOH:O	2.20	0.41
6:F:52:THR:N	6:F:70:GLY:O	2.53	0.41
10:J:82:LYS:NZ	10:J:82:LYS:CB	2.84	0.41
15:O:64:SER:C	15:O:66:LEU:N	2.74	0.41
16:P:98:LEU:O	16:P:102:ILE:HG13	2.20	0.41
19:S:119:VAL:CG1	19:S:119:VAL:O	2.68	0.41
21:U:16:LEU:HA	21:U:16:LEU:HD23	1.85	0.41
24:X:122:ARG:NH1	24:X:152:ALA:O	2.54	0.41
24:X:73:LEU:HA	24:X:73:LEU:HD12	1.90	0.41
28:2:10:LYS:CB	37:2:2979:HOH:O	2.68	0.41
1:A:1909:A:HO2'	1:A:2266:A:HO2'	1.67	0.41
1:A:2434:A:O3'	30:4:28:GLY:CA	2.63	0.41
1:A:470:U:H2'	1:A:471:G:O4'	2.21	0.41
1:A:90:A:H2'	1:A:91:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:5876:HOH:O	3:C:185:LYS:HE2	2.20	0.41
3:C:53:ALA:HB1	3:C:54:PRO:HD2	2.02	0.41
4:D:189:ALA:HB1	37:D:8564:HOH:O	2.20	0.41
4:D:162:MET:HE1	4:D:308:LEU:HD21	2.01	0.41
4:D:312:ARG:HG2	4:D:313:PRO:N	2.33	0.41
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.50	0.41
7:G:9:GLU:HG3	7:G:10:ASP:N	2.36	0.41
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.03	0.41
10:J:30:GLN:H	10:J:65:ARG:NH1	2.18	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.89	0.41
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.51	0.41
14:N:74:ARG:O	14:N:88:VAL:HG13	2.20	0.41
15:O:74:PRO:HG2	15:O:159:TYR:CZ	2.56	0.41
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.04	0.41
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.51	0.41
25:Y:70:ILE:HG23	25:Y:70:ILE:O	2.20	0.41
37:A:9657:HOH:O	26:Z:163:THR:HG23	2.21	0.41
1:A:396:U:H5'	30:4:42:ARG:NH1	2.35	0.41
1:A:1188:A:C5	1:A:1189:A:C2	3.09	0.41
1:A:904:U:O2	1:A:1354:G:H3'	2.20	0.41
1:A:177:A:H2'	1:A:178:U:O4'	2.21	0.41
1:A:1951:G:N2	37:A:6241:HOH:O	2.52	0.41
1:A:1973:A:H8	1:A:1973:A:H5'	1.85	0.41
1:A:2011:A:O4'	1:A:2013:G:C8	2.74	0.41
1:A:2094:G:H4'	4:D:245:SER:CB	2.50	0.41
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.21	0.41
1:A:2397:G:C5	1:A:2465:A:C6	3.09	0.41
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.54	0.41
1:A:331:A:H1'	37:A:4765:HOH:O	2.19	0.41
3:C:130:THR:HG22	3:C:131:HIS:O	2.20	0.41
7:G:11:VAL:HG11	7:G:22:VAL:CG1	2.51	0.41
1:A:2274:A:N3	14:N:86:MET:CE	2.84	0.41
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.53	0.41
17:Q:125:LYS:NZ	17:Q:140:TYR:OH	2.46	0.41
24:X:85:ALA:HB2	24:X:91:ASP:O	2.21	0.41
30:4:74:CYS:SG	30:4:76:LYS:HD2	2.61	0.41
1:A:1684:A:O2'	1:A:1685:A:H5''	2.21	0.41
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.41
1:A:1840:A:H4'	1:A:1841:C:O5'	2.21	0.41
1:A:2012:U:C2'	1:A:2013:G:OP1	2.69	0.41
1:A:2072:G:C6	1:A:2533:C:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:G:N2	1:A:316:A:H3'	2.36	0.41
1:A:485:A:H4'	1:A:486:A:OP1	2.21	0.41
1:A:74:A:H2'	1:A:75:U:C6	2.56	0.41
1:A:814:G:H8	37:A:7194:HOH:O	2.02	0.41
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.54	0.41
2:B:3014:G:H2'	2:B:3015:C:C5'	2.51	0.41
4:D:185:GLY:HA2	37:D:8633:HOH:O	2.21	0.41
4:D:279:THR:OG1	4:D:290:VAL:HB	2.21	0.41
4:D:321:PRO:HG3	37:D:8597:HOH:O	2.20	0.41
4:D:55:ASN:HB3	4:D:64:GLY:N	2.35	0.41
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.35	0.41
15:O:110:THR:HA	15:O:111:PRO:HD3	1.95	0.41
15:O:73:ALA:HB1	15:O:74:PRO:HD2	2.02	0.41
1:A:1352:A:P	5:E:92:PRO:HG3	2.61	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.21	0.41
1:A:1882:C:O2'	1:A:2012:U:OP2	2.31	0.41
1:A:2453:G:H3'	37:A:5897:HOH:O	2.20	0.41
1:A:553:G:O4'	1:A:1325:G:H5'	2.20	0.41
1:A:860:U:H2'	1:A:861:A:C8	2.56	0.41
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.02	0.41
3:C:19:PRO:HD3	37:C:8604:HOH:O	2.21	0.41
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.68	0.41
3:C:55:VAL:HG11	3:C:67:LEU:HD13	2.02	0.41
5:E:25:PRO:HG2	37:E:8322:HOH:O	2.20	0.41
6:F:64:ARG:HG2	6:F:66:GLY:O	2.21	0.41
8:H:32:GLY:N	37:H:3111:HOH:O	2.53	0.41
9:I:65:THR:O	9:I:69:ARG:HB2	2.20	0.41
9:I:66:LEU:O	9:I:69:ARG:HB3	2.21	0.41
1:A:1103:C:O2'	11:K:86:MET:HB3	2.21	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.03	0.41
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.42	0.41
21:U:71:VAL:CG1	21:U:72:ILE:N	2.83	0.41
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.21	0.41
24:X:21:LEU:HB3	24:X:26:ILE:HG12	2.03	0.41
1:A:1304:U:H2'	1:A:1305:C:C6	2.56	0.41
1:A:1444:G:O2'	1:A:1502:A:N1	2.46	0.41
1:A:1641:A:C2'	1:A:1642:A:H5'	2.50	0.41
1:A:1973:A:H2'	1:A:1974:G:O4'	2.21	0.41
1:A:2325:C:H2'	1:A:2326:U:C6	2.56	0.41
1:A:2781:U:H2'	1:A:2782:G:H5'	2.03	0.41
1:A:2793:A:H2'	37:A:4464:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:A:N6	16:P:65:LEU:HD13	2.36	0.41
1:A:932:U:O2'	1:A:1296:A:H1'	2.21	0.41
3:C:83:GLY:O	3:C:94:LEU:HB3	2.20	0.41
4:D:102:THR:HG23	4:D:182:VAL:CG1	2.51	0.41
1:A:1234:U:C4	4:D:244:PRO:HB3	2.56	0.41
5:E:78:ARG:CG	5:E:78:ARG:HH11	2.27	0.41
6:F:25:MET:SD	6:F:40:ILE:HD11	2.61	0.41
7:G:102:VAL:HG11	7:G:148:ILE:HD11	2.02	0.41
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.51	0.41
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.21	0.41
8:H:59:ILE:O	8:H:59:ILE:CG2	2.69	0.41
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.80	0.41
22:V:14:GLU:OE1	22:V:15:PRO:CD	2.65	0.41
24:X:5:VAL:O	24:X:52:VAL:CG2	2.69	0.41
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.36	0.41
27:1:60:CYS:SG	27:1:62:TYR:HB2	2.61	0.40
1:A:119:A:C2	1:A:122:C:C4	3.09	0.40
1:A:1877:G:C6	1:A:1878:G:C6	3.09	0.40
1:A:2107:U:O2'	1:A:2108:A:H5'	2.21	0.40
1:A:2300:A:C2	1:A:2306:U:C5	3.08	0.40
1:A:236:A:H2'	1:A:236:A:O5'	2.20	0.40
1:A:2073:G:C6	1:A:2607:U:C2	3.09	0.40
1:A:295:C:H2'	1:A:296:G:O4'	2.21	0.40
1:A:419:A:H1'	1:A:1921:A:C2	2.56	0.40
1:A:431:G:OP1	14:N:48:ARG:NH1	2.54	0.40
1:A:702:G:O2'	1:A:703:G:H5'	2.21	0.40
1:A:835:U:H3'	37:A:9360:HOH:O	2.21	0.40
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.49	0.40
3:C:179:MET:HG2	3:C:186:TRP:CG	2.56	0.40
6:F:173:GLU:O	6:F:174:VAL:C	2.59	0.40
8:H:101:ALA:HA	37:H:5413:HOH:O	2.21	0.40
1:A:1151:G:P	9:I:16:LYS:NZ	2.94	0.40
10:J:14:TYR:N	10:J:91:HIS:HE1	2.20	0.40
1:A:183:A:C5'	14:N:157:LEU:HD12	2.51	0.40
14:N:27:ARG:O	14:N:30:GLU:N	2.53	0.40
14:N:59:GLY:C	14:N:141:ILE:HD11	2.41	0.40
37:A:3140:HOH:O	14:N:87:MET:HE3	2.21	0.40
15:O:21:HIS:HB2	37:O:8532:HOH:O	2.22	0.40
16:P:22:GLY:CA	37:P:2823:HOH:O	2.69	0.40
17:Q:121:ASP:HB2	37:Q:5891:HOH:O	2.20	0.40
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:36:ILE:HA	30:4:36:ILE:HD12	1.95	0.40
1:A:10:U:HO2'	1:A:11:A:P	2.44	0.40
1:A:1159:G:H1	1:A:1208:C:H42	1.70	0.40
1:A:1291:A:H2	37:A:5266:HOH:O	2.05	0.40
1:A:1634:G:C3'	37:A:3866:HOH:O	2.53	0.40
1:A:164:G:O6	1:A:165:A:C6	2.74	0.40
1:A:1791:U:H2'	1:A:1792:C:C6	2.56	0.40
1:A:2071:C:H5'	37:A:9511:HOH:O	2.21	0.40
1:A:2783:A:O2'	1:A:2784:A:H5'	2.20	0.40
1:A:2898:G:H4'	4:D:288:GLY:HA2	2.03	0.40
1:A:590:A:H2'	1:A:591:A:C5'	2.51	0.40
3:C:1:GLY:HA2	3:C:197:VAL:HG23	2.03	0.40
4:D:234:ARG:NH1	37:D:8616:HOH:O	2.53	0.40
6:F:170:TYR:CD1	6:F:170:TYR:N	2.89	0.40
1:A:2780:C:C1'	7:G:143:GLN:NE2	2.83	0.40
10:J:11:LYS:NZ	37:J:8336:HOH:O	2.45	0.40
37:A:9744:HOH:O	13:M:41:HIS:HE1	2.04	0.40
14:N:122:GLU:HB2	14:N:126:HIS:O	2.22	0.40
14:N:12:TRP:CE2	14:N:20:ILE:CD1	3.02	0.40
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.54	0.40
17:Q:10:ALA:O	17:Q:13:VAL:HG12	2.21	0.40
17:Q:131:PHE:CE1	17:Q:137:LEU:HD13	2.56	0.40
1:A:840:U:H2'	19:S:128:ARG:NH1	2.36	0.40
21:U:105:ASP:OD1	21:U:107:LYS:N	2.54	0.40
24:X:101:LEU:HD23	24:X:101:LEU:HA	1.94	0.40
1:A:1495:C:H1'	1:A:1573:A:H1'	2.03	0.40
1:A:1494:A:O2'	1:A:1505:U:O2	2.24	0.40
1:A:1523:G:C6	1:A:1524:U:O4	2.74	0.40
1:A:154:C:H2'	1:A:155:C:C6	2.56	0.40
1:A:240:C:O2	1:A:240:C:H2'	2.22	0.40
1:A:2484:U:N3	37:A:9601:HOH:O	2.52	0.40
1:A:2729:C:H2'	1:A:2730:G:C8	2.48	0.40
1:A:2783:A:H2'	1:A:2784:A:C8	2.56	0.40
1:A:638:C:H2'	1:A:639:A:C8	2.56	0.40
1:A:821:U:H2'	1:A:822:C:C6	2.49	0.40
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.33	0.40
3:C:192:VAL:HG23	3:C:201:PHE:HB3	2.03	0.40
5:E:233:THR:HG22	5:E:234:VAL:H	1.84	0.40
6:F:128:LEU:C	6:F:128:LEU:HD23	2.42	0.40
1:A:2346:C:O3'	6:F:52:THR:CG2	2.69	0.40
7:G:119:HIS:HE1	7:G:147:ASP:OD2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:21:GLU:HA	8:H:24:ARG:HE	1.85	0.40
37:A:4945:HOH:O	10:J:57:ARG:HG3	2.21	0.40
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.20	0.40
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.83	0.40
27:1:81:LYS:HB2	27:1:82:ALA:H	1.76	0.40
30:4:71:CYS:SG	30:4:72:GLY:N	2.94	0.40
1:A:1336:U:C2	1:A:1337:A:C8	3.09	0.40
1:A:1815:A:HO2'	1:A:2750:G:HO2'	1.65	0.40
1:A:187:A:H3'	1:A:188:C:C6	2.56	0.40
1:A:2044:G:C6	1:A:2045:G:C5	3.09	0.40
1:A:2377:U:O5'	1:A:2377:U:H6	2.04	0.40
1:A:2815:G:N7	11:K:80:LYS:NZ	2.66	0.40
1:A:2851:G:C2'	1:A:2852:A:H5'	2.52	0.40
1:A:290:C:O2'	1:A:291:C:H5'	2.20	0.40
37:A:4379:HOH:O	3:C:11:ARG:CZ	2.70	0.40
3:C:228:ILE:O	3:C:229:ALA:C	2.60	0.40
3:C:36:ASP:HB2	3:C:84:VAL:N	2.37	0.40
4:D:312:ARG:HD3	4:D:315:VAL:HG13	2.02	0.40
4:D:57:GLU:HA	4:D:58:PRO:HD2	1.94	0.40
6:F:19:GLU:O	6:F:133:ASN:HB3	2.21	0.40
10:J:113:ALA:N	10:J:114:PRO:HD3	2.36	0.40
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.72	0.40
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.41	0.40
37:B:5071:HOH:O	15:O:20:TYR:HE2	1.98	0.40
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.03	0.40
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.87	0.40
37:A:5961:HOH:O	30:4:31:THR:HA	2.20	0.40
1:A:1127:C:C5	1:A:1128:U:C4	3.09	0.40
1:A:1552:G:C2	1:A:1553:C:C2	3.10	0.40
1:A:1549:C:N3	1:A:1637:A:C2	2.89	0.40
1:A:2088:C:H1'	1:A:2841:A:C2	2.56	0.40
1:A:2379:G:H4'	1:A:2380:A:H5''	2.04	0.40
1:A:2588:G:H5''	1:A:2589:U:OP2	2.22	0.40
1:A:2782:G:O6	1:A:2790:C:H5''	2.21	0.40
1:A:440:C:O2'	1:A:441:A:H5'	2.21	0.40
3:C:93:THR:HG23	3:C:154:ALA:O	2.22	0.40
7:G:149:GLU:HG3	7:G:166:VAL:O	2.21	0.40
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.37	0.40
11:K:40:ASN:OD1	11:K:106:GLY:HA2	2.22	0.40
11:K:51:GLU:O	11:K:55:GLU:HG3	2.21	0.40
11:K:70:PHE:CD2	11:K:70:PHE:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:71:TYR:CG	11:K:72:PRO:HD2	2.56	0.40
12:L:98:VAL:HG13	12:L:99:ASP:N	2.36	0.40
17:Q:141:ILE:C	17:Q:143:ALA:H	2.25	0.40
37:D:8625:HOH:O	22:V:17:THR:HG21	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	9	39
4	D	335/337 (99%)	304 (91%)	22 (7%)	9 (3%)	5	26
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	34	72
6	F	134/176 (76%)	93 (69%)	30 (22%)	11 (8%)	1	4
7	G	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
8	H	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	9	39
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	131 (86%)	14 (9%)	7 (5%)	2	14
11	K	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	4	24
12	L	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	10	42
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	22	60
14	N	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	15	53
15	O	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	3	18
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	22	60
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	148/154 (96%)	139 (94%)	9 (6%)	0	100	100
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17	55
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	22
24	X	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	12	45
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	5	28
26	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11	43
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	6	31
All	All	3633/4235 (86%)	3300 (91%)	271 (8%)	62 (2%)	9	39

