



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:39 pm BST

PDB ID : 1KC8  
Title : Co-crystal Structure of Blastocidin S Bound to the 50S Ribosomal Subunit  
Authors : Hansen, J.L.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2001-11-07  
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

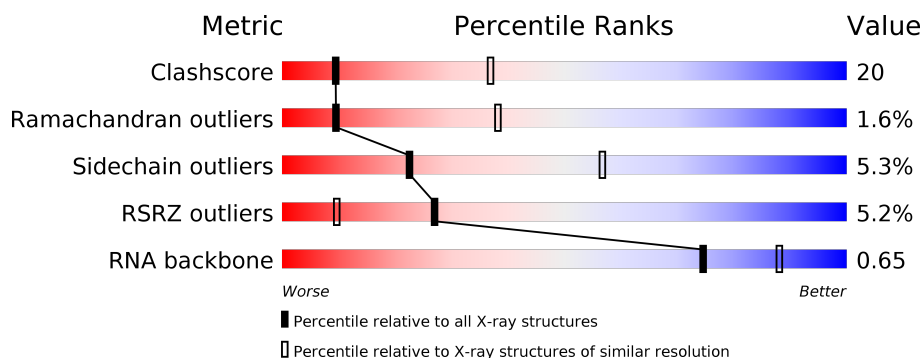
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)
RNA backbone	3102	1066 (3.30-2.74)

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>4%</div> <div>54% 32% 7% 6%</div> </div>
2	B	122	<div> <div>4%</div> <div>49% 37% 9% 5%</div> </div>
3	C	239	<div> <div>3%</div> <div>56% 38% 5%</div> </div>
4	D	337	<div> <div></div> <div>57% 37% 6%</div> </div>
5	E	246	<div> <div></div> <div>55% 40%</div> </div>
6	F	176	<div> <div>23%</div> <div>28% 43% 7% 20%</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
32	MG	A	8102	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	4	8504	-	-	-	X
35	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 98590 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	S	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	S	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	S	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			

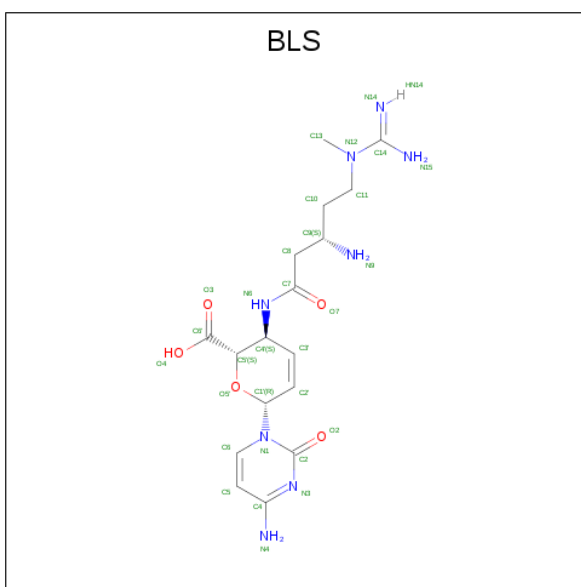
There is a discrepancy between the modelled and reference sequences:

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 BLASTICIDIN S (three-letter code: BLS) (formula: C<sub>17</sub>H<sub>26</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total 30	C 17	N 8	O 5	0	0
31	A	1	Total 30	C 17	N 8	O 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	110	Total Mg 110 110	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	Z	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	9	Total 9	Cl 9	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	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	5909	Total 5909	O 5909	0	0
37	B	147	Total 147	O 147	0	0
37	C	127	Total 127	O 127	0	0
37	D	142	Total 142	O 142	0	0
37	E	168	Total 168	O 168	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	43	Total 43	O 43	0	0
37	H	28	Total 28	O 28	0	0
37	I	21	Total 21	O 21	0	0
37	J	78	Total 78	O 78	0	0
37	K	55	Total 55	O 55	0	0
37	L	65	Total 65	O 65	0	0
37	M	85	Total 85	O 85	0	0
37	N	134	Total 134	O 134	0	0
37	O	66	Total 66	O 66	0	0
37	P	41	Total 41	O 41	0	0
37	Q	64	Total 64	O 64	0	0
37	R	57	Total 57	O 57	0	0
37	S	85	Total 85	O 85	0	0
37	T	35	Total 35	O 35	0	0
37	U	38	Total 38	O 38	0	0
37	V	26	Total 26	O 26	0	0
37	W	16	Total 16	O 16	0	0
37	X	69	Total 69	O 69	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	94	Total 94	O 94	0	0
37	1	37	Total 37	O 37	0	0

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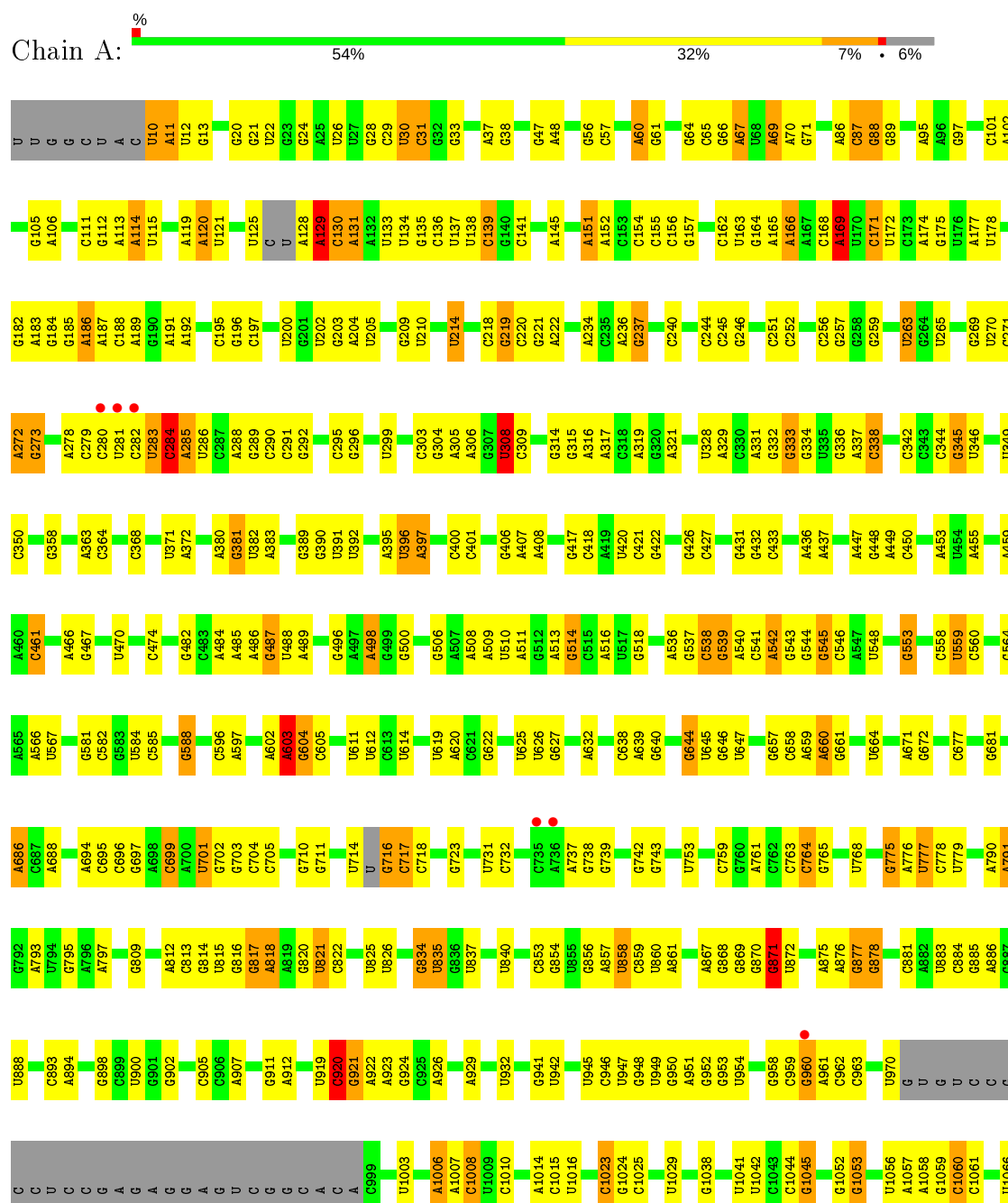
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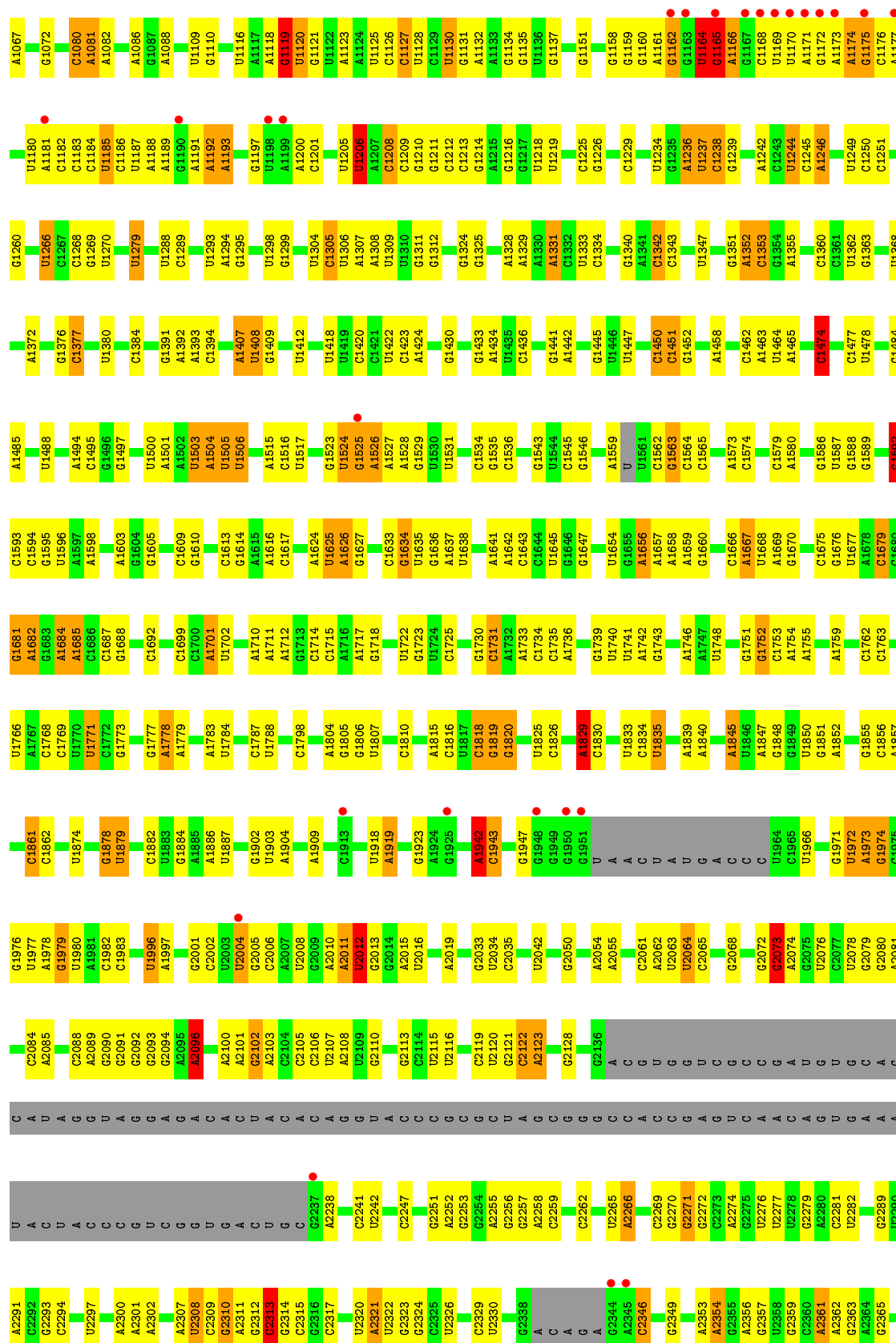
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	56	Total 56	O 56	0	0
37	3	40	Total 40	O 40	0	0
37	4	73	Total 73	O 73	0	0

### 3 Residue-property plots

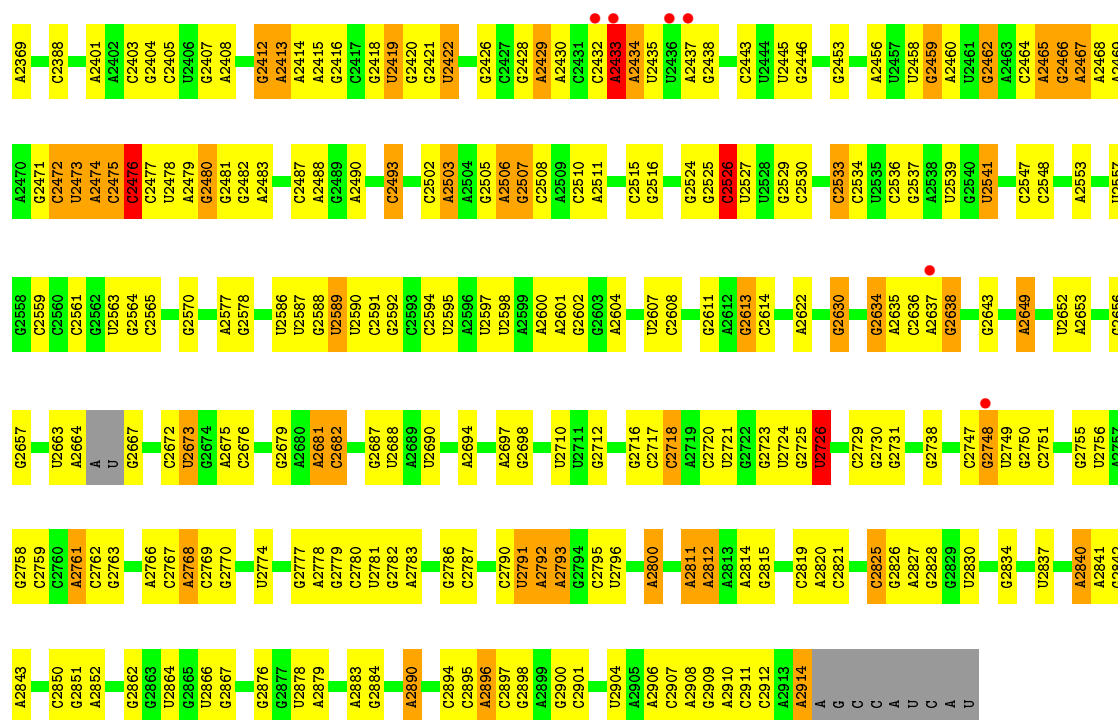
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 23S rRNA