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
10	J	164	ALA
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
23	W	43	PRO
24	X	77	ALA
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
4	D	184	ASP
6	F	11	HIS
6	F	20	LYS
6	F	137	PRO

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Mol	Chain	Res	Type
11	K	5	GLU
11	K	143	LYS
12	L	119	GLN
17	Q	116	SER
30	4	57	GLY
3	C	132	ASP
6	F	16	PRO
6	F	171	ASP
8	H	64	PRO
10	J	40	PRO
10	J	138	PRO
11	K	7	ASP
14	N	140	ALA
15	O	162	ASP
15	O	181	ASP
24	X	49	ASN
27	1	81	LYS
30	4	56	PRO
3	C	119	ALA
10	J	72	VAL
11	K	76	ASP
12	L	126	SER
14	N	165	SER
15	O	65	ASP
15	O	167	ASP
21	U	114	SER
25	Y	77	PHE
4	D	2	GLN
4	D	206	THR
5	E	232	LEU
6	F	60	GLU
6	F	147	ALA
6	F	170	TYR
10	J	128	ALA
18	R	54	PRO
23	W	40	PRO
4	D	107	SER
4	D	185	GLY
10	J	140	PRO
4	D	5	ARG
25	Y	70	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	14	44
4	D	282/282 (100%)	265 (94%)	17 (6%)	19	53
5	E	193/193 (100%)	176 (91%)	17 (9%)	10	36
6	F	117/147 (80%)	108 (92%)	9 (8%)	13	42
7	G	152/155 (98%)	147 (97%)	5 (3%)	38	73
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	110 (90%)	12 (10%)	8	30
11	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	77
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	70
14	N	166/166 (100%)	158 (95%)	8 (5%)	25	62
15	O	149/149 (100%)	143 (96%)	6 (4%)	31	68
16	P	93/93 (100%)	92 (99%)	1 (1%)	73	90
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	77
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	112 (96%)	5 (4%)	29	66
20	T	71/73 (97%)	70 (99%)	1 (1%)	67	88
21	U	105/105 (100%)	102 (97%)	3 (3%)	42	76
22	V	44/52 (85%)	42 (96%)	2 (4%)	27	64
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	83
24	X	130/130 (100%)	121 (93%)	9 (7%)	15	48
25	Y	66/73 (90%)	62 (94%)	4 (6%)	18	53
26	Z	120/195 (62%)	113 (94%)	7 (6%)	20	55
27	1	56/56 (100%)	50 (89%)	6 (11%)	6	26
28	2	46/46 (100%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	3	42/44 (96%)	41 (98%)	1 (2%)	49 79
30	4	79/79 (100%)	73 (92%)	6 (8%)	13 43
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	22 58

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	8	ARG
3	C	33	GLU
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	120	ARG
3	C	131	HIS
3	C	153	ARG
3	C	179	MET
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	84	LEU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	234	ARG
4	D	251	VAL
4	D	254	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	42	ARG
5	E	57	PRO

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Mol	Chain	Res	Type
5	E	67	GLN
5	E	76	ARG
5	E	78	ARG
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
6	F	24	HIS
6	F	61	PHE
6	F	99	ASP
6	F	100	ASP
6	F	131	THR
6	F	133	ASN
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	7	ILE
7	G	12	ASP
7	G	54	ASP
7	G	102	VAL
7	G	164	ASP
8	H	100	ASP
10	J	1	LYS
10	J	30	GLN
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN

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Mol	Chain	Res	Type
11	K	74	ARG
11	K	76	ASP
11	K	79	PHE
11	K	107	ASN
11	K	112	ASP
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	30	ARG
13	M	35	ARG
13	M	80	ASP
13	M	117	GLU
14	N	38	VAL
14	N	46	LEU
14	N	68	ARG
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
19	S	130	MET

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Mol	Chain	Res	Type
19	S	132	ARG
20	T	10	VAL
21	U	39	ASN
21	U	73	HIS
21	U	96	VAL
22	V	9	CYS
22	V	32	CYS
23	W	43	PRO
24	X	4	LEU
24	X	26	ILE
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	49	ARG
25	Y	72	VAL
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	32	LYS
27	1	42	CYS
27	1	49	ARG
27	1	60	CYS
27	1	64	ILE
29	3	18	ASN
30	4	14	CYS
30	4	38	ARG
30	4	42	ARG
30	4	56	PRO
30	4	65	THR
30	4	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such

sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	HIS
3	C	47	HIS
3	C	92	ASN
3	C	125	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	191	ASN
4	D	221	GLN
4	D	238	ASN
4	D	260	HIS
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
5	E	163	HIS
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	119	HIS
7	G	143	GLN
8	H	80	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	35	ASN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	80	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
12	L	10	GLN
13	M	18	HIS

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Mol	Chain	Res	Type
13	M	41	HIS
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	GLN
15	O	107	ASN
15	O	140	GLN
15	O	153	GLN
16	P	53	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	122	GLN
19	S	123	GLN
20	T	53	ASN
21	U	39	ASN
22	V	38	ASN
22	V	39	ASN
23	W	60	GLN
24	X	14	HIS
24	X	28	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	189	ASN
27	1	33	HIS
28	2	8	GLN

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Mol	Chain	Res	Type
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	41	HIS
29	3	45	ASN
30	4	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	33 (1%)
2	B	121/122 (99%)	16 (13%)	6 (4%)
All	All	2868/3044 (94%)	260 (9%)	39 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G

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Mol	Chain	Res	Type
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G

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Mol	Chain	Res	Type
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1083	C
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1129	C
1	A	1130	U
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U

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Mol	Chain	Res	Type
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A

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Mol	Chain	Res	Type
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
1	A	2103	A

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Mol	Chain	Res	Type
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G

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Mol	Chain	Res	Type
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3011	A
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3040	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G

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Mol	Chain	Res	Type
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1261	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1506	U
1	A	1563	G
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2102	G
1	A	2103	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2791	U
2	B	3002	U
2	B	3023	U
2	B	3026	C
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 235 ligands modelled in this entry, 234 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	$\# Z  > 2$
31	TYK	A	9000	1	67,67,67	3.43	31 (46%)	83,97,97	2.34	23 (27%)

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
31	TYK	A	9000	1	-	9/67/126/126	0/3/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	O1C-C1C	12.47	1.61	1.40
31	A	9000	TYK	O9-C9	9.87	1.37	1.22
31	A	9000	TYK	C22-C12	8.42	1.68	1.50
31	A	9000	TYK	C8-C9	6.67	1.62	1.51
31	A	9000	TYK	C4-C3	-6.43	1.41	1.54
31	A	9000	TYK	C7-C6	6.24	1.66	1.53
31	A	9000	TYK	O4C-C4C	5.85	1.56	1.43
31	A	9000	TYK	C4A-C5A	5.52	1.62	1.52
31	A	9000	TYK	C14-C15	5.34	1.63	1.54
31	A	9000	TYK	C6-C5	4.64	1.61	1.52
31	A	9000	TYK	C7-C8	4.25	1.65	1.54
31	A	9000	TYK	C19-C6	3.67	1.64	1.54
31	A	9000	TYK	C3C-C2C	3.51	1.59	1.52
31	A	9000	TYK	C23-C14	3.20	1.56	1.52
31	A	9000	TYK	C2-C3	-3.17	1.48	1.53
31	A	9000	TYK	C1C-C2C	3.15	1.60	1.52
31	A	9000	TYK	C2B-C1B	3.11	1.58	1.51
31	A	9000	TYK	C16-C15	3.11	1.63	1.52
31	A	9000	TYK	C4C-C5C	-3.07	1.45	1.52
31	A	9000	TYK	O5A-C5A	-3.04	1.37	1.44
31	A	9000	TYK	O5B-C1B	2.99	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	O2C-C2C	-2.97	1.35	1.42
31	A	9000	TYK	O20-C20	2.94	1.36	1.19
31	A	9000	TYK	C3A-N3A	2.93	1.55	1.48
31	A	9000	TYK	O3-C3	2.91	1.49	1.43
31	A	9000	TYK	C6A-C5A	-2.90	1.44	1.51
31	A	9000	TYK	C2A-C3A	2.49	1.57	1.53
31	A	9000	TYK	C3B-C4B	2.48	1.58	1.53
31	A	9000	TYK	O3C-C3C	2.44	1.48	1.42
31	A	9000	TYK	C18-C4	2.15	1.57	1.53
31	A	9000	TYK	C4C-C3C	-2.09	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	TYK	O20-C20-C19	-11.11	93.06	125.43
31	A	9000	TYK	O15-C15-C16	-6.77	96.12	106.92
31	A	9000	TYK	C6C-C5C-C4C	-6.10	101.81	113.07
31	A	9000	TYK	O1A-C5-C4	4.69	113.87	108.22
31	A	9000	TYK	C10-C11-C12	-4.46	119.50	126.23
31	A	9000	TYK	O5C-C1C-C2C	-4.44	100.72	109.51
31	A	9000	TYK	O15-C15-C14	3.90	115.97	107.42
31	A	9000	TYK	C17-C16-C15	3.71	123.49	113.27
31	A	9000	TYK	C18-C4-C3	-3.08	106.34	111.17
31	A	9000	TYK	C3B-C2B-C1B	-3.06	108.95	114.82
31	A	9000	TYK	O4C-C4C-C5C	3.01	116.33	109.67
31	A	9000	TYK	O4A-C4A-C5A	2.88	114.29	106.79
31	A	9000	TYK	O5C-C5C-C6C	2.82	112.78	106.70
31	A	9000	TYK	O5A-C5A-C4A	2.75	114.27	109.13
31	A	9000	TYK	O3-C3-C2	-2.58	103.35	109.56
31	A	9000	TYK	O4A-C1B-C2B	2.57	113.45	109.01
31	A	9000	TYK	O3B-C3B-C4B	2.57	112.25	107.48
31	A	9000	TYK	O3C-C3C-C2C	-2.36	103.38	108.94
31	A	9000	TYK	O5C-C1C-O1C	-2.19	104.79	109.97
31	A	9000	TYK	C2A-C3A-C4A	-2.15	107.38	110.44
31	A	9000	TYK	C8C-O3C-C3C	2.13	120.11	114.52
31	A	9000	TYK	O2C-C2C-C1C	2.11	117.10	111.04
31	A	9000	TYK	O15-C1-O1	2.09	128.76	123.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