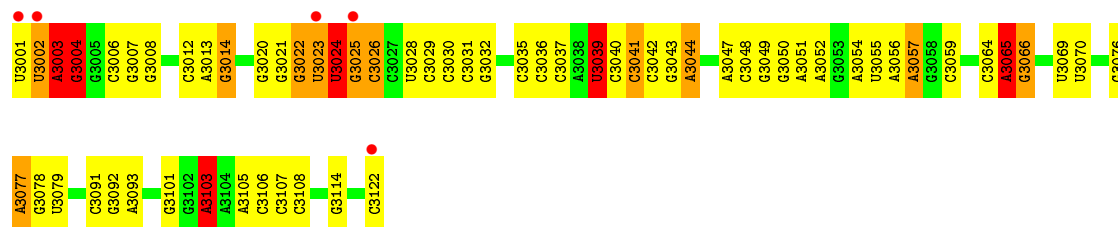




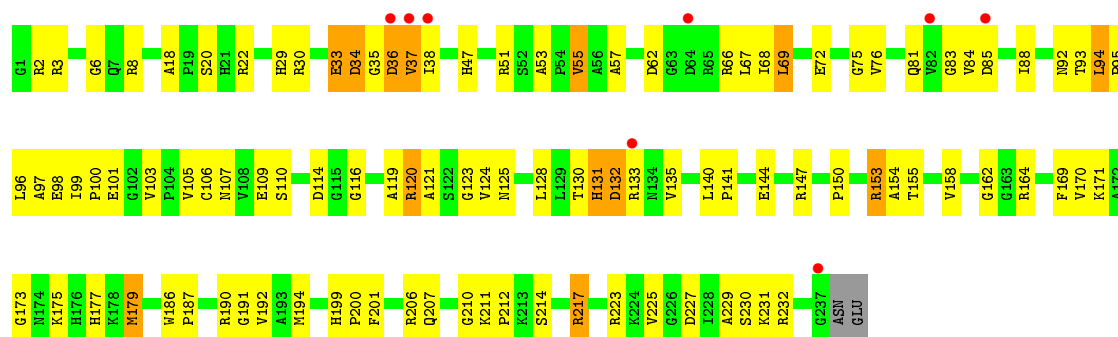




### • Molecule 2: 5S rRNA

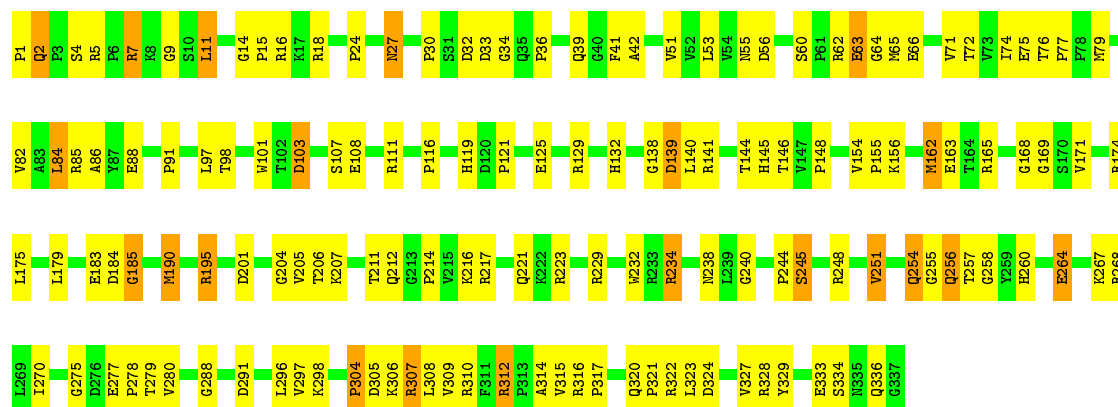


### • Molecule 3: RIBOSOMAL PROTEIN L2

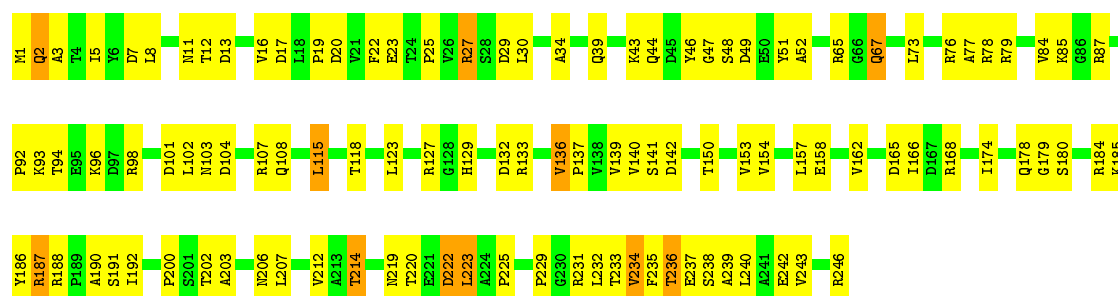


### • Molecule 4: RIBOSOMAL PROTEIN L3

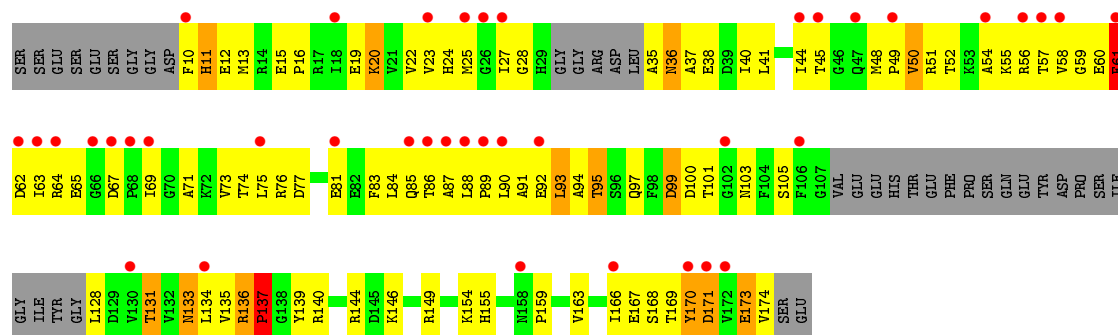




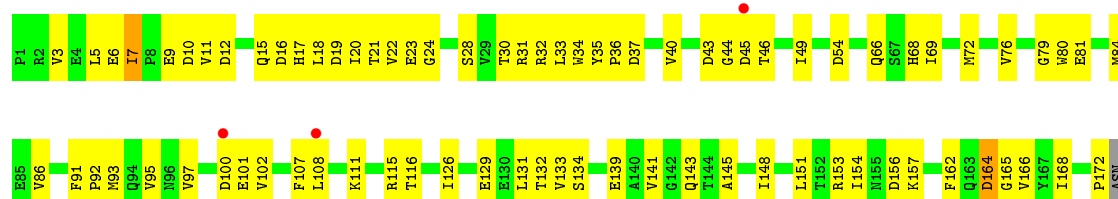
• Molecule 5: RIBOSOMAL PROTEIN L4



• Molecule 6: RIBOSOMAL PROTEIN L5

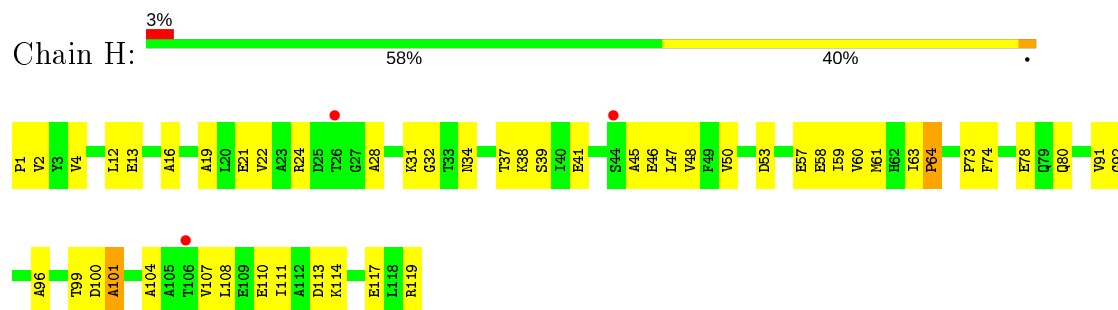


• Molecule 7: RIBOSOMAL PROTEIN L6

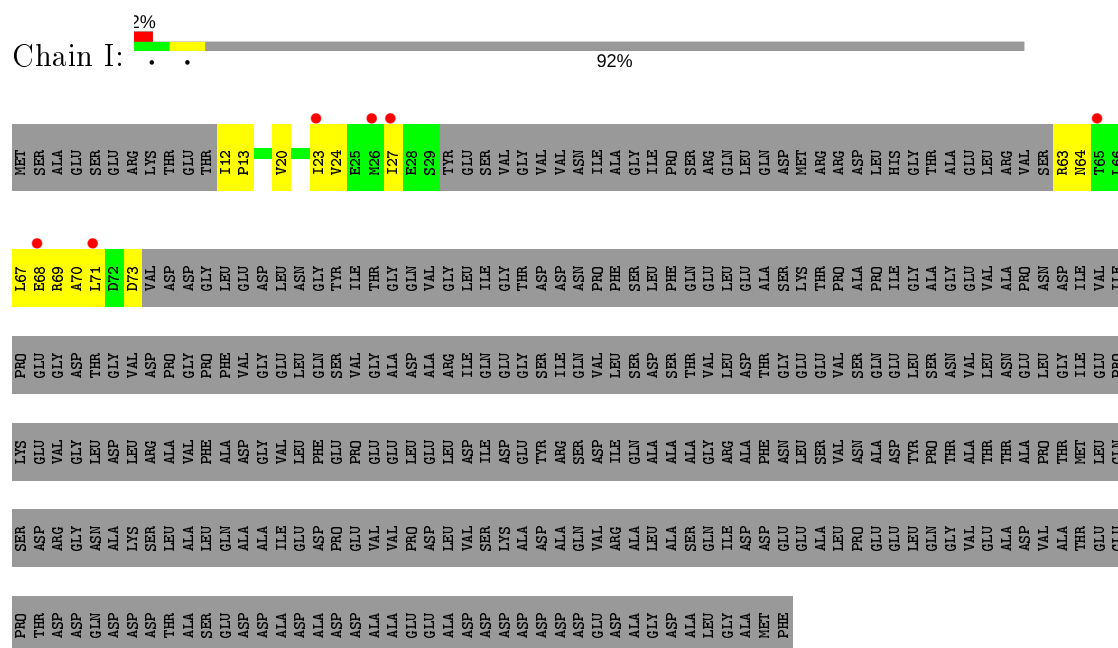


ARG  
GLY  
ASP  
ALA

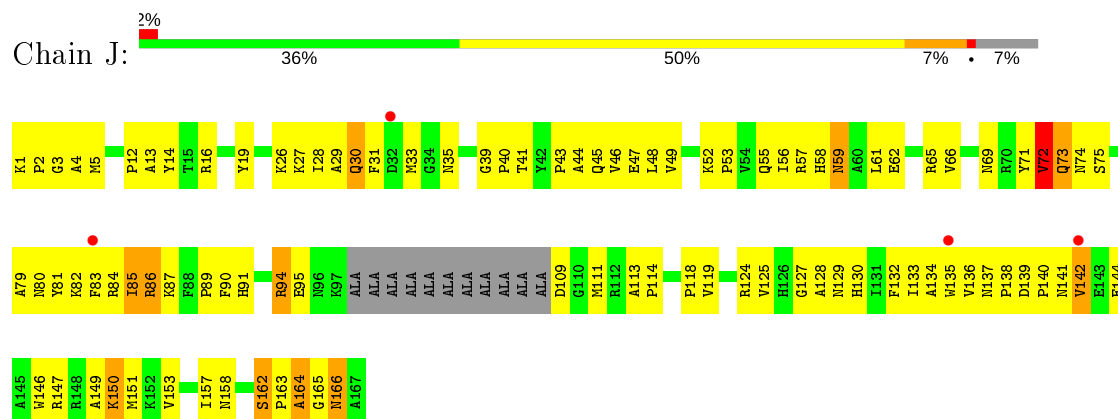
- Molecule 8: RIBOSOMAL PROTEIN L7AE



- Molecule 9: RIBOSOMAL PROTEIN L10

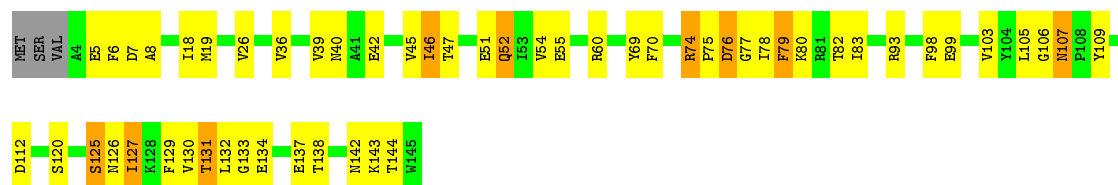


- Molecule 10: RIBOSOMAL PROTEIN L10E



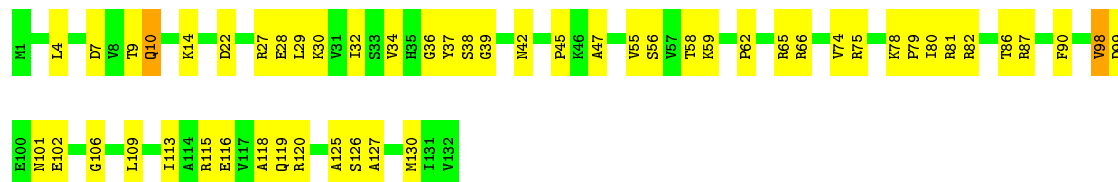
- Molecule 11: RIBOSOMAL PROTEIN L13





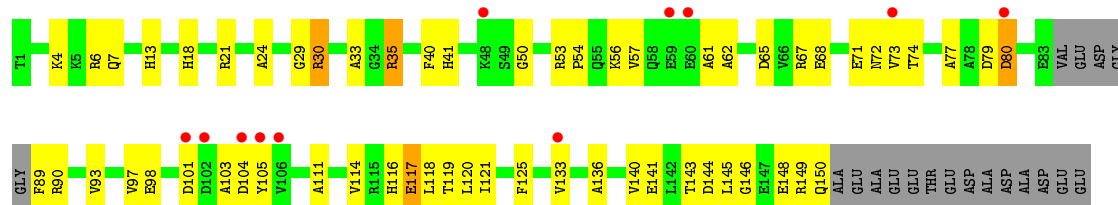
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 61% 38% .



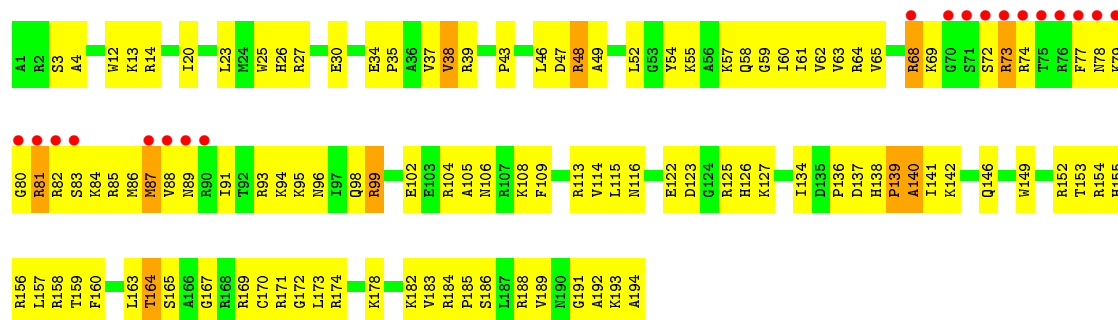
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M: 52% 34% 7% 12%



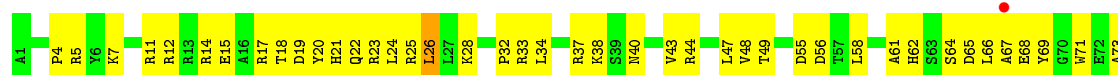
• Molecule 14: RIBOSOMAL PROTEIN L15E

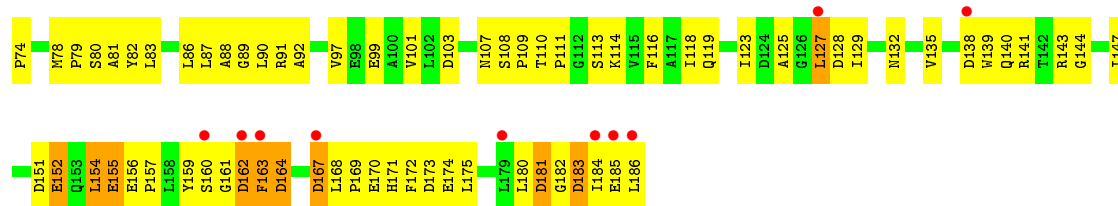
Chain N: 41% 54% 10% 5%



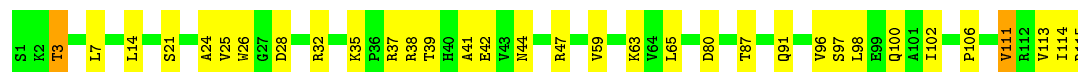
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O: 40% 54% 6% 6%