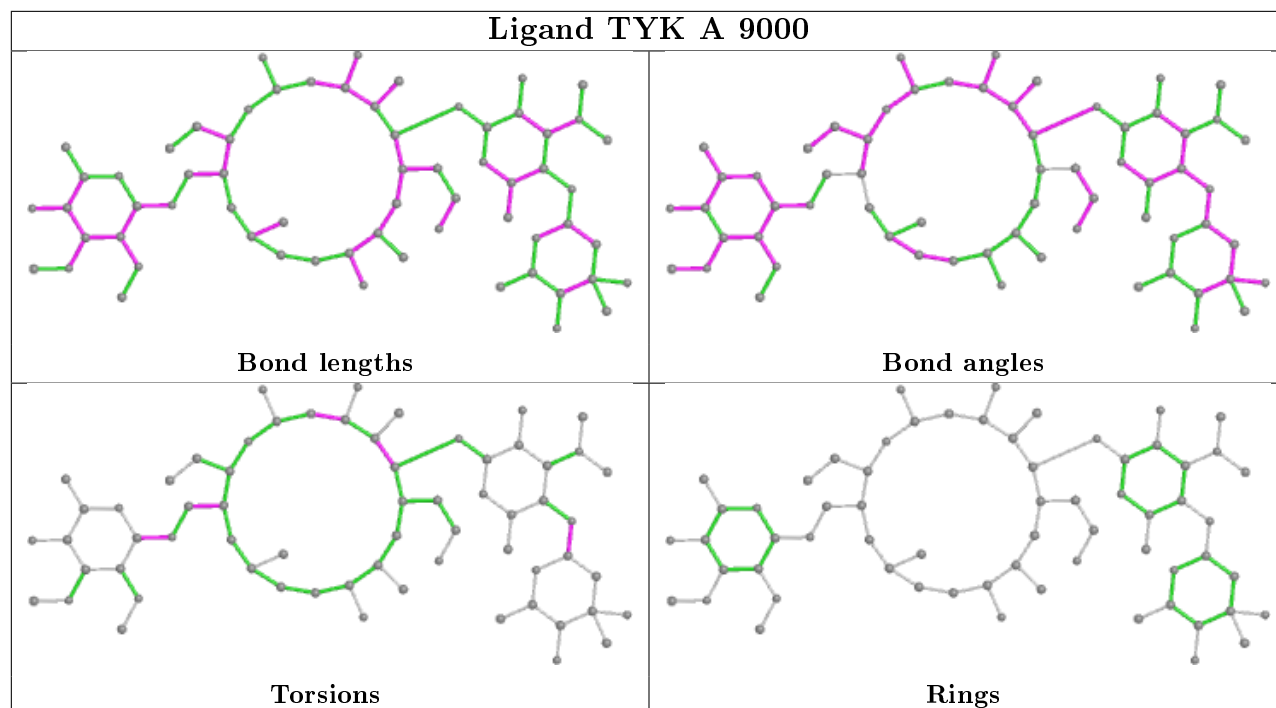
Mol	Chain	Res	Type	Atoms
31	A	9000	TYK	C2B-C1B-O4A-C4A
31	A	9000	TYK	O5C-C1C-O1C-C23
31	A	9000	TYK	C2C-C1C-O1C-C23
31	A	9000	TYK	O5B-C1B-O4A-C4A
31	A	9000	TYK	C1-C2-C3-C4
31	A	9000	TYK	C18-C4-C5-C6
31	A	9000	TYK	C3-C4-C5-C6
31	A	9000	TYK	C1-C2-C3-O3
31	A	9000	TYK	C13-C14-C23-O1C

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	TYK	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.04	66 (2%) 59 30	20, 47, 93, 139	0
2	B	122/122 (100%)	0.22	5 (4%) 37 14	31, 65, 95, 145	0
3	C	237/239 (99%)	0.22	16 (6%) 17 5	27, 61, 90, 109	0
4	D	337/337 (100%)	-0.07	1 (0%) 94 84	20, 54, 81, 90	0
5	E	246/246 (100%)	-0.15	2 (0%) 86 65	19, 49, 72, 81	0
6	F	140/176 (79%)	1.49	40 (28%) 0 0	54, 101, 118, 126	0
7	G	172/177 (97%)	0.60	7 (4%) 37 14	39, 65, 88, 94	0
8	H	119/119 (100%)	0.79	10 (8%) 11 3	56, 78, 99, 103	0
9	I	29/348 (8%)	2.05	14 (48%) 0 0	68, 91, 100, 101	0
10	J	156/167 (93%)	0.23	6 (3%) 40 16	32, 55, 79, 88	0
11	K	142/145 (97%)	-0.10	0 100 100	32, 47, 71, 82	0
12	L	132/132 (100%)	-0.00	1 (0%) 86 65	30, 53, 76, 82	0
13	M	145/164 (88%)	0.58	17 (11%) 4 1	23, 72, 105, 115	0
14	N	194/194 (100%)	0.09	11 (5%) 23 8	34, 53, 83, 88	0
15	O	186/186 (100%)	0.70	24 (12%) 3 1	41, 69, 107, 119	0
16	P	115/115 (100%)	-0.06	0 100 100	38, 57, 76, 80	0
17	Q	143/148 (96%)	0.05	2 (1%) 75 49	33, 58, 73, 81	0
18	R	95/95 (100%)	-0.21	1 (1%) 80 56	33, 48, 59, 73	0
19	S	150/154 (97%)	-0.12	0 100 100	27, 42, 66, 74	0
20	T	81/84 (96%)	0.13	1 (1%) 79 54	47, 62, 80, 84	0
21	U	119/119 (100%)	0.37	3 (2%) 57 29	37, 58, 81, 91	0
22	V	53/66 (80%)	3.14	41 (77%) 0 0	81, 91, 97, 105	0
23	W	65/70 (92%)	1.17	12 (18%) 1 0	52, 77, 106, 113	0
24	X	154/154 (100%)	-0.31	0 100 100	31, 46, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.30	2 (2%) 59 30	39, 55, 81, 93	0
26	Z	142/240 (59%)	-0.01	3 (2%) 63 34	25, 45, 69, 85	0
27	1	73/73 (100%)	2.99	43 (58%) 0 0	79, 92, 98, 99	0
28	2	56/56 (100%)	-0.50	0 100 100	26, 34, 41, 47	0
29	3	46/48 (95%)	0.11	2 (4%) 35 13	33, 59, 85, 97	0
30	4	92/92 (100%)	6.13	92 (100%) 0 0	90, 101, 105, 107	0
All	All	6577/7279 (90%)	0.25	422 (6%) 19 6	19, 54, 99, 145	0

All (422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	14.5
30	4	62	THR	13.3
30	4	82	GLY	12.7
30	4	83	TRP	11.3
30	4	38	ARG	11.2
27	1	11	THR	11.1
30	4	11	CYS	10.7
30	4	33	MET	10.3
30	4	2	GLN	9.5
30	4	35	TRP	9.5
30	4	1	MET	9.5
30	4	56	PRO	9.2
30	4	59	ASP	9.1
30	4	91	GLN	9.0
30	4	84	ARG	8.9
30	4	65	THR	8.9
30	4	14	CYS	8.5
30	4	32	GLY	8.4
30	4	8	ASN	8.4
30	4	41	GLU	8.2
23	W	1	THR	8.1
30	4	85	ALA	8.0
14	N	71	SER	8.0
30	4	34	LYS	7.9
27	1	15	GLY	7.9
27	1	12	GLY	7.8
27	1	22	ILE	7.6
30	4	86	GLY	7.4
27	1	26	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
30	4	31	THR	7.3
30	4	71	CYS	7.3
30	4	47	GLY	7.2
1	A	1173	A	7.2
22	V	40	ALA	7.2
30	4	42	ARG	7.1
30	4	4	PRO	7.0
30	4	60	LYS	7.0
22	V	55	ALA	7.0
30	4	3	MET	6.9
27	1	16	PRO	6.9
30	4	9	THR	6.9
30	4	43	ASN	6.7
30	4	40	ARG	6.6
30	4	88	LEU	6.6
30	4	74	CYS	6.4
30	4	57	GLY	6.4
30	4	53	SER	6.3
30	4	81	GLU	6.3
15	O	186	LEU	6.3
30	4	78	HIS	6.2
30	4	18	GLN	6.0
9	I	24	VAL	6.0
30	4	61	PRO	5.9
30	4	77	ALA	5.9
30	4	22	VAL	5.9
27	1	30	GLU	5.8
30	4	75	GLY	5.8
27	1	44	PHE	5.8
30	4	20	HIS	5.8
30	4	48	ASN	5.8
27	1	23	ARG	5.8
22	V	51	TRP	5.8
9	I	27	ILE	5.7
22	V	9	CYS	5.7
22	V	54	THR	5.6
27	1	39	CYS	5.6
30	4	25	VAL	5.6
22	V	53	ASP	5.6
6	F	57	THR	5.6
21	U	119	ALA	5.5
30	4	36	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
30	4	58	GLY	5.5
30	4	27	SER	5.5
30	4	76	LYS	5.5
1	A	1198	U	5.4
30	4	68	LYS	5.4
6	F	88	LEU	5.3
6	F	10	PHE	5.3
27	1	20	LEU	5.2
30	4	67	LEU	5.2
22	V	52	THR	5.2
30	4	10	TYR	5.2
15	O	162	ASP	5.2
30	4	39	GLN	5.2
27	1	19	GLY	5.1
27	1	17	ARG	5.1
30	4	44	SER	5.0
27	1	21	LYS	5.0
27	1	24	VAL	5.0
9	I	23	ILE	4.9
14	N	89	ASN	4.9
22	V	33	SER	4.9
30	4	55	VAL	4.9
1	A	1172	G	4.8
30	4	13	HIS	4.8
14	N	70	GLY	4.8
30	4	21	GLU	4.8
30	4	17	HIS	4.7
1	A	1175	G	4.7
30	4	15	ASN	4.7
27	1	13	ARG	4.6
30	4	80	ARG	4.6
22	V	41	ASP	4.6
30	4	24	LYS	4.6
30	4	45	GLY	4.6
30	4	5	ARG	4.6
15	O	157	PRO	4.6
22	V	50	GLU	4.6
30	4	19	GLU	4.6
22	V	39	ASN	4.6
30	4	7	PHE	4.5
30	4	63	LYS	4.5
1	A	735	C	4.5

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Mol	Chain	Res	Type	RSRZ
30	4	16	GLU	4.5
30	4	51	LYS	4.5
27	1	34	LYS	4.5
30	4	12	PRO	4.5
30	4	72	GLY	4.5
30	4	87	ARG	4.4
22	V	12	ASP	4.4
1	A	1168	C	4.3
8	H	90	GLU	4.3
30	4	89	GLU	4.3
6	F	26	GLY	4.2
27	1	35	LYS	4.2
22	V	6	CYS	4.2
2	B	3001	U	4.2
1	A	285	A	4.2
27	1	40	PRO	4.2
30	4	30	GLN	4.2
30	4	92	GLU	4.2
1	A	1199	A	4.2
27	1	18	TYR	4.2
15	O	160	SER	4.2
27	1	45	LYS	4.1
15	O	147	ILE	4.1
22	V	32	CYS	4.1
26	Z	108	ASP	4.1
30	4	6	ARG	4.1
27	1	10	ARG	4.1
30	4	49	ASP	4.1
1	A	1171	A	4.1
22	V	11	THR	4.1
3	C	85	ASP	4.0
27	1	28	ASP	4.0
27	1	33	HIS	4.0
1	A	1192	A	4.0
1	A	1948	G	3.9
27	1	31	ILE	3.9
30	4	46	ILE	3.9
15	O	179	LEU	3.9
23	W	39	ALA	3.9
6	F	96	SER	3.8
30	4	69	TYR	3.8
1	A	1177	A	3.8

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Mol	Chain	Res	Type	RSRZ
30	4	52	PHE	3.8
15	O	150	TYR	3.8
15	O	184	ILE	3.8
6	F	102	GLY	3.8
8	H	86	ALA	3.8
3	C	37	VAL	3.7
27	1	42	CYS	3.7
22	V	4	ARG	3.7
22	V	29	THR	3.7
27	1	29	VAL	3.7
6	F	58	VAL	3.7
27	1	25	ARG	3.7
3	C	62	ASP	3.6
6	F	18	ILE	3.6
15	O	159	TYR	3.6
13	M	104	ASP	3.6
27	1	59	HIS	3.6
3	C	64	ASP	3.6
22	V	49	LEU	3.5
27	1	41	VAL	3.5
30	4	23	GLU	3.5
22	V	10	GLY	3.5
30	4	64	LYS	3.5
1	A	1951	G	3.5
6	F	16	PRO	3.5
13	M	102	ASP	3.5
8	H	106	THR	3.5
6	F	84	LEU	3.4
9	I	26	MET	3.4
1	A	1949	G	3.4
1	A	1169	U	3.4
27	1	58	GLY	3.4
22	V	48	ASN	3.4
8	H	15	ASP	3.4
1	A	1188	A	3.4
7	G	10	ASP	3.3
30	4	66	ASP	3.3
27	1	27	ALA	3.3
15	O	158	LEU	3.3
1	A	1204	C	3.3
30	4	79	LEU	3.3
1	A	1167	G	3.3

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Mol	Chain	Res	Type	RSRZ
22	V	19	THR	3.3
1	A	960	G	3.3
27	1	14	PHE	3.3
3	C	82	VAL	3.3
30	4	26	ARG	3.2
1	A	1190	G	3.2
1	A	1525	G	3.2
17	Q	1	THR	3.2
27	1	36	LYS	3.2
22	V	47	ARG	3.2
8	H	107	VAL	3.2
1	A	1279	U	3.1
1	A	1205	U	3.1
30	4	54	LYS	3.1
6	F	56	ARG	3.1
1	A	2345	A	3.1
1	A	2344	G	3.1
3	C	36	ASP	3.1
10	J	83	PHE	3.1
4	D	1	PRO	3.1
27	1	80	MET	3.1
8	H	19	ALA	3.1
6	F	63	ILE	3.0
22	V	25	ASP	3.0
6	F	104	PHE	3.0
1	A	713	U	3.0
6	F	69	ILE	3.0
23	W	8	ILE	3.0
23	W	40	PRO	3.0
13	M	80	ASP	3.0
14	N	72	SER	3.0
27	1	37	HIS	3.0
6	F	11	HIS	3.0
20	T	81	ILE	3.0
9	I	68	GLU	3.0
1	A	2433	A	3.0
9	I	20	VAL	2.9
22	V	46	ALA	2.9
23	W	2	VAL	2.9
6	F	62	ASP	2.9
8	H	20	LEU	2.9
22	V	28	THR	2.9