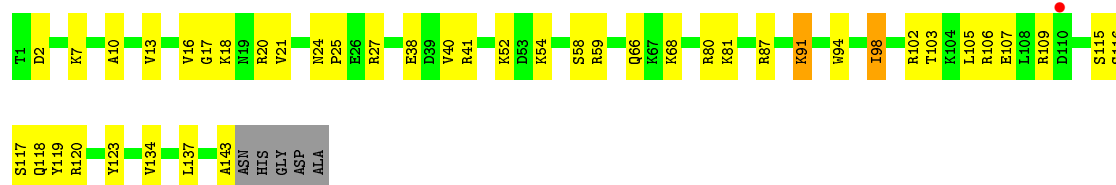




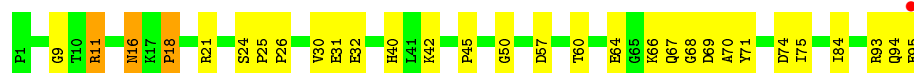
• Molecule 16: RIBOSOMAL PROTEIN L18E



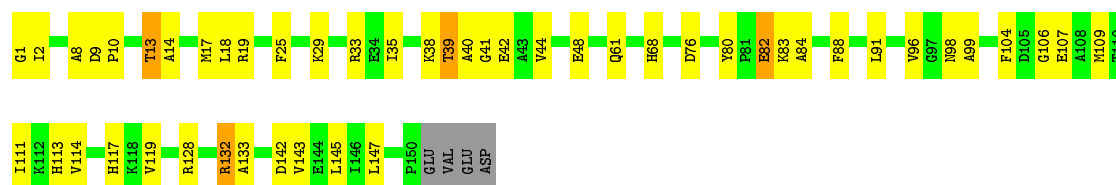
• Molecule 17: RIBOSOMAL PROTEIN L19E



• Molecule 18: RIBOSOMAL PROTEIN L21E



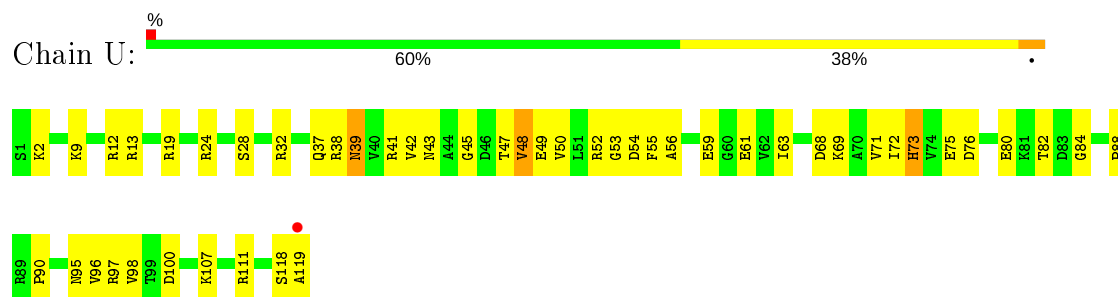
• Molecule 19: RIBOSOMAL PROTEIN L22



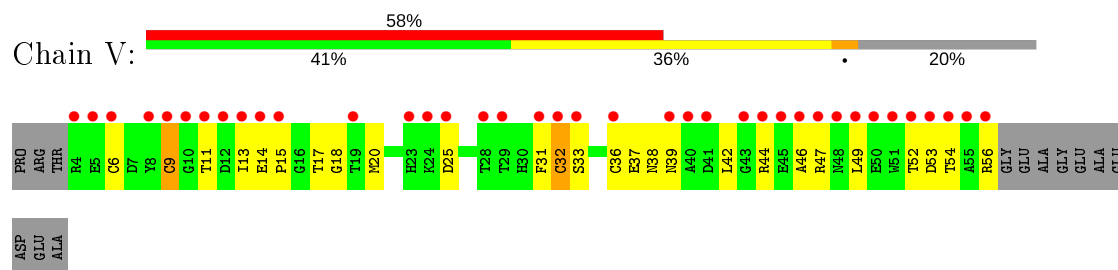
• Molecule 20: RIBOSOMAL PROTEIN L23



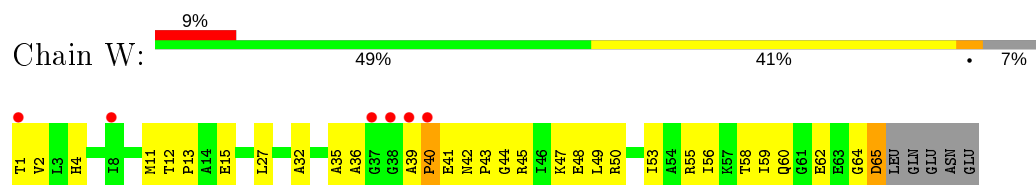
• Molecule 21: RIBOSOMAL PROTEIN L24



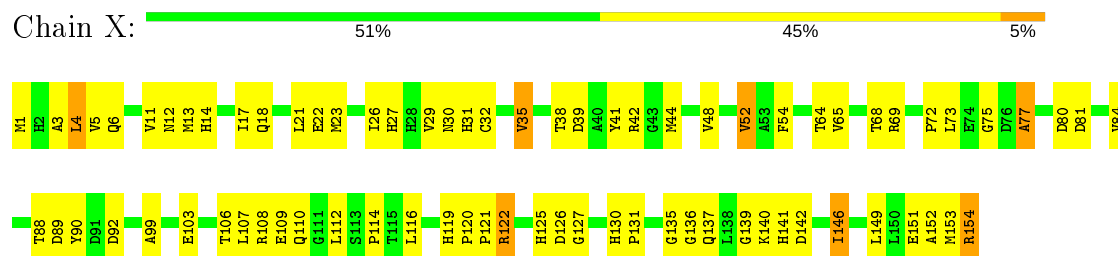
• Molecule 22: RIBOSOMAL PROTEIN L24E



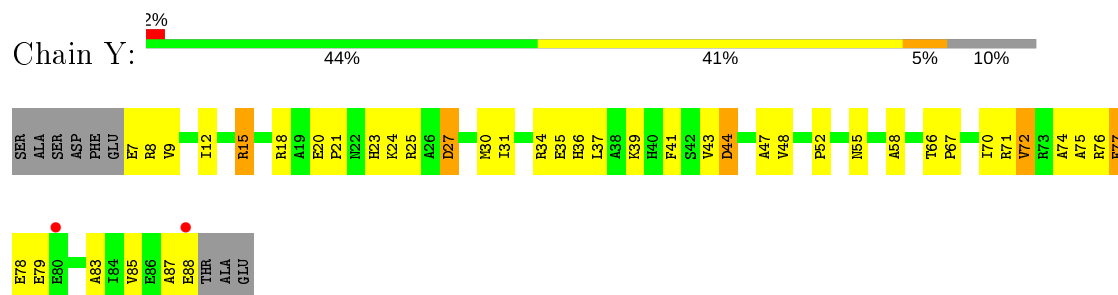
• Molecule 23: RIBOSOMAL PROTEIN L29



• Molecule 24: RIBOSOMAL PROTEIN L30

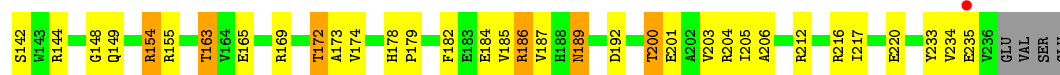
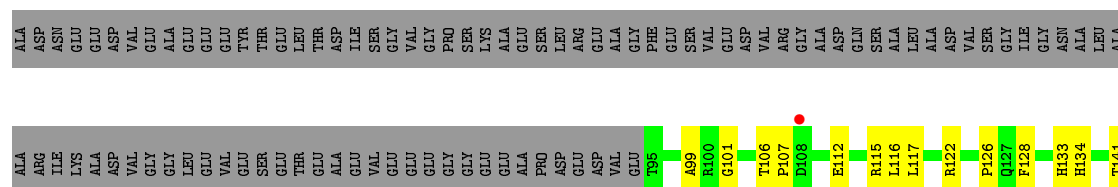


• Molecule 25: RIBOSOMAL PROTEIN L31E

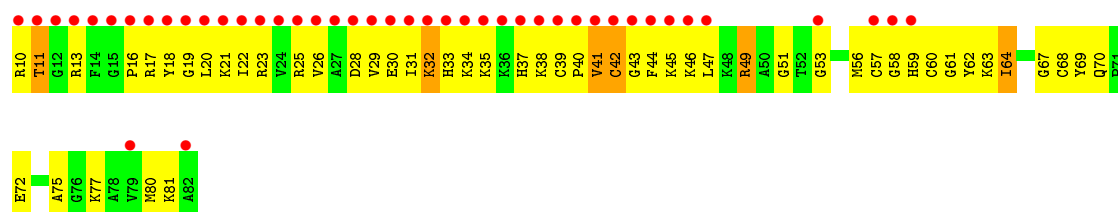


• Molecule 26: RIBOSOMAL PROTEIN L32E

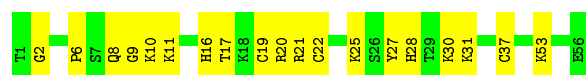




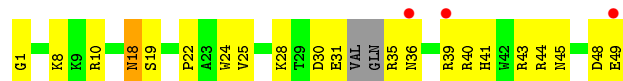
• Molecule 27: RIBOSOMAL PROTEIN L37Ae



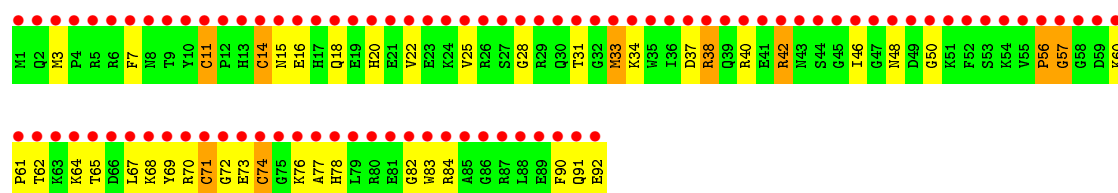
• Molecule 28: RIBOSOMAL PROTEIN L37E



• 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 – 3.01 50.08 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.99-3.01) 94.6 (50.08-3.01)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.195 , 0.235 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	98590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, BLS, 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	16/66076 (0.0%)	0.77	49/103052 (0.0%)
2	B	0.57	3/2905 (0.1%)	0.81	6/4528 (0.1%)
3	C	0.48	0/1787	0.76	0/2409
4	D	0.46	0/2689	0.71	0/3652
5	E	0.50	0/1883	0.76	0/2551
6	F	0.39	0/1111	0.63	0/1498
7	G	0.46	0/1382	0.64	0/1880
8	H	0.39	0/896	0.62	0/1219
9	I	0.33	0/241	0.53	0/324
10	J	0.50	0/1246	0.82	1/1686 (0.1%)
11	K	0.47	0/1135	0.69	0/1530
12	L	0.46	0/1003	0.75	0/1351
13	M	0.48	0/1126	0.74	0/1504
14	N	0.69	0/1633	0.85	2/2180 (0.1%)
15	O	0.49	2/1473 (0.1%)	0.72	0/1999
16	P	0.47	0/873	0.71	0/1181
17	Q	0.47	0/1143	0.63	0/1521
18	R	0.44	0/748	0.76	1/1005 (0.1%)
19	S	0.51	0/1172	0.74	0/1578
20	T	0.42	0/648	0.65	0/875
21	U	0.43	0/957	0.70	0/1289
22	V	0.76	0/417	0.82	1/562 (0.2%)
23	W	0.42	0/502	0.60	0/675
24	X	0.51	0/1218	0.75	0/1655
25	Y	0.48	0/664	0.69	0/895
26	Z	0.49	0/1146	0.71	0/1536
27	1	0.79	0/575	0.82	0/763
28	2	0.57	0/437	0.81	0/578
29	3	0.44	0/398	0.61	0/527
30	4	1.04	1/771 (0.1%)	0.84	2/1024 (0.2%)
All	All	0.57	22/98255 (0.0%)	0.76	62/147027 (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	143
2	B	1	4
All	All	2	147

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2472	C	O3'-P	16.93	1.81	1.61
1	A	2472	C	C2'-O2'	12.85	1.58	1.41
1	A	2473	U	P-OP2	-9.23	1.33	1.49
1	A	2475	C	O3'-P	9.11	1.72	1.61
1	A	2472	C	P-OP2	-7.59	1.36	1.49
1	A	2473	U	P-O5'	-6.94	1.52	1.59
2	B	3003	A	C3'-O3'	6.30	1.50	1.42
2	B	3003	A	C2'-O2'	-6.07	1.33	1.41
1	A	2473	U	C2-N3	5.97	1.42	1.37
1	A	2433	A	C5-C6	5.90	1.46	1.41
1	A	1206	U	C3'-O3'	5.63	1.50	1.42
15	O	20	TYR	CD1-CE1	5.61	1.47	1.39
30	4	33	MET	SD-CE	5.48	2.08	1.77
1	A	2474	A	P-O5'	-5.35	1.54	1.59
1	A	2433	A	N9-C4	5.31	1.41	1.37
1	A	1206	U	P-OP2	5.19	1.57	1.49
1	A	2471	G	C4'-C3'	-5.15	1.47	1.52
1	A	2476	C	O3'-P	-5.14	1.54	1.61
1	A	2473	U	C5'-C4'	5.09	1.57	1.51
15	O	20	TYR	CD2-CE2	5.06	1.47	1.39
2	B	3004	G	P-OP2	-5.04	1.40	1.49
1	A	2477	C	C4'-O4'	5.03	1.52	1.45

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.78	63.88	105.20
1	A	1164	U	OP2-P-O3'	-18.07	65.44	105.20
1	A	1165	G	O5'-P-OP1	-15.12	92.10	105.70
1	A	1979	G	C2'-C3'-O3'	9.86	131.18	109.50
1	A	2476	C	C5'-C4'-O4'	9.81	120.87	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1563	G	C2'-C3'-O3'	9.52	130.44	109.50
2	B	3024	U	C2'-C3'-O3'	9.42	130.23	109.50
1	A	2472	C	O5'-P-OP2	-9.21	97.41	105.70
1	A	1165	G	O5'-P-OP2	-8.77	97.81	105.70
1	A	1942	A	C5'-C4'-O4'	8.64	119.47	109.10
1	A	1942	A	C5'-C4'-C3'	8.46	129.54	116.00
22	V	36	CYS	CA-CB-SG	-8.30	99.06	114.00
1	A	2472	C	C5'-C4'-O4'	-8.05	99.44	109.10
1	A	2473	U	C4-C5-C6	7.58	124.25	119.70
2	B	3004	G	O5'-P-OP1	-7.09	99.32	105.70
1	A	1120	U	C5'-C4'-C3'	-6.98	104.83	116.00
1	A	2122	C	OP2-P-O3'	6.92	120.42	105.20
1	A	2473	U	C5'-C4'-C3'	6.75	126.80	116.00
2	B	3039	U	N1-C1'-C2'	6.75	122.77	114.00
1	A	2471	G	C2'-C3'-O3'	6.62	124.29	113.70
1	A	2473	U	P-O5'-C5'	6.61	131.48	120.90
2	B	3103	A	C5'-C4'-O4'	6.33	116.69	109.10
1	A	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
30	4	11	CYS	CA-CB-SG	-6.08	103.06	114.00
1	A	2477	C	O4'-C4'-C3'	-6.05	97.95	104.00
1	A	2313	C	C5'-C4'-O4'	6.04	116.34	109.10
1	A	2473	U	N3-C4-O4	6.01	123.61	119.40
1	A	1165	G	OP1-P-OP2	5.94	128.51	119.60
2	B	3003	A	C5'-C4'-C3'	5.83	125.33	116.00
1	A	1819	G	C5'-C4'-C3'	5.77	125.24	116.00
1	A	459	A	N9-C1'-C2'	5.76	121.49	114.00
1	A	1829	A	N9-C1'-C2'	-5.74	105.69	112.00
1	A	129	A	C2'-C3'-O3'	5.71	122.83	113.70
14	N	73	ARG	N-CA-C	-5.62	95.82	111.00
30	4	71	CYS	CA-CB-SG	-5.60	103.92	114.00
1	A	2476	C	O5'-C5'-C4'	-5.60	101.06	111.70
1	A	2465	A	N9-C1'-C2'	-5.59	105.85	112.00
1	A	2012	U	N1-C1'-C2'	5.59	121.26	114.00
1	A	2472	C	N1-C1'-C2'	-5.58	105.86	112.00
1	A	2493	C	O4'-C1'-N1	5.53	112.63	108.20
1	A	1819	G	C4'-C3'-C2'	-5.46	97.14	102.60
1	A	2726	U	N1-C1'-C2'	5.43	121.06	114.00
10	J	74	ASN	N-CA-C	-5.38	96.46	111.00
1	A	2477	C	P-O5'-C5'	-5.36	112.33	120.90
1	A	871	G	C5'-C4'-O4'	-5.35	102.68	109.10
1	A	1592	G	N9-C1'-C2'	5.34	120.94	114.00
2	B	3003	A	OP1-P-O3'	5.30	116.86	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1579	C	N1-C1'-C2'	5.28	120.86	114.00
1	A	2419	U	N1-C1'-C2'	5.27	120.85	114.00
1	A	2313	C	O4'-C4'-C3'	-5.26	98.74	104.00
1	A	2476	C	OP1-P-O3'	5.25	116.76	105.20
14	N	139	PRO	N-CA-C	-5.24	98.49	112.10
18	R	68	GLY	N-CA-C	-5.17	100.17	113.10
1	A	2433	A	N9-C1'-C2'	5.16	120.71	114.00
1	A	2096	A	N9-C1'-C2'	5.14	120.69	114.00
1	A	389	G	C5'-C4'-C3'	-5.10	107.84	116.00
1	A	1819	G	C1'-O4'-C4'	-5.08	105.83	109.90
1	A	699	C	C1'-O4'-C4'	-5.05	105.86	109.90
1	A	2476	C	C4'-C3'-C2'	-5.03	97.57	102.60
1	A	920	C	N1-C1'-C2'	5.02	120.53	114.00
1	A	284	C	N1-C1'-C2'	5.02	120.52	114.00
1	A	2313	C	C1'-O4'-C4'	-5.01	105.89	109.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	C	Sidechain
1	A	1038	G	Sidechain
1	A	1053	G	Sidechain
1	A	1082	A	Sidechain
1	A	1119	G	Sidechain
1	A	1127	C	Sidechain
1	A	1206	U	Sidechain
1	A	1226	G	Sidechain
1	A	1236	A	Sidechain
1	A	1244	U	Sidechain
1	A	1260	G	Sidechain
1	A	1266	U	Sidechain
1	A	1288	U	Sidechain
1	A	1305	C	Sidechain
1	A	1309	U	Sidechain
1	A	131	A	Sidechain
1	A	1340	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1347	U	Sidechain
1	A	1355	A	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1408	U	Sidechain
1	A	1418	U	Sidechain
1	A	1430	G	Sidechain
1	A	1433	G	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	1474	C	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1531	U	Sidechain
1	A	1645	U	Sidechain
1	A	1647	G	Sidechain
1	A	1679	C	Sidechain
1	A	1681	G	Sidechain
1	A	1688	G	Sidechain
1	A	169	A	Sidechain
1	A	171	C	Sidechain
1	A	174	A	Sidechain
1	A	1771	U	Sidechain
1	A	1777	G	Sidechain
1	A	1816	C	Sidechain
1	A	1818	C	Sidechain
1	A	1830	C	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1845	A	Sidechain
1	A	1848	G	Sidechain
1	A	1861	C	Sidechain
1	A	1878	G	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	2035	C	Sidechain
1	A	2042	U	Sidechain
1	A	2063	U	Sidechain
1	A	2068	G	Sidechain
1	A	2073	G	Sidechain
1	A	2076	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2078	U	Sidechain
1	A	2092	G	Sidechain
1	A	2096	A	Sidechain
1	A	2123	A	Sidechain
1	A	214	U	Sidechain
1	A	22	U	Sidechain
1	A	2266	A	Sidechain
1	A	2308	U	Sidechain
1	A	2310	G	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	24	G	Sidechain
1	A	2412	G	Sidechain
1	A	2413	A	Sidechain
1	A	2429	A	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2458	U	Sidechain
1	A	2459	G	Sidechain
1	A	2480	G	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2525	G	Sidechain
1	A	2526	C	Sidechain
1	A	2539	U	Sidechain
1	A	2557	U	Sidechain
1	A	26	U	Sidechain
1	A	263	U	Sidechain
1	A	2630	G	Sidechain
1	A	2634	G	Sidechain
1	A	2643	G	Sidechain
1	A	265	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2675	A	Sidechain
1	A	2726	U	Sidechain
1	A	2774	U	Sidechain
1	A	2793	A	Sidechain
1	A	28	G	Sidechain
1	A	2800	A	Sidechain
1	A	2811	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2864	U	Sidechain
1	A	30	U	Sidechain
1	A	308	U	Sidechain
1	A	315	G	Sidechain
1	A	321	A	Sidechain
1	A	33	G	Sidechain
1	A	333	G	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	436	A	Sidechain
1	A	48	A	Sidechain
1	A	486	A	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	603	A	Sidechain
1	A	614	U	Sidechain
1	A	619	U	Sidechain
1	A	664	U	Sidechain
1	A	686	A	Sidechain
1	A	701	U	Sidechain
1	A	723	G	Sidechain
1	A	742	G	Sidechain
1	A	743	G	Sidechain
1	A	753	U	Sidechain
1	A	761	A	Sidechain
1	A	763	C	Sidechain
1	A	764	C	Sidechain
1	A	768	U	Sidechain
1	A	775	G	Sidechain
1	A	791	A	Sidechain
1	A	815	U	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	837	U	Sidechain
1	A	867	A	Sidechain
1	A	881	C	Sidechain
1	A	888	U	Sidechain
1	A	893	C	Sidechain
1	A	900	U	Sidechain
1	A	919	U	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain