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Mol	Chain	Res	Type	RSRZ
13	M	73	VAL	2.9
1	A	1197	G	2.9
15	O	67	ALA	2.9
1	A	284	C	2.9
6	F	171	ASP	2.9
8	H	44	SER	2.9
22	V	43	GLY	2.9
9	I	72	ASP	2.8
14	N	74	ARG	2.8
22	V	8	TYR	2.8
27	1	46	LYS	2.8
22	V	34	SER	2.8
6	F	24	HIS	2.8
18	R	95	GLU	2.8
13	M	105	TYR	2.8
2	B	3024	U	2.8
30	4	29	ARG	2.8
9	I	71	LEU	2.8
23	W	7	GLU	2.8
25	Y	80	GLU	2.8
1	A	2004	U	2.8
6	F	89	PRO	2.8
6	F	90	LEU	2.8
6	F	15	GLU	2.8
27	1	68	CYS	2.8
23	W	38	GLY	2.8
5	E	135	GLU	2.7
1	A	1950	G	2.7
27	1	47	LEU	2.7
29	3	35	ARG	2.7
30	4	90	PHE	2.7
13	M	123	ASP	2.7
15	O	167	ASP	2.7
10	J	32	ASP	2.7
14	N	90	ARG	2.7
15	O	146	HIS	2.7
23	W	52	ALA	2.7
3	C	32	VAL	2.7
6	F	132	VAL	2.7
13	M	106	VAL	2.7
15	O	155	GLU	2.7
1	A	1182	C	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	28	GLU	2.7
27	1	57	CYS	2.7
14	N	78	ASN	2.7
22	V	56	ARG	2.7
1	A	1166	A	2.7
1	A	2436	U	2.6
30	4	70	ARG	2.6
6	F	98	PHE	2.6
15	O	152	GLU	2.6
15	O	138	ASP	2.6
22	V	15	PRO	2.6
6	F	59	GLY	2.6
6	F	134	LEU	2.6
30	4	28	GLY	2.6
1	A	1180	U	2.6
6	F	129	ASP	2.6
22	V	7	ASP	2.6
22	V	13	ILE	2.5
6	F	170	TYR	2.5
9	I	67	LEU	2.5
1	A	1203	G	2.5
6	F	87	ALA	2.5
30	4	50	GLY	2.5
1	A	1200	A	2.5
7	G	100	ASP	2.5
30	4	73	GLU	2.5
23	W	10	ASP	2.5
22	V	23	HIS	2.5
2	B	3002	U	2.5
13	M	140	VAL	2.5
1	A	1193	A	2.4
1	A	2637	A	2.4
1	A	1174	A	2.4
1	A	1181	A	2.4
12	L	119	GLN	2.4
13	M	59	GLU	2.4
6	F	106	PHE	2.4
3	C	110	SER	2.4
22	V	45	GLU	2.4
26	Z	235	GLU	2.4
10	J	135	TRP	2.4
15	O	127	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	368	C	2.4
22	V	36	CYS	2.4
1	A	1176	C	2.4
3	C	83	GLY	2.3
23	W	11	MET	2.3
8	H	49	PHE	2.3
3	C	154	ALA	2.3
27	1	38	LYS	2.3
3	C	34	ASP	2.3
13	M	60	GLU	2.3
1	A	736	A	2.3
1	A	371	U	2.3
8	H	18	GLU	2.3
1	A	2237	G	2.3
13	M	120	LEU	2.3
15	O	183	ASP	2.3
27	1	32	LYS	2.3
7	G	108	LEU	2.3
23	W	3	LEU	2.3
13	M	81	VAL	2.3
6	F	85	GLN	2.3
15	O	80	SER	2.3
6	F	27	ILE	2.3
21	U	37	GLN	2.3
14	N	80	GLY	2.3
6	F	48	MET	2.3
6	F	17	ARG	2.3
1	A	970	U	2.3
13	M	130	ARG	2.3
10	J	80	ASN	2.2
6	F	92	GLU	2.2
7	G	28	SER	2.2
22	V	42	LEU	2.2
7	G	122	THR	2.2
1	A	2338	G	2.2
1	A	282	C	2.2
3	C	38	ILE	2.2
9	I	65	THR	2.2
22	V	26	GLY	2.2
26	Z	103	THR	2.2
10	J	146	TRP	2.2
1	A	601	G	2.2

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Mol	Chain	Res	Type	RSRZ
7	G	131	LEU	2.2
6	F	166	ILE	2.2
17	Q	130	GLU	2.2
1	A	130	C	2.2
1	A	1522	A	2.2
9	I	13	PRO	2.2
9	I	21	ASP	2.2
1	A	138	U	2.2
13	M	133	VAL	2.2
1	A	2432	C	2.2
3	C	61	GLU	2.2
22	V	22	VAL	2.2
1	A	1913	C	2.1
25	Y	88	GLU	2.1
1	A	370	G	2.1
13	M	62	ALA	2.1
2	B	3122	C	2.1
6	F	44	ILE	2.1
14	N	83	SER	2.1
15	O	64	SER	2.1
27	1	79	VAL	2.1
6	F	25	MET	2.1
15	O	95	ALA	2.1
1	A	2249	G	2.1
2	B	3023	U	2.1
10	J	81	TYR	2.1
13	M	61	ALA	2.1
22	V	24	LYS	2.1
22	V	14	GLU	2.1
3	C	84	VAL	2.1
5	E	143	ASP	2.1
1	A	1947	G	2.1
3	C	31	LYS	2.1
15	O	72	GLU	2.1
15	O	166	ALA	2.1
6	F	47	GLN	2.1
3	C	60	PHE	2.1
7	G	129	GLU	2.1
1	A	1201	C	2.1
1	A	1162	G	2.1
1	A	372	A	2.1
1	A	1184	C	2.1