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Mol	Chain	Res	Type	Group
2	B	3024	U	Sidechain
2	B	3039	U	Sidechain
2	B	3059	C	Sidechain
2	B	3065	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	29803	1049	0
2	B	2600	0	1326	86	0
3	C	1754	0	1763	129	0
4	D	2624	0	2533	160	0
5	E	1858	0	1816	127	0
6	F	1094	0	1085	128	0
7	G	1357	0	1266	86	0
8	H	885	0	854	60	0
9	I	240	0	231	20	0
10	J	1215	0	1215	156	0
11	K	1119	0	1098	69	0
12	L	993	0	1027	58	0
13	M	1114	0	1072	59	0
14	N	1605	0	1676	182	0
15	O	1444	0	1401	141	0
16	P	864	0	873	32	0
17	Q	1133	0	1127	52	0
18	R	734	0	729	24	0
19	S	1149	0	1122	56	0
20	T	641	0	605	28	0
21	U	949	0	923	50	0
22	V	410	0	368	37	0
23	W	499	0	511	33	0
24	X	1195	0	1137	98	0
25	Y	654	0	653	47	0
26	Z	1130	0	1133	65	0
27	1	563	0	601	81	0
28	2	430	0	426	22	0
29	3	393	0	406	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4	755	0	731	56	0
31	A	60	0	50	5	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	110	0	0	2	0
32	B	1	0	0	0	0
32	C	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	3	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	2	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	2	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	1	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	13	0
37	2	56	0	0	2	0
37	3	40	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4	73	0	0	6	0
37	A	5909	0	0	231	0
37	B	147	0	0	14	0
37	C	127	0	0	15	0
37	D	142	0	0	29	0
37	E	168	0	0	31	0
37	F	51	0	0	18	0
37	G	43	0	0	11	0
37	H	28	0	0	8	0
37	I	21	0	0	6	0
37	J	78	0	0	23	0
37	K	55	0	0	3	0
37	L	65	0	0	16	0
37	M	85	0	0	17	0
37	N	134	0	0	33	0
37	O	66	0	0	16	0
37	P	41	0	0	8	0
37	Q	64	0	0	5	0
37	R	57	0	0	4	0
37	S	85	0	0	10	0
37	T	35	0	0	5	0
37	U	38	0	0	5	0
37	V	26	0	0	5	0
37	W	16	0	0	5	0
37	X	69	0	0	10	0
37	Y	29	0	0	5	0
37	Z	94	0	0	20	0
All	All	98590	0	59561	2936	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 (2936) 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)
14:N:86:MET:CE	14:N:86:MET:SD	2.01	1.48
30:4:33:MET:CE	30:4:33:MET:SD	2.08	1.40
1:A:2122:C:OP2	37:A:6550:HOH:O	1.60	1.17
1:A:2121:G:OP2	37:A:3496:HOH:O	1.61	1.13
5:E:236:THR:HG22	5:E:239:ALA:H	1.06	1.10
10:J:165:GLY:HA3	37:J:8398:HOH:O	1.51	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:G:H4'	10:J:151:MET:HE1	1.29	1.09
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.66	1.09
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.36	1.08
1:A:1160:G:H5'	1:A:1161:A:H5'	1.34	1.07
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.71	1.04
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.38	1.04
14:N:164:THR:HG22	14:N:167:GLY:H	1.21	1.04
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.87	1.03
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.73	1.02
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.40	1.02
1:A:172:U:OP2	37:A:6185:HOH:O	1.77	1.02
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.39	1.02
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.40	1.02
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.41	1.02
1:A:2466:G:H5''	37:A:3634:HOH:O	1.60	1.01
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.42	1.00
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.25	1.00
11:K:76:ASP:HA	37:K:5907:HOH:O	1.62	1.00
1:A:156:C:H5''	14:N:171:ARG:HD3	1.44	1.00
1:A:21:G:H5'	19:S:2:ILE:HA	1.45	0.99
1:A:856:G:H2'	37:A:5407:HOH:O	1.61	0.99
12:L:10:GLN:H	12:L:10:GLN:HE21	1.01	0.99
1:A:1835:U:H5	1:A:1840:A:N7	1.61	0.98
1:A:1751:G:H2'	1:A:1752:G:H5''	1.41	0.98
24:X:88:THR:HB	37:X:6679:HOH:O	1.64	0.98
1:A:1474:C:H5'	1:A:1474:C:H6	1.28	0.97
1:A:2717:C:H2'	1:A:2718:C:H5''	1.45	0.97
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.43	0.97
1:A:1242:A:H5'	11:K:82:THR:HG23	1.45	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.44	0.97
5:E:2:GLN:HB3	37:E:8335:HOH:O	1.65	0.97
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.44	0.97
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.46	0.96
12:L:10:GLN:NE2	12:L:10:GLN:H	1.64	0.96
37:A:3713:HOH:O	14:N:157:LEU:HD11	1.64	0.96
1:A:870:G:H2'	1:A:871:G:H5''	1.46	0.96
2:B:3056:A:H2'	2:B:3057:A:H5''	1.48	0.96
37:A:4835:HOH:O	14:N:14:ARG:HG2	1.64	0.95
2:B:3076:G:H3'	2:B:3077:A:H5''	1.49	0.95
1:A:871:G:H8	1:A:871:G:H5'	1.31	0.94
14:N:146:GLN:HG2	37:N:8582:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.32	0.94
4:D:86:ALA:HA	37:D:8580:HOH:O	1.67	0.93
20:T:57:THR:HG22	20:T:59:ASP:H	1.31	0.93
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.08	0.93
1:A:542:A:H8	1:A:542:A:H5'	1.34	0.93
14:N:79:LYS:HD3	37:N:8559:HOH:O	1.69	0.93
1:A:962:C:H1'	15:O:5:ARG:NH1	1.83	0.93
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.81	0.93
17:Q:115:SER:H	17:Q:118:GLN:HE21	0.94	0.93
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.50	0.93
4:D:140:LEU:HA	37:D:8580:HOH:O	1.68	0.93
13:M:68:GLU:HA	37:M:8549:HOH:O	1.66	0.93
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.47	0.93
2:B:3023:U:H4'	2:B:3024:U:OP2	1.66	0.92
10:J:27:LYS:H	10:J:58:HIS:HD2	1.14	0.92
1:A:1205:U:H2'	1:A:1206:U:H5'	1.51	0.92
14:N:69:LYS:O	14:N:73:ARG:NH2	2.02	0.92
1:A:2717:C:C2'	1:A:2718:C:H5''	1.99	0.92
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.52	0.91
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.48	0.91
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.51	0.91
1:A:871:G:C8	1:A:871:G:H5'	2.04	0.91
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.51	0.91
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.52	0.90
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.12	0.90
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.32	0.90
32:A:8011:MG:MG	37:A:3964:HOH:O	1.15	0.90
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.53	0.90
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.70	0.90
1:A:1372:A:H3'	37:A:7167:HOH:O	1.71	0.89
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.52	0.89
9:I:12:ILE:HA	37:I:4499:HOH:O	1.72	0.89
12:L:39:GLY:HA2	37:L:4183:HOH:O	1.72	0.89
1:A:2468:A:H61	30:4:48:ASN:HD21	1.18	0.89
6:F:25:MET:HE2	6:F:41:LEU:HG	1.55	0.89
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.03	0.89
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.55	0.89
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.72	0.89
1:A:2426:G:H1'	37:A:6065:HOH:O	1.71	0.88
14:N:52:LEU:HD11	37:N:8619:HOH:O	1.73	0.88
1:A:2748:G:H2'	37:A:7524:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:C:H1'	37:A:7447:HOH:O	1.73	0.88
1:A:960:G:H4'	37:A:7410:HOH:O	1.71	0.88
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.53	0.88
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.15	0.88
6:F:105:SER:HB2	6:F:131:THR:HG23	1.55	0.88
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.57	0.87
24:X:88:THR:HG22	24:X:89:ASP:H	1.39	0.87
5:E:236:THR:HG22	5:E:239:ALA:N	1.89	0.87
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.56	0.87
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.57	0.87
37:A:7541:HOH:O	30:4:60:LYS:HG3	1.75	0.86
15:O:144:GLY:O	15:O:147:ILE:HG22	1.74	0.86
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.19	0.86
1:A:2467:A:H2'	37:A:5435:HOH:O	1.73	0.86
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.57	0.86
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.76	0.86
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.40	0.86
1:A:545:G:H8	1:A:545:G:H5'	1.41	0.86
1:A:1701:A:H5'	37:A:6258:HOH:O	1.75	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.11	0.86
3:C:199:HIS:HD2	3:C:201:PHE:H	1.23	0.85
3:C:223:ARG:HG3	37:C:8607:HOH:O	1.76	0.85
10:J:150:LYS:HE2	37:J:8383:HOH:O	1.75	0.85
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.57	0.85
6:F:154:LYS:H	6:F:154:LYS:HD2	1.38	0.85
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.57	0.85
1:A:2533:C:H6	1:A:2533:C:H5'	1.41	0.85
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.92	0.84
1:A:346:U:H4'	37:A:6815:HOH:O	1.78	0.84
14:N:164:THR:HG23	14:N:165:SER:N	1.90	0.83
10:J:142:VAL:HG13	37:J:8381:HOH:O	1.79	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.79	0.83
29:3:41:HIS:H	29:3:45:ASN:HD22	1.25	0.83
1:A:1701:A:H4'	1:A:1702:U:H5''	1.60	0.83
1:A:1165:G:H4'	1:A:1174:A:O2'	1.78	0.83
5:E:236:THR:HG21	37:E:8373:HOH:O	1.77	0.83
12:L:10:GLN:HE21	12:L:10:GLN:N	1.77	0.83
1:A:1450:C:H4'	1:A:1451:C:OP2	1.80	0.82
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.78	0.82
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.78	0.82
1:A:1116:U:O2'	1:A:1118:A:H2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1603:A:H5'	1:A:1605:G:O4'	1.79	0.82
1:A:2812:A:H2	1:A:2814:A:H62	1.27	0.82
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.45	0.82
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.78	0.82
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.61	0.82
1:A:2506:A:HO2'	1:A:2507:G:H8	0.83	0.82
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.61	0.82
1:A:541:C:H2'	1:A:542:A:H5''	1.60	0.82
10:J:139:ASP:N	10:J:140:PRO:HD3	1.94	0.82
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.80	0.82
18:R:25:PRO:HB2	37:R:4350:HOH:O	1.79	0.82
1:A:2123:A:OP2	37:A:5268:HOH:O	1.96	0.82
37:A:4926:HOH:O	2:B:3103:A:H4'	1.80	0.82
5:E:140:VAL:HB	37:E:8449:HOH:O	1.80	0.81
6:F:27:ILE:HG22	6:F:28:GLY:H	1.44	0.81
10:J:136:VAL:HG23	37:J:8343:HOH:O	1.81	0.81
10:J:162:SER:HB2	10:J:163:PRO:CD	2.08	0.81
20:T:57:THR:HG22	20:T:59:ASP:N	1.94	0.81
26:Z:141:THR:HG23	37:Z:8587:HOH:O	1.81	0.81
1:A:2716:G:H5''	4:D:206:THR:HG21	1.63	0.81
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.63	0.81
1:A:1474:C:H5'	1:A:1474:C:C6	2.14	0.81
1:A:272:A:H3'	37:A:7512:HOH:O	1.79	0.80
1:A:541:C:C2'	1:A:542:A:H5''	2.11	0.80
3:C:192:VAL:HB	37:C:8599:HOH:O	1.80	0.80
1:A:645:U:OP2	13:M:4:LYS:HE2	1.82	0.80
22:V:9:CYS:SG	22:V:11:THR:HG23	2.20	0.80
13:M:133:VAL:HA	37:M:8578:HOH:O	1.78	0.80
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.76	0.80
1:A:1116:U:H3	1:A:1246:A:H62	1.28	0.80
19:S:9:ASP:O	19:S:13:THR:HB	1.82	0.80
4:D:238:ASN:HD22	4:D:240:GLY:H	1.30	0.80
1:A:820:G:OP1	27:1:17:ARG:NH2	2.13	0.80
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.64	0.80
1:A:560:C:H42	1:A:597:A:H61	1.29	0.80
1:A:2420:G:O2'	1:A:2421:G:H5'	1.80	0.80
23:W:1:THR:HG23	23:W:2:VAL:H	1.47	0.80
1:A:1116:U:HO2'	1:A:1118:A:H2	0.82	0.79
1:A:870:G:C2'	1:A:871:G:H5''	2.12	0.79
15:O:7:LYS:HE3	18:R:21:ARG:O	1.80	0.79
27:1:42:CYS:SG	27:1:44:PHE:N	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.47	0.79
10:J:2:PRO:HB2	37:J:8364:HOH:O	1.82	0.79
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.46	0.79
1:A:877:G:H5'	1:A:878:G:OP1	1.83	0.79
4:D:321:PRO:HA	37:D:8656:HOH:O	1.82	0.79
19:S:17:MET:SD	37:S:8546:HOH:O	2.39	0.79
21:U:9:LYS:HE3	21:U:13:ARG:NH1	1.98	0.79
1:A:2586:U:H3	1:A:2592:G:H22	1.28	0.79
14:N:87:MET:CG	30:4:46:ILE:HG21	2.12	0.79
1:A:2271:G:OP2	37:A:9424:HOH:O	2.00	0.79
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.13	0.79
1:A:2466:G:OP1	37:A:3634:HOH:O	2.00	0.78
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.47	0.78
1:A:289:G:H22	1:A:363:A:H2	1.32	0.78
37:A:6270:HOH:O	6:F:99:ASP:HA	1.82	0.78
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.65	0.78
1:A:871:G:C5'	1:A:871:G:H8	1.97	0.78
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.65	0.78
1:A:1118:A:H3'	1:A:1118:A:H8	1.48	0.78
1:A:381:G:H5''	37:A:4298:HOH:O	1.83	0.78
37:A:3772:HOH:O	14:N:189:VAL:HG21	1.82	0.78
26:Z:212:ARG:HD2	37:Z:8599:HOH:O	1.83	0.78
1:A:1160:G:C5'	1:A:1161:A:H5'	2.13	0.78
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.83	0.78
11:K:74:ARG:HH11	11:K:74:ARG:HB3	1.46	0.78
1:A:506:G:H22	1:A:509:A:C5'	1.95	0.78
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.65	0.78
12:L:30:LYS:O	12:L:55:VAL:HG13	1.84	0.78
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.13	0.78
19:S:39:THR:HB	19:S:42:GLU:HG3	1.64	0.78
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.78
10:J:139:ASP:HA	37:J:8369:HOH:O	1.82	0.78
13:M:79:ASP:HB3	37:M:8563:HOH:O	1.84	0.78
14:N:74:ARG:O	14:N:88:VAL:HG13	1.84	0.78
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.64	0.77
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.47	0.77
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.66	0.77
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.48	0.77
37:A:9114:HOH:O	14:N:82:ARG:HD2	1.84	0.77
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.84	0.77
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:59:ASN:H	10:J:59:ASN:HD22	1.33	0.77
14:N:164:THR:HG22	14:N:167:GLY:N	1.98	0.77
3:C:35:GLY:O	3:C:36:ASP:HB3	1.84	0.77
8:H:91:VAL:HG12	8:H:92:GLY:H	1.50	0.77
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.84	0.77
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.66	0.77
1:A:1918:U:OP2	37:A:4008:HOH:O	2.03	0.77
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.83	0.77
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.64	0.77
4:D:145:HIS:HD2	4:D:146:THR:O	1.68	0.77
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.12	0.77
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.50	0.77
1:A:2506:A:O2'	1:A:2507:G:H8	1.65	0.77
1:A:2064:U:H4'	1:A:2653:A:OP1	1.85	0.77
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.48	0.77
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.50	0.77
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.98	0.77
1:A:1058:A:H2'	1:A:1060:C:H5''	1.65	0.76
1:A:2467:A:OP1	37:A:9043:HOH:O	2.03	0.76
1:A:1886:A:N3	37:A:4794:HOH:O	2.18	0.76
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.32	0.76
1:A:288:A:H61	1:A:364:C:H42	1.33	0.76
3:C:199:HIS:CD2	3:C:201:PHE:H	2.03	0.76
5:E:132:ASP:HB3	37:E:8362:HOH:O	1.85	0.76
8:H:96:ALA:HA	37:H:3111:HOH:O	1.84	0.76
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.66	0.76
2:B:3056:A:C2'	2:B:3057:A:H5''	2.16	0.76
14:N:186:SER:O	14:N:189:VAL:HG12	1.84	0.76
1:A:1667:A:H8	1:A:1667:A:H5'	1.50	0.76
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.66	0.76
1:A:516:A:OP2	37:A:5620:HOH:O	2.04	0.76
37:A:4808:HOH:O	11:K:47:THR:HB	1.85	0.76
1:A:2432:C:O4'	37:A:9724:HOH:O	2.02	0.76
2:B:3024:U:O2'	2:B:3025:G:H4'	1.85	0.76
1:A:2004:U:H4'	37:A:5286:HOH:O	1.86	0.76
1:A:506:G:H22	1:A:509:A:H5'	1.48	0.76
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.68	0.76
1:A:1164:U:H3	1:A:1192:A:H2	1.31	0.75
1:A:1666:C:O2'	1:A:1667:A:H5''	1.86	0.75
3:C:121:ALA:O	3:C:124:VAL:HG22	1.86	0.75
8:H:91:VAL:HG12	8:H:92:GLY:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.16	0.75
4:D:179:LEU:O	4:D:183:GLU:HG2	1.87	0.75
4:D:62:ARG:HA	4:D:65:MET:HE3	1.66	0.75
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.65	0.75
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.67	0.75
14:N:152:ARG:HG3	37:N:8556:HOH:O	1.84	0.75
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.67	0.75
15:O:113:SER:HB2	37:O:8558:HOH:O	1.85	0.75
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.69	0.75
2:B:3025:G:H3'	2:B:3026:C:H5'	1.66	0.75
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.68	0.75
2:B:3025:G:H3'	2:B:3026:C:C5'	2.15	0.75
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.69	0.75
1:A:962:C:H1'	15:O:5:ARG:HH12	1.52	0.75
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.85	0.74
1:A:1751:G:C2'	1:A:1752:G:H5''	2.17	0.74
22:V:9:CYS:HA	22:V:52:THR:HG23	1.68	0.74
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.68	0.74
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.50	0.74
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.70	0.74
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.27	0.74
11:K:131:THR:HG22	11:K:134:GLU:H	1.52	0.74
27:1:49:ARG:HD2	37:1:8427:HOH:O	1.87	0.74
19:S:99:ALA:HB1	19:S:109:MET:CE	2.17	0.74
27:1:29:VAL:O	27:1:33:HIS:HB2	1.88	0.74
1:A:2291:A:C8	1:A:2309:C:H5'	2.23	0.74
10:J:141:ASN:HA	37:J:8365:HOH:O	1.88	0.74
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.70	0.74
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.52	0.74
1:A:111:C:O2'	28:2:20:ARG:HG2	1.88	0.74
5:E:219:ASN:O	5:E:222:ASP:OD1	2.06	0.74
11:K:19:MET:CE	11:K:132:LEU:HD11	2.18	0.74
1:A:2064:U:H5'	1:A:2652:U:O3'	1.88	0.74
2:B:3023:U:H6	2:B:3023:U:H5''	1.52	0.74
9:I:12:ILE:N	9:I:13:PRO:HD3	2.03	0.74
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.70	0.74
24:X:13:MET:HE1	24:X:18:GLN:HA	1.69	0.74
1:A:541:C:H2'	1:A:542:A:C5'	2.17	0.73
2:B:3023:U:H3'	37:B:8482:HOH:O	1.88	0.73
13:M:67:ARG:O	13:M:71:GLU:HG3	1.87	0.73
26:Z:216:ARG:HD3	37:Z:8568:HOH:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:C:H4'	37:A:7404:HOH:O	1.88	0.73
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.68	0.73
1:A:559:U:H6	1:A:559:U:H5'	1.53	0.73
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.71	0.73
1:A:2432:C:O2'	1:A:2433:A:H5'	1.89	0.73
1:A:450:C:OP1	5:E:184:ARG:NH2	2.19	0.73
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.53	0.73
1:A:284:C:H4'	1:A:285:A:O5'	1.87	0.73
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.70	0.73
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.87	0.73
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.71	0.73
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.69	0.73
1:A:1080:C:H4'	1:A:1081:A:OP1	1.88	0.73
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.73
1:A:1743:G:N7	37:A:9251:HOH:O	2.20	0.73
1:A:2768:A:H2'	1:A:2769:C:O4'	1.88	0.73
10:J:26:LYS:HG2	10:J:28:ILE:H	1.54	0.73
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.86	0.73
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.18	0.73
1:A:282:C:H1'	1:A:368:C:N4	2.03	0.72
19:S:39:THR:HG23	19:S:107:GLU:O	1.89	0.72
12:L:81:ARG:HB2	12:L:87:ARG:NH1	2.04	0.72
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.89	0.72
20:T:43:GLU:HB3	37:T:7106:HOH:O	1.88	0.72
1:A:2638:G:H5'	37:A:4904:HOH:O	1.90	0.72
14:N:139:PRO:O	14:N:140:ALA:HB3	1.89	0.72
1:A:1974:G:OP1	37:A:6835:HOH:O	2.08	0.72
1:A:31:C:H2'	37:A:7674:HOH:O	1.89	0.72
1:A:542:A:C8	1:A:542:A:H5'	2.23	0.72
1:A:820:G:C6	3:C:171:LYS:HB2	2.25	0.72
37:A:7404:HOH:O	21:U:9:LYS:HB2	1.89	0.72
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.20	0.72
10:J:5:MET:HG3	37:J:8364:HOH:O	1.87	0.72
1:A:1679:C:H5'	37:A:9317:HOH:O	1.87	0.72
10:J:137:ASN:O	10:J:139:ASP:N	2.23	0.72
10:J:59:ASN:N	10:J:59:ASN:HD22	1.85	0.72
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.71	0.72
11:K:99:GLU:HA	37:K:7377:HOH:O	1.89	0.72
13:M:143:THR:HG22	13:M:144:ASP:N	2.04	0.72
6:F:19:GLU:O	6:F:20:LYS:HG2	1.90	0.71
29:3:18:ASN:HD21	29:3:40:ARG:H	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:H5'	37:A:5135:HOH:O	1.88	0.71
1:A:21:G:C5'	19:S:2:ILE:HA	2.19	0.71
4:D:248:ARG:NH2	37:D:8524:HOH:O	2.23	0.71
1:A:2054:A:N3	19:S:128:ARG:NH2	2.39	0.71
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.55	0.71
7:G:11:VAL:HG12	7:G:12:ASP:N	2.06	0.71
10:J:14:TYR:H	10:J:91:HIS:CE1	2.09	0.71
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.26	0.71
37:A:6251:HOH:O	16:P:7:LEU:HD22	1.91	0.71
5:E:76:ARG:HD2	37:E:8432:HOH:O	1.90	0.71
37:A:5769:HOH:O	14:N:170:CYS:SG	2.48	0.71
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.71	0.71
23:W:39:ALA:N	23:W:40:PRO:HD2	2.06	0.71
1:A:2466:G:C5'	37:A:3634:HOH:O	2.27	0.71
1:A:2508:C:H2'	37:A:6725:HOH:O	1.91	0.71
4:D:51:VAL:HG23	4:D:329:TYR:O	1.90	0.71
19:S:132:ARG:NH2	37:S:8583:HOH:O	2.22	0.71
1:A:1209:C:H4'	37:A:5259:HOH:O	1.90	0.71
1:A:1595:G:O2'	1:A:1596:U:H5'	1.91	0.71
11:K:45:VAL:HG23	11:K:130:VAL:O	1.90	0.71
2:B:3029:C:H2'	2:B:3030:C:H5'	1.72	0.71
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.22	0.70
23:W:12:THR:HG22	23:W:15:GLU:CG	2.19	0.70
1:A:236:A:H4'	1:A:237:G:H5'	1.73	0.70
1:A:544:G:H2'	1:A:545:G:H5''	1.72	0.70
20:T:23:LYS:HE2	37:T:3430:HOH:O	1.91	0.70
2:B:3014:G:H8	2:B:3014:G:H5'	1.56	0.70
4:D:258:GLY:H	4:D:260:HIS:CE1	2.09	0.70
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.72	0.70
14:N:138:HIS:ND1	14:N:139:PRO:O	2.23	0.70
1:A:2597:U:OP2	37:A:3814:HOH:O	2.08	0.70
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.57	0.70
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.74	0.70
14:N:60:ILE:C	14:N:61:ILE:HD12	2.11	0.70
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.74	0.70
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.72	0.70
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.21	0.70
14:N:169:ARG:HD2	37:N:8593:HOH:O	1.92	0.70
14:N:139:PRO:O	14:N:140:ALA:CB	2.40	0.70
1:A:338:C:H4'	5:E:174:ILE:CD1	2.21	0.70
4:D:305:ASP:O	4:D:306:LYS:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.22	0.70
24:X:26:ILE:O	24:X:26:ILE:HG13	1.90	0.70
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.56	0.69
24:X:88:THR:HG22	24:X:89:ASP:N	2.07	0.69
1:A:2533:C:C6	1:A:2533:C:H5'	2.27	0.69
1:A:2710:U:H1'	37:A:7608:HOH:O	1.92	0.69
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.07	0.69
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.33	0.69
11:K:133:GLY:O	11:K:137:GLU:HG3	1.92	0.69
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.69
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.25	0.69
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.92	0.69
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.07	0.69
1:A:447:A:OP1	21:U:2:LYS:HG2	1.92	0.69
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.22	0.69
14:N:87:MET:CB	30:4:46:ILE:HD13	2.22	0.69
1:A:1625:U:H4'	37:A:4642:HOH:O	1.91	0.69
1:A:299:U:H5'	37:A:7315:HOH:O	1.93	0.69
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.74	0.69
10:J:69:ASN:O	10:J:72:VAL:HG12	1.92	0.69
16:P:47:ARG:HG3	16:P:47:ARG:HH11	1.57	0.69
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.92	0.69
1:A:1170:U:O2'	1:A:1172:G:N7	2.23	0.69
1:A:1835:U:C5	1:A:1840:A:N7	2.53	0.69
7:G:6:GLU:HA	7:G:46:THR:HG22	1.75	0.69
6:F:97:GLN:O	6:F:97:GLN:HG2	1.93	0.69
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.22	0.69
29:3:41:HIS:N	29:3:45:ASN:HD22	1.90	0.69
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.28	0.69
1:A:1191:A:H3'	1:A:1192:A:H5''	1.73	0.69
5:E:115:LEU:O	5:E:118:THR:HB	1.91	0.69
1:A:1329:A:H2	37:A:4659:HOH:O	1.75	0.69
1:A:2281:C:C2'	1:A:2282:U:H5'	2.22	0.69
10:J:27:LYS:H	10:J:58:HIS:CD2	2.05	0.69
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.74	0.69
1:A:2433:A:H2'	1:A:2434:A:C8	2.28	0.69
1:A:2346:C:O2'	6:F:52:THR:HG21	1.93	0.69
10:J:27:LYS:N	10:J:58:HIS:HD2	1.88	0.69
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.58	0.69
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.93	0.69
1:A:1741:U:O2'	1:A:2723:G:H4'	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:LEU:HD23	3:C:94:LEU:N	2.07	0.68
8:H:58:GLU:HA	8:H:61:MET:HG3	1.74	0.68
14:N:164:THR:CG2	14:N:165:SER:N	2.56	0.68
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.75	0.68
3:C:33:GLU:O	3:C:34:ASP:HB2	1.93	0.68
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.75	0.68
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.94	0.68
1:A:1874:U:OP1	37:A:4301:HOH:O	2.11	0.68
3:C:131:HIS:O	3:C:132:ASP:HB2	1.93	0.68
5:E:236:THR:H	5:E:239:ALA:HB3	1.58	0.68
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.75	0.68
1:A:2094:G:H4'	4:D:245:SER:HB3	1.74	0.68
10:J:41:THR:HA	37:J:8396:HOH:O	1.92	0.68
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.29	0.68
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.76	0.68
1:A:2433:A:H2'	1:A:2434:A:H8	1.56	0.68
1:A:558:C:H5'	37:A:5236:HOH:O	1.94	0.68
27:1:28:ASP:O	27:1:31:ILE:HG22	1.94	0.68
3:C:8:ARG:HG2	37:C:8553:HOH:O	1.93	0.68
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.94	0.68
1:A:1887:U:OP1	27:1:21:LYS:HE3	1.93	0.68
1:A:1209:C:H2'	1:A:1210:G:H8	1.56	0.68
29:3:35:ARG:HB2	37:3:2691:HOH:O	1.92	0.68
10:J:71:TYR:C	10:J:73:GLN:H	1.97	0.68
37:A:6846:HOH:O	14:N:178:LYS:HB2	1.92	0.68
1:A:1118:A:H62	1:A:1244:U:H3	1.42	0.68
1:A:2812:A:N7	37:A:7499:HOH:O	2.27	0.68
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.76	0.68
1:A:1119:G:H22	1:A:1246:A:H2	1.42	0.67
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.58	0.67
6:F:91:ALA:HB1	37:F:5198:HOH:O	1.94	0.67
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.76	0.67
24:X:154:ARG:C	37:X:4276:HOH:O	2.32	0.67
1:A:1534:C:N3	37:A:9471:HOH:O	2.27	0.67
1:A:1829:A:H61	27:1:18:TYR:HA	1.60	0.67
1:A:1834:C:H2'	1:A:1840:A:N6	2.09	0.67
37:A:7435:HOH:O	4:D:211:THR:HG21	1.95	0.67
8:H:99:THR:HA	37:H:3461:HOH:O	1.94	0.67
1:A:2421:G:H3'	1:A:2422:U:H5"	1.75	0.67
4:D:36:PRO:HA	4:D:168:GLY:CA	2.23	0.67
6:F:23:VAL:HG23	6:F:23:VAL:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:164:ASP:CG	15:O:167:ASP:HA	2.14	0.67
6:F:95:THR:O	6:F:97:GLN:N	2.24	0.67
10:J:46:VAL:O	10:J:146:TRP:HH2	1.77	0.67
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.09	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.58	0.67
3:C:179:MET:HG2	3:C:186:TRP:CB	2.25	0.67
1:A:820:G:C5	3:C:171:LYS:HB2	2.29	0.67
5:E:78:ARG:NH1	5:E:78:ARG:HG3	2.09	0.67
14:N:104:ARG:O	14:N:108:LYS:HG2	1.94	0.67
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.76	0.67
37:A:6743:HOH:O	15:O:4:PRO:HD2	1.94	0.67
24:X:65:VAL:HA	24:X:68:THR:HG22	1.77	0.67
1:A:711:G:H1'	37:A:7070:HOH:O	1.95	0.67
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.27	0.67
1:A:2475:C:H2'	1:A:2476:C:O5'	1.94	0.67
6:F:55:LYS:HA	37:F:6752:HOH:O	1.95	0.67
10:J:109:ASP:HB2	37:J:8345:HOH:O	1.94	0.67
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.29	0.67
30:4:65:THR:HG23	30:4:67:LEU:HG	1.77	0.67
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.25	0.67
37:L:1387:HOH:O	22:V:20:MET:HE1	1.94	0.67
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.07	0.67
14:N:87:MET:CB	30:4:46:ILE:HG21	2.24	0.66
1:A:1942:A:H3'	37:A:7325:HOH:O	1.95	0.66
1:A:545:G:H5'	1:A:545:G:C8	2.29	0.66
2:B:3039:U:H1'	2:B:3044:A:H61	1.58	0.66
4:D:85:ARG:NH1	37:D:8634:HOH:O	2.28	0.66
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.93	0.66
1:A:281:U:H2'	1:A:282:C:O4'	1.95	0.66
4:D:41:PHE:HA	4:D:79:MET:HE2	1.77	0.66
12:L:55:VAL:HG12	12:L:56:SER:N	2.10	0.66
19:S:39:THR:HG22	19:S:42:GLU:H	1.60	0.66
1:A:1130:U:H2'	1:A:1131:G:O4'	1.96	0.66
4:D:62:ARG:HA	4:D:65:MET:CE	2.24	0.66
5:E:242:GLU:HG3	37:E:8381:HOH:O	1.95	0.66
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.58	0.66
11:K:107:ASN:ND2	11:K:109:TYR:H	1.93	0.66
14:N:84:LYS:HE2	37:N:8579:HOH:O	1.95	0.66
1:A:1829:A:N6	27:1:18:TYR:HA	2.10	0.66
30:4:74:CYS:SG	30:4:76:LYS:HG3	2.35	0.66
1:A:1172:G:H1'	37:A:4949:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:C:H6	1:A:2346:C:O5'	1.77	0.66
6:F:135:VAL:HG22	6:F:136:ARG:H	1.58	0.66
11:K:93:ARG:HH11	11:K:93:ARG:HB3	1.59	0.66
14:N:104:ARG:O	14:N:108:LYS:HE2	1.95	0.66
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.10	0.66
30:4:74:CYS:SG	30:4:76:LYS:CG	2.84	0.66
10:J:162:SER:CB	10:J:163:PRO:HD3	2.22	0.66
27:1:23:ARG:NH1	37:1:8404:HOH:O	2.29	0.66
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.26	0.66
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.96	0.66
1:A:558:C:O2'	1:A:559:U:H5''	1.95	0.66
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.31	0.66
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.78	0.66
10:J:140:PRO:HB3	37:J:8381:HOH:O	1.95	0.66
14:N:35:PRO:O	37:N:8539:HOH:O	2.13	0.66
1:A:661:G:C5	1:A:686:A:C2	2.83	0.66
2:B:3023:U:H5''	2:B:3023:U:C6	2.31	0.66
7:G:69:ILE:HA	7:G:72:MET:CE	2.26	0.66
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.96	0.66
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.76	0.66
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.77	0.66
10:J:127:GLY:O	10:J:128:ALA:HB3	1.95	0.66
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.77	0.65
1:A:1741:U:H5'	1:A:1742:A:OP1	1.95	0.65
1:A:1919:A:H4'	37:A:4821:HOH:O	1.95	0.65
1:A:282:C:O2'	1:A:283:U:H5'	1.96	0.65
5:E:139:VAL:HG13	37:E:8446:HOH:O	1.95	0.65
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.93	0.65
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.97	0.65
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.95	0.65
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.29	0.65
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.77	0.65
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.61	0.65
35:A:8505:CL:CL	37:A:4908:HOH:O	2.51	0.65
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.09	0.65
1:A:183:A:H5'	14:N:157:LEU:HD12	1.79	0.65
1:A:396:U:H1'	37:A:7616:HOH:O	1.95	0.65
1:A:2637:A:H8	31:A:9002:BLS:H2'	1.60	0.65
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.22	0.65
5:E:12:THR:HB	37:E:8439:HOH:O	1.96	0.65
6:F:101:THR:HG22	37:F:7400:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:148:GLU:HA	37:M:8577:HOH:O	1.95	0.65
1:A:902:G:N7	13:M:18:HIS:HD2	1.93	0.65
37:B:8476:HOH:O	15:O:23:ARG:HD3	1.95	0.65
1:A:739:G:C5	37:A:7526:HOH:O	2.50	0.65
5:E:236:THR:HA	37:E:8449:HOH:O	1.96	0.65
16:P:32:ARG:O	16:P:32:ARG:HD3	1.94	0.65
1:A:125:U:H2'	37:A:3755:HOH:O	1.97	0.65