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Mol	Chain	Res	Type	RSRZ
14	N	73	ARG	2.0
1	A	362	G	2.0
1	A	1165	G	2.0
6	F	93	LEU	2.0
9	I	64	ASN	2.0
15	O	75	THR	2.0
23	W	63	GLU	2.0
13	M	119	THR	2.0
14	N	26	HIS	2.0
22	V	5	GLU	2.0
1	A	514	G	2.0
1	A	1158	G	2.0
6	F	28	GLY	2.0
21	U	80	GLU	2.0
29	3	36	ASN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	A	8384	1/1	0.27	1.11	106,106,106,106	0
33	NA	S	8337	1/1	0.47	0.33	34,34,34,34	0
34	CL	4	8504	1/1	0.48	1.29	112,112,112,112	0
33	NA	E	8304	1/1	0.62	0.16	32,32,32,32	0
33	NA	J	8322	1/1	0.63	0.46	56,56,56,56	0
33	NA	S	8386	1/1	0.64	0.54	75,75,75,75	0
36	CD	V	8401	1/1	0.68	0.41	142,142,142,142	0
33	NA	T	8312	1/1	0.70	0.79	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CD	P	8405	1/1	0.72	0.20	154,154,154,154	0
32	MG	A	8112	1/1	0.73	0.19	58,58,58,58	0
36	CD	4	8404	1/1	0.74	0.52	148,148,148,148	0
32	MG	A	8104	1/1	0.75	0.38	51,51,51,51	0
33	NA	A	8357	1/1	0.77	0.10	53,53,53,53	0
33	NA	B	8351	1/1	0.77	0.18	58,58,58,58	0
33	NA	A	8373	1/1	0.77	0.49	37,37,37,37	0
34	CL	A	8505	1/1	0.78	0.53	83,83,83,83	0
33	NA	A	8356	1/1	0.78	0.73	57,57,57,57	0
33	NA	A	8332	1/1	0.79	0.18	34,34,34,34	0
32	MG	A	8050	1/1	0.80	0.21	77,77,77,77	0
33	NA	B	8383	1/1	0.81	0.19	54,54,54,54	0
33	NA	A	8382	1/1	0.81	0.30	41,41,41,41	0
33	NA	A	8326	1/1	0.81	0.25	56,56,56,56	0
32	MG	A	8071	1/1	0.82	0.11	84,84,84,84	0
32	MG	A	8001	1/1	0.82	0.11	38,38,38,38	0
32	MG	A	8070	1/1	0.83	0.80	70,70,70,70	0
33	NA	A	8310	1/1	0.84	0.20	31,31,31,31	0
33	NA	A	8377	1/1	0.84	0.32	77,77,77,77	0
32	MG	D	8055	1/1	0.84	0.17	84,84,84,84	0
32	MG	A	8118	1/1	0.84	0.33	31,31,31,31	0
34	CL	M	8510	1/1	0.85	0.33	75,75,75,75	0
33	NA	A	8354	1/1	0.85	0.20	40,40,40,40	0
32	MG	A	8101	1/1	0.85	0.16	38,38,38,38	0
32	MG	A	8081	1/1	0.85	0.18	64,64,64,64	0
33	NA	A	8362	1/1	0.85	0.32	63,63,63,63	0
33	NA	A	8369	1/1	0.85	0.23	53,53,53,53	0
33	NA	A	8303	1/1	0.85	0.26	53,53,53,53	0
34	CL	A	8503	1/1	0.86	0.26	55,55,55,55	0
32	MG	A	8023	1/1	0.86	0.10	42,42,42,42	0
32	MG	A	8090	1/1	0.87	0.21	11,11,11,11	0
33	NA	A	8371	1/1	0.87	0.21	31,31,31,31	0
33	NA	A	8321	1/1	0.87	0.29	45,45,45,45	0
33	NA	A	8364	1/1	0.87	0.23	39,39,39,39	0
33	NA	A	8301	1/1	0.87	0.17	20,20,20,20	0
33	NA	A	8311	1/1	0.87	0.22	50,50,50,50	0
32	MG	A	8087	1/1	0.87	0.18	52,52,52,52	0
33	NA	A	8370	1/1	0.87	0.37	55,55,55,55	0
34	CL	A	8522	1/1	0.88	0.74	80,80,80,80	0
32	MG	A	8024	1/1	0.88	0.55	99,99,99,99	0
32	MG	A	8116	1/1	0.88	0.21	80,80,80,80	0
33	NA	A	8323	1/1	0.88	0.29	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8082	1/1	0.89	0.23	59,59,59,59	0
35	K	A	8602	1/1	0.89	0.13	56,56,56,56	0
33	NA	A	8341	1/1	0.89	0.10	17,17,17,17	0
32	MG	B	8095	1/1	0.89	0.06	68,68,68,68	0
32	MG	A	8046	1/1	0.89	0.07	62,62,62,62	0
34	CL	A	8513	1/1	0.89	0.19	64,64,64,64	0
33	NA	A	8376	1/1	0.89	0.33	80,80,80,80	0
33	NA	A	8366	1/1	0.89	0.28	43,43,43,43	0
33	NA	A	8372	1/1	0.89	0.48	53,53,53,53	0
34	CL	K	8502	1/1	0.90	0.12	56,56,56,56	0
32	MG	A	8100	1/1	0.90	0.15	48,48,48,48	0
33	NA	A	8374	1/1	0.90	0.30	41,41,41,41	0
32	MG	A	8066	1/1	0.90	0.07	70,70,70,70	0
32	MG	A	8059	1/1	0.90	0.09	33,33,33,33	0
33	NA	A	8331	1/1	0.91	0.18	46,46,46,46	0
32	MG	A	8115	1/1	0.91	0.10	46,46,46,46	0
33	NA	A	8368	1/1	0.91	0.16	43,43,43,43	0
33	NA	A	8308	1/1	0.91	0.12	50,50,50,50	0
33	NA	A	8307	1/1	0.91	0.10	20,20,20,20	0
33	NA	A	8365	1/1	0.91	0.33	41,41,41,41	0
32	MG	A	8045	1/1	0.91	0.11	61,61,61,61	0
32	MG	A	8061	1/1	0.91	0.06	35,35,35,35	0
33	NA	A	8330	1/1	0.91	0.18	46,46,46,46	0
32	MG	A	8041	1/1	0.91	0.34	62,62,62,62	0
34	CL	A	8515	1/1	0.91	0.49	97,97,97,97	0
35	K	A	8603	1/1	0.91	0.44	76,76,76,76	0
34	CL	Z	8520	1/1	0.91	0.14	30,30,30,30	0
33	NA	A	8355	1/1	0.91	0.68	55,55,55,55	0
33	NA	A	8324	1/1	0.92	0.12	42,42,42,42	0
33	NA	A	8305	1/1	0.92	0.13	33,33,33,33	0
33	NA	A	8359	1/1	0.92	0.44	52,52,52,52	0
33	NA	A	8333	1/1	0.92	0.16	26,26,26,26	0
33	NA	A	8342	1/1	0.92	0.17	39,39,39,39	0
32	MG	A	8027	1/1	0.92	0.06	51,51,51,51	0
32	MG	Z	8109	1/1	0.92	0.14	39,39,39,39	0
34	CL	R	8511	1/1	0.92	0.13	57,57,57,57	0
32	MG	4	8078	1/1	0.92	0.42	91,91,91,91	0
32	MG	A	8092	1/1	0.92	0.16	83,83,83,83	0
33	NA	A	8302	1/1	0.92	0.16	24,24,24,24	0
32	MG	A	8053	1/1	0.92	0.10	52,52,52,52	0
33	NA	A	8336	1/1	0.92	0.16	46,46,46,46	0
33	NA	A	8378	1/1	0.92	0.30	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8064	1/1	0.92	0.15	18,18,18,18	0
33	NA	M	8380	1/1	0.93	0.25	49,49,49,49	0
33	NA	A	8338	1/1	0.93	0.12	59,59,59,59	0
32	MG	A	8040	1/1	0.93	0.10	84,84,84,84	0
32	MG	A	8114	1/1	0.93	0.23	82,82,82,82	0
33	NA	A	8363	1/1	0.93	0.19	49,49,49,49	0
33	NA	A	8327	1/1	0.93	0.15	28,28,28,28	0
32	MG	A	8103	1/1	0.93	0.20	69,69,69,69	0
33	NA	A	8340	1/1	0.93	0.37	31,31,31,31	0
36	CD	1	8403	1/1	0.93	0.21	139,139,139,139	0
32	MG	A	8088	1/1	0.93	0.07	28,28,28,28	0
32	MG	A	8106	1/1	0.93	0.13	62,62,62,62	0
34	CL	K	8516	1/1	0.93	0.19	40,40,40,40	0
32	MG	A	8108	1/1	0.93	0.11	73,73,73,73	0
33	NA	A	8350	1/1	0.93	0.21	24,24,24,24	0
34	CL	A	8517	1/1	0.93	0.24	49,49,49,49	0
32	MG	A	8089	1/1	0.94	0.11	64,64,64,64	0
32	MG	A	8085	1/1	0.94	0.11	79,79,79,79	0
33	NA	A	8319	1/1	0.94	0.14	39,39,39,39	0
32	MG	U	8073	1/1	0.94	0.12	38,38,38,38	0
33	NA	A	8367	1/1	0.94	0.15	37,37,37,37	0
34	CL	N	8518	1/1	0.94	0.17	38,38,38,38	0
32	MG	A	8022	1/1	0.94	0.18	39,39,39,39	0
33	NA	A	8343	1/1	0.94	0.08	11,11,11,11	0
32	MG	A	8049	1/1	0.94	0.16	62,62,62,62	0
31	TYK	A	9000	64/64	0.94	0.21	33,43,48,51	0
35	K	A	8601	1/1	0.94	0.12	62,62,62,62	0
32	MG	A	8111	1/1	0.94	0.06	54,54,54,54	0
33	NA	A	8375	1/1	0.94	0.25	53,53,53,53	0
32	MG	A	8113	1/1	0.94	0.13	40,40,40,40	0
33	NA	A	8334	1/1	0.94	0.06	26,26,26,26	0
32	MG	A	8067	1/1	0.94	0.26	49,49,49,49	0
32	MG	A	8084	1/1	0.94	0.09	40,40,40,40	0
34	CL	A	8512	1/1	0.94	0.15	32,32,32,32	0
32	MG	A	8075	1/1	0.94	0.11	38,38,38,38	0
33	NA	A	8352	1/1	0.94	0.47	37,37,37,37	0
32	MG	A	8062	1/1	0.94	0.11	46,46,46,46	0
32	MG	A	8057	1/1	0.95	0.18	34,34,34,34	0
34	CL	O	8507	1/1	0.95	0.14	54,54,54,54	0
34	CL	K	8521	1/1	0.95	0.21	50,50,50,50	0
32	MG	A	8102	1/1	0.95	0.86	82,82,82,82	0
33	NA	N	8347	1/1	0.95	0.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8018	1/1	0.95	0.08	32,32,32,32	0
32	MG	A	8044	1/1	0.95	0.17	44,44,44,44	0
32	MG	A	8048	1/1	0.95	0.15	47,47,47,47	0
33	NA	A	8385	1/1	0.95	0.25	28,28,28,28	0
32	MG	A	8093	1/1	0.95	0.12	38,38,38,38	0
32	MG	A	8096	1/1	0.95	0.10	54,54,54,54	0
34	CL	D	8519	1/1	0.95	0.49	59,59,59,59	0
32	MG	A	8110	1/1	0.95	0.11	23,23,23,23	0
33	NA	A	8320	1/1	0.95	0.11	32,32,32,32	0
33	NA	A	8325	1/1	0.95	0.15	47,47,47,47	0
32	MG	A	8072	1/1	0.96	0.15	88,88,88,88	0
32	MG	A	8031	1/1	0.96	0.04	14,14,14,14	0
32	MG	A	8079	1/1	0.96	0.09	24,24,24,24	0
32	MG	A	8003	1/1	0.96	0.12	19,19,19,19	0
33	NA	A	8317	1/1	0.96	0.11	9,9,9,9	0
33	NA	A	8361	1/1	0.96	0.13	48,48,48,48	0
33	NA	A	8316	1/1	0.96	0.12	31,31,31,31	0
34	CL	A	8514	1/1	0.96	0.12	51,51,51,51	0
33	NA	A	8328	1/1	0.96	0.13	24,24,24,24	0
32	MG	A	8006	1/1	0.96	0.06	48,48,48,48	0
32	MG	I	8105	1/1	0.96	0.18	42,42,42,42	0
33	NA	K	8346	1/1	0.96	0.12	17,17,17,17	0
33	NA	A	8318	1/1	0.96	0.14	37,37,37,37	0
32	MG	A	8002	1/1	0.96	0.12	42,42,42,42	0
34	CL	P	8508	1/1	0.96	0.24	83,83,83,83	0
32	MG	A	8052	1/1	0.96	0.05	36,36,36,36	0
33	NA	A	8360	1/1	0.96	0.54	38,38,38,38	0
33	NA	A	8344	1/1	0.96	0.07	16,16,16,16	0
33	NA	A	8314	1/1	0.96	0.14	45,45,45,45	0
32	MG	A	8042	1/1	0.96	0.13	31,31,31,31	0
32	MG	A	8007	1/1	0.96	0.06	24,24,24,24	0
33	NA	A	8379	1/1	0.96	0.15	32,32,32,32	0
33	NA	A	8306	1/1	0.96	0.37	36,36,36,36	0
32	MG	A	8097	1/1	0.96	0.23	37,37,37,37	0
32	MG	A	8119	1/1	0.96	0.10	30,30,30,30	0
32	MG	C	8065	1/1	0.97	0.07	52,52,52,52	0
32	MG	L	8069	1/1	0.97	0.10	72,72,72,72	0
32	MG	A	8107	1/1	0.97	0.06	51,51,51,51	0
32	MG	A	8004	1/1	0.97	0.11	35,35,35,35	0
33	NA	A	8313	1/1	0.97	0.17	64,64,64,64	0
34	CL	S	8506	1/1	0.97	0.14	42,42,42,42	0
32	MG	A	8033	1/1	0.97	0.09	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8076	1/1	0.97	0.13	61,61,61,61	0
32	MG	A	8039	1/1	0.97	0.09	54,54,54,54	0
32	MG	A	8011	1/1	0.97	0.07	25,25,25,25	0
33	NA	A	8329	1/1	0.97	0.09	33,33,33,33	0
32	MG	A	8025	1/1	0.97	0.09	54,54,54,54	0
32	MG	A	8077	1/1	0.97	0.09	28,28,28,28	0
32	MG	A	8021	1/1	0.97	0.08	27,27,27,27	0
32	MG	A	8099	1/1	0.97	0.09	46,46,46,46	0
34	CL	C	8509	1/1	0.97	0.33	74,74,74,74	0
32	MG	A	8051	1/1	0.97	0.07	66,66,66,66	0
32	MG	A	8060	1/1	0.97	0.10	48,48,48,48	0
33	NA	A	8349	1/1	0.97	0.29	33,33,33,33	0
32	MG	A	8016	1/1	0.97	0.08	43,43,43,43	0
33	NA	A	8335	1/1	0.97	0.18	45,45,45,45	0
32	MG	A	8068	1/1	0.97	0.12	40,40,40,40	0
33	NA	A	8339	1/1	0.97	0.16	22,22,22,22	0
32	MG	A	8028	1/1	0.97	0.07	43,43,43,43	0
32	MG	A	8094	1/1	0.97	0.05	60,60,60,60	0
32	MG	A	8032	1/1	0.97	0.10	29,29,29,29	0
32	MG	A	8054	1/1	0.97	0.08	50,50,50,50	0
32	MG	A	8017	1/1	0.98	0.05	28,28,28,28	0
32	MG	A	8083	1/1	0.98	0.07	47,47,47,47	0
32	MG	A	8037	1/1	0.98	0.12	45,45,45,45	0
32	MG	A	8047	1/1	0.98	0.14	45,45,45,45	0
32	MG	A	8034	1/1	0.98	0.05	32,32,32,32	0
36	CD	2	8402	1/1	0.98	0.08	52,52,52,52	0
32	MG	A	8008	1/1	0.98	0.08	41,41,41,41	0
33	NA	J	8309	1/1	0.98	0.13	25,25,25,25	0
32	MG	A	8035	1/1	0.98	0.06	48,48,48,48	0
32	MG	A	8014	1/1	0.98	0.05	13,13,13,13	0
32	MG	A	8038	1/1	0.98	0.05	14,14,14,14	0
32	MG	A	8005	1/1	0.98	0.14	47,47,47,47	0
32	MG	A	8058	1/1	0.98	0.11	34,34,34,34	0
32	MG	A	8029	1/1	0.98	0.12	51,51,51,51	0
33	NA	C	8345	1/1	0.98	0.10	34,34,34,34	0
32	MG	A	8086	1/1	0.98	0.11	40,40,40,40	0
32	MG	A	8074	1/1	0.98	0.07	12,12,12,12	0
32	MG	A	8015	1/1	0.98	0.08	46,46,46,46	0
33	NA	R	8348	1/1	0.98	0.06	15,15,15,15	0
32	MG	A	8091	1/1	0.98	0.07	45,45,45,45	0
32	MG	A	8056	1/1	0.98	0.07	41,41,41,41	0
32	MG	A	8063	1/1	0.98	0.09	73,73,73,73	0