1:A:2359:G:N7	37:A:3690:HOH:O	2.29	0.65
1:A:2578:G:H8	1:A:2578:G:H5'	1.61	0.65
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.25	0.65
1:A:2281:C:H2'	1:A:2282:U:H5'	1.78	0.65
4:D:41:PHE:HB3	4:D:190:MET:HE3	1.79	0.65
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.79	0.65
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.78	0.65
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.12	0.65
27:1:30:GLU:HA	27:1:33:HIS:CB	2.27	0.65
1:A:2827:A:H2'	1:A:2828:G:O4'	1.95	0.65
4:D:254:GLN:HG3	37:D:8530:HOH:O	1.96	0.65
7:G:69:ILE:HA	7:G:72:MET:HE3	1.79	0.65
1:A:2011:A:P	37:A:5931:HOH:O	2.54	0.65
4:D:223:ARG:HG3	4:D:232:TRP:O	1.97	0.65
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.11	0.65
30:4:74:CYS:SG	30:4:76:LYS:CB	2.85	0.65
1:A:2276:U:H2'	1:A:2277:U:C6	2.32	0.65
6:F:25:MET:CE	6:F:41:LEU:HG	2.27	0.65
24:X:26:ILE:O	24:X:26:ILE:CG1	2.44	0.65
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.62	0.64
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.98	0.64
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.79	0.64
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.32	0.64
1:A:2622:A:OP2	37:A:9147:HOH:O	2.15	0.64
9:I:12:ILE:N	9:I:13:PRO:CD	2.61	0.64
13:M:136:ALA:HB3	37:M:8578:HOH:O	1.97	0.64
14:N:52:LEU:HD21	37:N:8619:HOH:O	1.98	0.64
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.97	0.64
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.79	0.64
22:V:6:CYS:SG	22:V:31:PHE:HA	2.37	0.64
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.27	0.64
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.78	0.64
1:A:1205:U:H2'	1:A:1206:U:C5'	2.26	0.64
1:A:2361:A:H5''	37:A:9003:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:9:CYS:CA	22:V:52:THR:HG23	2.27	0.64
37:A:4049:HOH:O	4:D:27:ASN:HB2	1.96	0.64
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.80	0.64
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.25	0.64
14:N:172:GLY:O	14:N:183:VAL:HG11	1.97	0.64
23:W:64:GLY:O	23:W:65:ASP:HB2	1.97	0.64
1:A:2769:C:H2'	1:A:2770:G:O4'	1.98	0.64
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.95	0.64
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.28	0.64
37:A:6975:HOH:O	18:R:9:GLY:HA2	1.98	0.64
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.97	0.64
1:A:544:G:C2'	1:A:545:G:H5''	2.27	0.64
5:E:168:ARG:NH2	5:E:190:ALA:O	2.31	0.64
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.33	0.64
10:J:45:GLN:HE21	10:J:135:TRP:HE1	1.46	0.64
24:X:122:ARG:HH22	24:X:154:ARG:C	2.01	0.64
1:A:2755:G:H1'	37:A:4658:HOH:O	1.97	0.64
1:A:383:A:H4'	37:A:5309:HOH:O	1.97	0.63
1:A:603:A:H5''	1:A:604:G:OP1	1.97	0.63
14:N:154:ARG:HD3	37:N:8645:HOH:O	1.97	0.63
15:O:73:ALA:N	37:O:8565:HOH:O	2.31	0.63
29:3:41:HIS:H	29:3:45:ASN:ND2	1.96	0.63
32:A:8029:MG:MG	37:A:7802:HOH:O	1.41	0.63
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.80	0.63
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.45	0.63
6:F:37:ALA:O	6:F:40:ILE:HG12	1.98	0.63
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.80	0.63
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.80	0.63
37:A:4702:HOH:O	15:O:21:HIS:HD2	1.81	0.63
1:A:625:U:H5''	1:A:1044:C:N4	2.12	0.63
1:A:553:G:P	26:Z:204:ARG:HH22	2.22	0.63
4:D:204:GLY:HA3	37:D:8652:HOH:O	1.99	0.63
6:F:69:ILE:O	6:F:69:ILE:HG22	1.97	0.63
12:L:58:THR:HG22	12:L:59:LYS:HG3	1.80	0.63
1:A:157:G:H4'	14:N:95:LYS:HE3	1.80	0.63
1:A:1730:G:H5'	1:A:1731:C:C5	2.34	0.63
1:A:2419:U:H5''	1:A:2420:G:H5'	1.79	0.63
2:B:3092:G:H2'	2:B:3093:A:C8	2.33	0.63
4:D:138:GLY:O	4:D:139:ASP:O	2.16	0.63
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.13	0.63
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:145:LEU:O	13:M:148:GLU:HG3	1.98	0.63
14:N:30:GLU:O	14:N:34:GLU:HG3	1.98	0.63
24:X:38:THR:HG22	37:X:3580:HOH:O	1.98	0.63
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.79	0.63
2:B:3049:G:H5'	37:B:8467:HOH:O	1.98	0.63
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.43	0.63
15:O:151:ASP:O	15:O:154:LEU:HB2	1.99	0.63
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.28	0.63
1:A:1634:G:H3'	37:A:3880:HOH:O	1.97	0.63
1:A:2121:G:O2'	1:A:2122:C:H5'	1.99	0.63
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.97	0.63
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.17	0.63
7:G:23:GLU:HG2	7:G:28:SER:CB	2.29	0.63
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.99	0.63
37:A:6678:HOH:O	26:Z:165:GLU:HB3	1.99	0.63
37:A:4172:HOH:O	26:Z:186:ARG:HD2	1.98	0.63
1:A:1268:C:O2'	1:A:1269:G:H5'	1.99	0.62
1:A:20:G:H21	19:S:117:HIS:HD2	1.47	0.62
1:A:2119:C:O2'	1:A:2120:U:H5'	1.98	0.62
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.14	0.62
30:4:62:THR:HB	37:4:8555:HOH:O	1.98	0.62
1:A:1293:U:O2'	26:Z:149:GLN:NE2	2.29	0.62
24:X:119:HIS:HD2	24:X:120:PRO:O	1.83	0.62
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.28	0.62
1:A:1362:U:H5'	37:A:3249:HOH:O	1.99	0.62
1:A:189:A:OP1	14:N:171:ARG:NH2	2.31	0.62
2:B:3039:U:H1'	2:B:3044:A:N6	2.14	0.62
3:C:69:LEU:CD2	3:C:120:ARG:HB3	2.27	0.62
5:E:127:ARG:HH11	5:E:127:ARG:HG2	1.64	0.62
37:A:4522:HOH:O	10:J:151:MET:HE2	1.99	0.62
11:K:74:ARG:O	11:K:78:ILE:HG12	1.98	0.62
19:S:44:VAL:O	19:S:48:GLU:HG3	1.99	0.62
1:A:2279:G:OP1	37:A:5073:HOH:O	2.16	0.62
7:G:79:GLY:HA3	37:G:7046:HOH:O	2.00	0.62
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.11	0.62
1:A:1116:U:O2'	1:A:1118:A:C2	2.45	0.62
1:A:182:G:O3'	14:N:157:LEU:CD1	2.48	0.62
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.81	0.62
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.29	0.62
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.01	0.62
1:A:1060:C:H6	1:A:1060:C:H5'	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:O3'	14:N:157:LEU:HD13	2.00	0.62
22:V:14:GLU:O	22:V:17:THR:HB	1.99	0.62
23:W:4:HIS:HB3	37:W:6622:HOH:O	2.00	0.62
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.81	0.62
1:A:1123:A:C6	1:A:1238:C:H5'	2.35	0.62
4:D:41:PHE:CD2	4:D:190:MET:HE3	2.34	0.62
5:E:214:THR:HG21	37:E:8403:HOH:O	1.98	0.62
10:J:75:SER:O	10:J:79:ALA:HB2	2.00	0.62
37:B:8467:HOH:O	15:O:147:ILE:HD12	1.98	0.62
5:E:246:ARG:NH1	5:E:246:ARG:HB3	2.15	0.62
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.82	0.62
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.82	0.62
27:I:18:TYR:HB3	27:I:22:ILE:HG21	1.80	0.62
1:A:2301:A:H5''	1:A:2302:A:H5'	1.81	0.62
2:B:3013:A:O2'	2:B:3014:G:H5''	2.00	0.62
2:B:3025:G:C3'	2:B:3026:C:H5'	2.29	0.62
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.81	0.62
5:E:16:VAL:HG12	5:E:17:ASP:N	2.15	0.62
5:E:79:ARG:O	5:E:87:ARG:HG2	2.00	0.62
12:L:115:ARG:HG3	12:L:116:GLU:N	2.15	0.62
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.65	0.62
15:O:119:GLN:O	15:O:123:ILE:HG13	2.00	0.62
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.82	0.61
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.30	0.61
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.81	0.61
1:A:1086:A:N6	24:X:11:VAL:HG11	2.15	0.61
1:A:2421:G:H3'	1:A:2422:U:C5'	2.31	0.61
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.29	0.61
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.83	0.61
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.30	0.61
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.31	0.61
1:A:182:G:H4'	14:N:157:LEU:HD13	1.82	0.61
1:A:214:U:H5'	37:A:6114:HOH:O	1.99	0.61
1:A:714:U:H3'	37:A:6916:HOH:O	2.01	0.61
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.82	0.61
14:N:106:ASN:ND2	35:N:8518:CL:CL	2.69	0.61
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.81	0.61
19:S:132:ARG:CZ	37:S:8583:HOH:O	2.48	0.61
23:W:42:ASN:HB3	37:W:7247:HOH:O	2.00	0.61
1:A:2271:G:P	37:A:9424:HOH:O	2.58	0.61
1:A:2464:C:H5''	1:A:2465:A:OP1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2505:G:O2'	1:A:2506:A:H5'	2.01	0.61
1:A:871:G:C5'	1:A:871:G:C8	2.75	0.61
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.82	0.61
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.51	0.61
14:N:61:ILE:N	14:N:61:ILE:HD12	2.14	0.61
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.63	0.61
3:C:192:VAL:O	3:C:192:VAL:HG12	2.00	0.61
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.82	0.61
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.83	0.61
1:A:431:G:P	14:N:48:ARG:HH12	2.23	0.61
16:P:87:THR:O	16:P:91:GLN:HG3	2.00	0.61
1:A:1187:U:O2'	1:A:1189:A:H2	1.84	0.61
1:A:263:U:O4'	8:H:59:ILE:HD13	2.00	0.61
1:A:657:G:OP1	5:E:27:ARG:NH2	2.30	0.61
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.33	0.61
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.33	0.61
1:A:1377:C:H5'	1:A:1377:C:H6	1.66	0.61
1:A:2324:G:H4'	1:A:2418:G:O2'	2.01	0.61
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.82	0.61
1:A:2840:A:OP1	4:D:211:THR:HG23	2.00	0.61
1:A:2878:U:H2'	1:A:2879:A:O4'	2.01	0.61
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.00	0.61
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.16	0.61
1:A:2717:C:H2'	1:A:2718:C:C5'	2.26	0.61
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.66	0.61
27:1:51:GLY:HA3	37:1:8416:HOH:O	2.01	0.61
1:A:1701:A:H4'	1:A:1702:U:C5'	2.31	0.61
3:C:192:VAL:O	3:C:207:GLN:HG2	2.00	0.61
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.83	0.61
5:E:1:MET:HG2	5:E:2:GLN:H	1.65	0.61
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.81	0.61
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.83	0.61
12:L:38:SER:O	37:L:4183:HOH:O	2.16	0.61
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.35	0.61
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.41	0.60
29:3:39:ARG:HG2	37:3:3143:HOH:O	2.01	0.60
6:F:105:SER:CB	6:F:131:THR:HG23	2.28	0.60
2:B:3001:U:O3'	2:B:3003:A:H5''	2.00	0.60
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.37	0.60
15:O:89:GLY:O	15:O:92:ALA:HB3	2.01	0.60
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1972:U:H2'	1:A:1973:A:H5'	1.83	0.60
1:A:2908:A:H2'	1:A:2909:G:O4'	2.01	0.60
2:B:3003:A:H2'	37:B:8422:HOH:O	2.01	0.60
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.34	0.60
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.82	0.60
1:A:797:A:C4'	27:1:10:ARG:N	2.64	0.60
1:A:926:A:O2'	13:M:41:HIS:HD2	1.85	0.60
6:F:25:MET:CE	6:F:37:ALA:HB1	2.30	0.60
37:A:4947:HOH:O	10:J:57:ARG:HG3	2.00	0.60
13:M:143:THR:HG22	13:M:145:LEU:H	1.65	0.60
14:N:72:SER:OG	14:N:74:ARG:HB2	2.00	0.60
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.29	0.60
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.82	0.60
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.31	0.60
1:A:1909:A:N1	1:A:2128:G:H1'	2.16	0.60
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.82	0.60
3:C:51:ARG:HB2	37:C:8611:HOH:O	2.01	0.60
6:F:99:ASP:CB	6:F:103:ASN:H	2.15	0.60
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.31	0.60
8:H:46:GLU:O	8:H:73:PRO:HD2	2.01	0.60
10:J:13:ALA:HA	10:J:91:HIS:HE1	1.65	0.60
23:W:44:GLY:O	23:W:48:GLU:HG2	2.01	0.60
1:A:2502:C:C2'	1:A:2503:A:H5'	2.31	0.60
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.60
1:A:2896:A:H5''	37:A:6072:HOH:O	2.00	0.60
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.34	0.60
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.82	0.60
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.31	0.60
18:R:11:ARG:HD3	37:R:5620:HOH:O	2.01	0.60
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.28	0.60
1:A:1766:U:O2	1:A:1778:A:H5'	2.02	0.60
1:A:1234:U:N3	4:D:244:PRO:HB3	2.17	0.60
10:J:44:ALA:HA	10:J:163:PRO:O	2.02	0.60
14:N:48:ARG:NH2	37:N:8563:HOH:O	2.34	0.60
23:W:39:ALA:C	23:W:41:GLU:H	2.05	0.60
24:X:149:LEU:HG	24:X:153:MET:HE2	1.84	0.60
27:1:10:ARG:HA	37:1:8414:HOH:O	2.02	0.60
1:A:113:A:OP2	1:A:114:A:H2'	2.02	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.01	0.60
13:M:114:VAL:HG11	37:M:8578:HOH:O	2.02	0.60
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2638:G:H1'	37:A:7746:HOH:O	2.02	0.59
4:D:145:HIS:CD2	4:D:146:THR:O	2.54	0.59
6:F:135:VAL:HG22	6:F:136:ARG:N	2.16	0.59
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.03	0.59
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.83	0.59
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.84	0.59
37:B:8467:HOH:O	15:O:147:ILE:HB	2.02	0.59
1:A:134:U:C2	1:A:145:A:C2	2.90	0.59
1:A:2604:A:H5'	37:A:5767:HOH:O	2.01	0.59
1:A:2830:U:H3'	37:A:5206:HOH:O	2.00	0.59
3:C:211:LYS:NZ	37:C:8576:HOH:O	2.35	0.59
5:E:107:ARG:HB3	5:E:107:ARG:NH1	2.17	0.59
6:F:174:VAL:HG13	37:F:6555:HOH:O	2.02	0.59
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.83	0.59
10:J:4:ALA:HB3	37:J:8364:HOH:O	2.01	0.59
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.16	0.59
37:A:3147:HOH:O	14:N:87:MET:HE3	2.01	0.59
15:O:37:ARG:NE	37:O:8533:HOH:O	2.35	0.59
27:I:53:GLY:HA2	27:I:67:GLY:O	2.01	0.59
1:A:1528:A:H2'	1:A:1529:G:O4'	2.02	0.59
1:A:2672:C:H1'	37:D:8634:HOH:O	2.02	0.59
1:A:536:A:H3'	37:A:5026:HOH:O	2.02	0.59
2:B:3023:U:H3'	2:B:3024:U:H5''	1.84	0.59
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.37	0.59
20:T:51:GLN:HE21	20:T:53:ASN:ND2	1.99	0.59
2:B:3003:A:N6	2:B:3022:G:H1'	2.17	0.59
3:C:105:VAL:HG13	3:C:155:THR:O	2.02	0.59
9:I:64:ASN:HD22	9:I:64:ASN:N	1.99	0.59
1:A:2502:C:H2'	1:A:2503:A:H5'	1.84	0.59
5:E:237:GLU:HB2	37:E:8429:HOH:O	2.02	0.59
1:A:2779:G:H21	7:G:143:GLN:NE2	2.01	0.59
10:J:150:LYS:NZ	37:J:8379:HOH:O	2.33	0.59
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.10	0.59
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.66	0.59
27:I:62:TYR:CE2	27:I:64:ILE:HG23	2.38	0.59
1:A:1441:G:O2'	1:A:1442:A:H5'	2.03	0.59
1:A:1641:A:H2'	1:A:1642:A:H5'	1.83	0.59
7:G:101:GLU:HB2	7:G:116:THR:O	2.02	0.59
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.83	0.59
19:S:104:PHE:HB2	19:S:109:MET:HE1	1.84	0.59
1:A:2488:A:H61	1:A:2534:C:H42	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.15	0.59
7:G:20:ILE:HD12	7:G:33:LEU:HD12	1.85	0.59
10:J:75:SER:C	10:J:79:ALA:HB2	2.23	0.59
30:4:73:GLU:HB3	37:4:8564:HOH:O	2.03	0.59
1:A:1168:C:H2'	1:A:1169:U:O4'	2.02	0.59
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.83	0.59
10:J:136:VAL:HG22	10:J:137:ASN:O	2.02	0.59
10:J:166:ASN:N	10:J:166:ASN:HD22	2.00	0.59
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.38	0.59
37:A:9524:HOH:O	17:Q:81:LYS:HG2	2.01	0.59
26:Z:187:VAL:HB	37:Z:8569:HOH:O	2.02	0.59
1:A:338:C:H5''	37:E:8420:HOH:O	2.02	0.59
3:C:211:LYS:NZ	37:C:8623:HOH:O	2.35	0.59