*Continued on next page...*

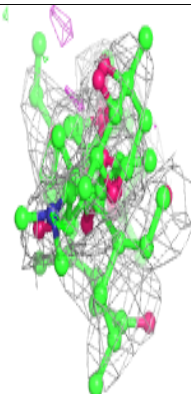
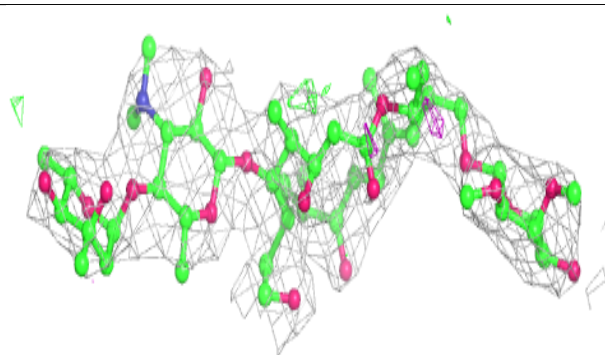
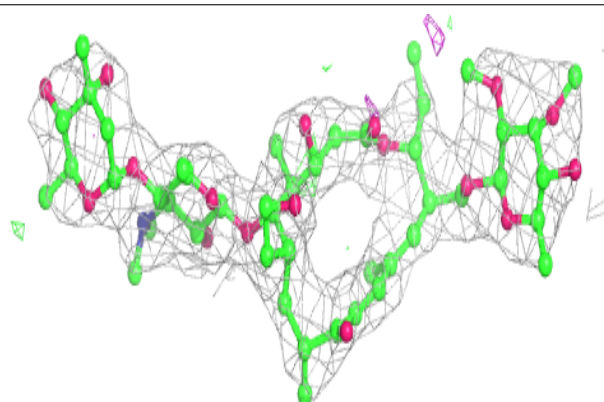
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8043	1/1	0.98	0.06	58,58,58,58	0
34	CL	K	8501	1/1	0.98	0.21	58,58,58,58	0
33	NA	A	8381	1/1	0.98	0.09	33,33,33,33	0
32	MG	A	8020	1/1	0.99	0.05	34,34,34,34	0
32	MG	A	8117	1/1	0.99	0.15	19,19,19,19	0
33	NA	A	8353	1/1	0.99	0.08	16,16,16,16	0
32	MG	A	8030	1/1	0.99	0.09	29,29,29,29	0
32	MG	A	8036	1/1	0.99	0.06	41,41,41,41	0
32	MG	A	8009	1/1	0.99	0.04	19,19,19,19	0
32	MG	A	8013	1/1	0.99	0.18	42,42,42,42	0
33	NA	A	8315	1/1	0.99	0.12	27,27,27,27	0
32	MG	A	8098	1/1	0.99	0.20	43,43,43,43	0
32	MG	A	8026	1/1	0.99	0.05	15,15,15,15	0
32	MG	A	8080	1/1	0.99	0.06	35,35,35,35	0
32	MG	A	8010	1/1	0.99	0.07	29,29,29,29	0
32	MG	A	8012	1/1	0.99	0.11	34,34,34,34	0
32	MG	A	8019	1/1	1.00	0.05	27,27,27,27	0

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

#### Electron density around TYK A 9000:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.