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.85	0.59
10:J:163:PRO:HG2	37:J:8338:HOH:O	2.01	0.59
15:O:12:ARG:HD3	15:O:18:THR:OG1	2.03	0.59
20:T:51:GLN:NE2	20:T:53:ASN:HD21	1.98	0.59
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.67	0.58
14:N:64:ARG:HD2	37:N:8588:HOH:O	2.02	0.58
19:S:39:THR:HB	19:S:42:GLU:CG	2.33	0.58
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.25	0.58
23:W:49:LEU:O	23:W:53:ILE:HG13	2.03	0.58
1:A:1086:A:C6	24:X:11:VAL:HG11	2.38	0.58
1:A:1183:C:N4	37:A:4379:HOH:O	2.32	0.58
1:A:1594:C:OP2	17:Q:120:ARG:HD2	2.02	0.58
1:A:1829:A:H5''	37:A:3064:HOH:O	2.03	0.58
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.03	0.58
2:B:3044:A:O4'	6:F:76:ARG:NE	2.36	0.58
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.38	0.58
1:A:2717:C:O2'	1:A:2718:C:H5''	2.02	0.58
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.16	0.58
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.85	0.58
15:O:80:SER:HB2	37:O:8535:HOH:O	2.02	0.58
1:A:2748:G:H5'	37:A:7524:HOH:O	2.04	0.58
4:D:156:LYS:HE3	37:D:8630:HOH:O	2.03	0.58
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.18	0.58
10:J:150:LYS:HE2	37:J:8379:HOH:O	2.03	0.58
1:A:121:U:OP2	29:3:10:ARG:NH2	2.36	0.58
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.68	0.58
1:A:2241:C:O2'	1:A:2242:U:H5'	2.03	0.58
1:A:56:G:H5''	23:W:50:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3014:G:H5'	2:B:3014:G:C8	2.37	0.58
6:F:64:ARG:O	6:F:67:ASP:OD2	2.21	0.58
7:G:20:ILE:CD1	7:G:33:LEU:HD12	2.33	0.58
27:1:31:ILE:O	27:1:35:LYS:HG3	2.04	0.58
1:A:1185:U:H5'	37:A:7447:HOH:O	2.03	0.58
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.67	0.58
1:A:184:G:H5''	14:N:153:THR:HG22	1.84	0.58
1:A:2718:C:H6	1:A:2718:C:H5'	1.68	0.58
1:A:272:A:H5'	1:A:273:G:OP2	2.03	0.58
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.33	0.58
6:F:95:THR:C	6:F:97:GLN:H	2.07	0.58
15:O:32:PRO:HD2	15:O:99:GLU:O	2.03	0.58
19:S:61:GLN:NE2	37:S:8539:HOH:O	2.36	0.58
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.03	0.58
1:A:1328:A:OP1	26:Z:169:ARG:HD2	2.03	0.58
1:A:289:G:N2	1:A:363:A:H2	1.99	0.58
10:J:53:PRO:HG3	10:J:127:GLY:H	1.68	0.58
1:A:1119:G:H8	11:K:52:GLN:HE22	1.51	0.58
1:A:926:A:O2'	13:M:41:HIS:CD2	2.56	0.58
2:B:3020:G:O2'	2:B:3021:G:H5'	2.03	0.58
3:C:37:VAL:HG22	37:C:8601:HOH:O	2.03	0.58
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.03	0.58
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.19	0.58
1:A:138:U:H5''	1:A:139:C:OP2	2.04	0.58
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.58
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.71	0.58
7:G:15:GLN:NE2	7:G:40:VAL:O	2.35	0.58
21:U:47:THR:HB	21:U:100:ASP:HB3	1.84	0.58
21:U:37:GLN:OE1	21:U:118:SER:HA	2.03	0.58
1:A:1819:G:H2'	1:A:1820:G:H4'	1.84	0.58
1:A:280:C:H2'	1:A:281:U:O4'	2.04	0.58
2:B:3029:C:C2'	2:B:3030:C:H5'	2.33	0.58
9:I:12:ILE:HD12	37:I:692:HOH:O	2.02	0.58
1:A:1134:G:H4'	10:J:151:MET:CE	2.19	0.57
1:A:1160:G:N3	37:A:5607:HOH:O	2.32	0.57
1:A:1185:U:H2'	1:A:1186:C:C6	2.39	0.57
1:A:1209:C:H2'	1:A:1210:G:C8	2.38	0.57
1:A:2089:A:O2'	1:A:2090:G:H5'	2.04	0.57
1:A:2506:A:O2'	1:A:2507:G:O5'	2.22	0.57
1:A:390:G:OP1	30:4:46:ILE:N	2.22	0.57
1:A:921:G:H4'	1:A:924:G:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:G:C4'	10:J:151:MET:HE1	2.19	0.57
13:M:143:THR:CG2	13:M:144:ASP:N	2.66	0.57
27:1:75:ALA:HB3	37:1:8436:HOH:O	2.03	0.57
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.03	0.57
5:E:133:ARG:NH2	37:E:8425:HOH:O	2.37	0.57
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.04	0.57
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.32	0.57
8:H:110:GLU:HG2	37:H:6926:HOH:O	2.02	0.57
14:N:38:VAL:C	14:N:63:VAL:HG13	2.25	0.57
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.72	0.57
1:A:1182:C:H1'	1:A:1192:A:H8	1.69	0.57
1:A:567:U:H5''	37:X:5817:HOH:O	2.04	0.57
5:E:233:THR:HG22	5:E:234:VAL:N	2.18	0.57
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.34	0.57
11:K:130:VAL:HG12	11:K:131:THR:N	2.18	0.57
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.85	0.57
22:V:9:CYS:HA	22:V:52:THR:CG2	2.34	0.57
27:1:25:ARG:O	27:1:29:VAL:HG23	2.04	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.20	0.57
3:C:53:ALA:HB3	37:C:8611:HOH:O	2.04	0.57
7:G:132:THR:HB	37:G:2227:HOH:O	2.03	0.57
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.57
1:A:2475:C:C2'	1:A:2476:C:O5'	2.53	0.57
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.34	0.57
1:A:558:C:C2'	1:A:559:U:H5''	2.34	0.57
5:E:118:THR:O	5:E:136:VAL:HG13	2.05	0.57
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.86	0.57
1:A:2502:C:H4'	10:J:151:MET:HG2	1.87	0.57
15:O:154:LEU:O	15:O:155:GLU:HB3	2.05	0.57
24:X:149:LEU:HG	24:X:153:MET:CE	2.35	0.57
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.86	0.57
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.05	0.57
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.69	0.57
1:A:283:U:H5''	1:A:284:C:P	2.44	0.57
4:D:72:THR:HB	37:D:8605:HOH:O	2.03	0.57
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	2.02	0.57
30:4:40:ARG:HD2	37:4:8553:HOH:O	2.03	0.57
1:A:1187:U:H2'	37:A:6869:HOH:O	2.04	0.57
1:A:1484:G:H2'	37:A:9101:HOH:O	2.04	0.57
1:A:282:C:H1'	1:A:368:C:H42	1.67	0.57
1:A:542:A:H2'	1:A:543:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3054:A:O2'	2:B:3055:U:H5'	2.04	0.57
12:L:28:GLU:OE2	12:L:58:THR:HG21	2.05	0.57
24:X:4:LEU:O	24:X:32:CYS:HA	2.05	0.57
1:A:1166:A:H1'	1:A:1192:A:N1	2.19	0.57
1:A:281:U:H3'	37:A:7185:HOH:O	2.05	0.57
1:A:474:C:O3'	5:E:73:LEU:HD21	2.04	0.57
4:D:2:GLN:CD	37:D:8620:HOH:O	2.42	0.57
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.57
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.05	0.57
37:A:7384:HOH:O	21:U:2:LYS:HE2	2.04	0.57
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.37	0.57
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.87	0.57
30:4:69:TYR:O	30:4:77:ALA:HA	2.05	0.57
8:H:28:ALA:HB3	8:H:99:THR:O	2.04	0.57
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.34	0.57
1:A:1886:A:O2'	27:1:20:LEU:HB2	2.05	0.57
1:A:1422:U:H2'	1:A:1423:C:C6	2.39	0.57
1:A:1477:C:O2'	1:A:1478:U:H5'	2.03	0.57
15:O:170:GLU:O	15:O:174:GLU:HG3	2.05	0.57
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	1.86	0.57
1:A:1923:G:H4'	30:4:31:THR:O	2.05	0.56
1:A:2507:G:H2'	1:A:2510:C:H42	1.70	0.56
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.35	0.56
3:C:191:GLY:HA2	3:C:194:MET:CE	2.35	0.56
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.87	0.56
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.88	0.56
1:A:1299:G:N2	37:A:4659:HOH:O	2.37	0.56
1:A:69:A:C8	1:A:69:A:H5'	2.40	0.56
4:D:2:GLN:HA	37:D:8620:HOH:O	2.05	0.56
4:D:305:ASP:O	4:D:306:LYS:CB	2.52	0.56
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.53	0.56
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.40	0.56
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.86	0.56
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.17	0.56
1:A:797:A:H4'	27:1:10:ARG:N	2.20	0.56
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.40	0.56
6:F:35:ALA:N	37:F:5576:HOH:O	2.37	0.56
15:O:58:LEU:HD12	15:O:58:LEU:N	2.21	0.56
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.04	0.56
1:A:21:G:H4'	19:S:2:ILE:HG22	1.87	0.56
23:W:39:ALA:N	23:W:40:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1773:G:C8	27:1:16:PRO:HA	2.39	0.56
1:A:558:C:H2'	1:A:559:U:H5'	1.88	0.56
1:A:2637:A:C8	31:A:9002:BLS:H2'	2.40	0.56
37:A:7666:HOH:O	14:N:154:ARG:HB2	2.05	0.56
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.87	0.56
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.19	0.56
1:A:1118:A:C8	1:A:1118:A:C3'	2.84	0.56
1:A:1667:A:H5'	1:A:1667:A:C8	2.38	0.56
1:A:1878:G:H1'	37:A:6094:HOH:O	2.05	0.56
1:A:2320:U:H4'	1:A:2321:A:O4'	2.05	0.56
1:A:2679:G:H2'	1:A:2681:A:OP2	2.06	0.56
1:A:835:U:H3'	37:A:9364:HOH:O	2.05	0.56
5:E:246:ARG:NE	37:E:8423:HOH:O	2.38	0.56
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.70	0.56
10:J:59:ASN:H	10:J:59:ASN:ND2	2.03	0.56
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.86	0.56
20:T:81:ILE:HG23	37:T:4527:HOH:O	2.05	0.56
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.41	0.56
1:A:2570:G:H5''	37:A:4887:HOH:O	2.05	0.56
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.40	0.56
1:A:671:A:O2'	1:A:672:G:H2'	2.06	0.56
1:A:777:U:O2'	28:2:11:LYS:HG2	2.06	0.56
4:D:162:MET:CE	4:D:308:LEU:HD21	2.36	0.56
1:A:154:C:H2'	1:A:155:C:H6	1.70	0.56
26:Z:189:ASN:ND2	26:Z:192:ASP:H	2.04	0.56
1:A:1197:G:N2	37:A:6207:HOH:O	2.39	0.56
2:B:3092:G:H22	10:J:52:LYS:NZ	2.04	0.56
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.36	0.56
4:D:175:LEU:HD23	4:D:175:LEU:C	2.26	0.56
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.20	0.56
4:D:82:VAL:O	4:D:82:VAL:HG12	2.04	0.56
1:A:240:C:H4'	14:N:146:GLN:NE2	2.21	0.56
14:N:74:ARG:NH2	37:N:8635:HOH:O	2.39	0.56
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.87	0.56
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.56
1:A:776:A:OP1	28:2:28:HIS:HE1	1.89	0.56
3:C:105:VAL:HG12	3:C:106:CYS:N	2.21	0.56
4:D:140:LEU:HD23	37:D:8580:HOH:O	2.06	0.56
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.26	0.56
14:N:84:LYS:O	37:N:8534:HOH:O	2.18	0.56
22:V:6:CYS:HA	22:V:13:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:29:VAL:O	24:X:30:ASN:HB2	2.05	0.56
26:Z:235:GLU:CD	26:Z:235:GLU:H	2.08	0.56
1:A:485:A:N3	1:A:487:G:H5''	2.21	0.56
5:E:162:VAL:O	5:E:162:VAL:HG12	2.06	0.56
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.21	0.56
37:E:8357:HOH:O	16:P:3:THR:HG21	2.06	0.56
19:S:132:ARG:HG2	19:S:133:ALA:N	2.20	0.56
23:W:64:GLY:O	23:W:65:ASP:CB	2.54	0.56
1:A:1205:U:C2'	1:A:1206:U:H5'	2.31	0.55
4:D:103:ASP:HB2	37:D:8592:HOH:O	2.04	0.55
15:O:110:THR:HB	15:O:113:SER:OG	2.06	0.55
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.06	0.55
1:A:113:A:H3'	1:A:114:A:H5''	1.88	0.55
1:A:349:U:O2'	1:A:350:C:H5'	2.06	0.55
1:A:516:A:P	37:A:5620:HOH:O	2.64	0.55
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.05	0.55
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.40	0.55
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
5:E:236:THR:CG2	5:E:239:ALA:H	1.97	0.55
6:F:86:THR:O	6:F:90:LEU:HG	2.06	0.55
1:A:188:C:H5''	14:N:163:LEU:HD21	1.89	0.55
23:W:55:ARG:NH2	37:W:4428:HOH:O	2.28	0.55
24:X:21:LEU:HD22	24:X:26:ILE:HD13	1.86	0.55
1:A:1120:U:H6	1:A:1120:U:H5''	1.72	0.55
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.55
1:A:2756:U:H3	1:A:2896:A:H2	1.49	0.55
1:A:69:A:H8	1:A:69:A:H5'	1.71	0.55
3:C:88:ILE:O	3:C:88:ILE:HG22	2.05	0.55
4:D:248:ARG:O	4:D:251:VAL:CG1	2.54	0.55
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.22	0.55
15:O:132:ASN:O	15:O:135:VAL:HG12	2.06	0.55
17:Q:143:ALA:HA	37:Q:165:HOH:O	2.06	0.55
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.04	0.55
1:A:2487:C:H5	37:A:4861:HOH:O	1.89	0.55
1:A:2763:G:OP1	12:L:9:THR:OG1	2.11	0.55
1:A:821:U:H2'	1:A:822:C:H6	1.70	0.55
4:D:205:VAL:O	4:D:307:ARG:NE	2.39	0.55
13:M:104:ASP:O	13:M:105:TYR:HB3	2.06	0.55
15:O:154:LEU:HG	15:O:155:GLU:H	1.71	0.55
1:A:1010:C:H4'	15:O:4:PRO:HB2	1.89	0.55
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.42	0.55
1:A:2791:U:H1'	1:A:2792:A:H5''	1.89	0.55
2:B:3076:G:C3'	2:B:3077:A:H5''	2.30	0.55
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.41	0.55
4:D:238:ASN:HD22	4:D:240:GLY:N	2.03	0.55
12:L:34:VAL:HB	37:L:7169:HOH:O	2.07	0.55
14:N:61:ILE:HA	37:N:8627:HOH:O	2.07	0.55
15:O:169:PRO:O	15:O:172:PHE:HB3	2.07	0.55
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.21	0.55
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.31	0.55
4:D:248:ARG:HG2	37:D:8575:HOH:O	2.06	0.55
5:E:27:ARG:HG3	5:E:29:ASP:OD1	2.06	0.55
6:F:27:ILE:HG22	6:F:28:GLY:N	2.16	0.55
8:H:107:VAL:O	8:H:111:ILE:HG13	2.06	0.55
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.36	0.55
17:Q:59:ARG:HH22	17:Q:66:GLN:HE22	1.55	0.55
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.72	0.55
24:X:130:HIS:O	24:X:136:GLY:HA3	2.07	0.55
1:A:105:G:O2'	1:A:106:A:H5'	2.05	0.55
1:A:2435:U:H1'	37:A:5409:HOH:O	2.05	0.55
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.07	0.55
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.88	0.55
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.37	0.55
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.89	0.55
37:A:4500:HOH:O	14:N:94:LYS:HE3	2.07	0.55
1:A:1699:C:H4'	37:A:6415:HOH:O	2.07	0.55
6:F:11:HIS:C	6:F:13:MET:H	2.10	0.55
10:J:49:VAL:O	10:J:157:ILE:HG23	2.07	0.55
11:K:103:VAL:HG12	37:K:5907:HOH:O	2.07	0.55
13:M:149:ARG:O	13:M:150:GLN:HB2	2.07	0.55
13:M:21:ARG:N	37:M:8534:HOH:O	2.40	0.55
14:N:39:ARG:NH2	37:N:8627:HOH:O	2.39	0.55
1:A:1120:U:H5''	1:A:1120:U:C6	2.42	0.55
1:A:1523:G:H2'	1:A:1524:U:C6	2.42	0.55
1:A:960:G:N3	1:A:960:G:H2'	2.22	0.55
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.88	0.55
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.55	0.55
20:T:80:ARG:HG2	37:T:4527:HOH:O	2.06	0.55
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.07	0.54
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.54
1:A:1667:A:H2'	1:A:1668:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:GLN:O	5:E:43:LYS:HD3	2.07	0.54
10:J:139:ASP:N	10:J:140:PRO:CD	2.69	0.54
15:O:141:ARG:HB3	37:O:8568:HOH:O	2.07	0.54
27:1:42:CYS:SG	27:1:43:GLY:N	2.80	0.54
1:A:1735:C:O2'	1:A:1736:A:H5'	2.07	0.54
1:A:506:G:H22	1:A:509:A:H5''	1.69	0.54
2:B:3002:U:H4'	2:B:3002:U:OP2	2.06	0.54
2:B:3025:G:N2	37:B:8512:HOH:O	2.40	0.54
1:A:2630:G:O6	3:C:206:ARG:NH2	2.40	0.54
4:D:144:THR:HG22	4:D:145:HIS:N	2.21	0.54
4:D:297:VAL:HB	37:D:8605:HOH:O	2.07	0.54
9:I:12:ILE:HG22	9:I:12:ILE:O	2.06	0.54
14:N:68:ARG:HD3	14:N:68:ARG:O	2.08	0.54
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.40	0.54
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.37	0.54
1:A:1159:G:H21	1:A:1189:A:H8	1.54	0.54
1:A:1189:A:O2'	1:A:1208:C:H2'	2.07	0.54
1:A:2783:A:H3'	37:A:5210:HOH:O	2.06	0.54
14:N:61:ILE:HG13	37:N:8627:HOH:O	2.06	0.54
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.90	0.54
27:1:19:GLY:O	27:1:23:ARG:HG2	2.07	0.54
2:B:3042:C:H2'	37:B:8505:HOH:O	2.07	0.54
4:D:162:MET:CE	4:D:310:ARG:HD3	2.37	0.54
6:F:36:ASN:HA	37:F:7500:HOH:O	2.06	0.54
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.88	0.54
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.43	0.54
1:A:2502:C:C4'	10:J:151:MET:HG2	2.38	0.54
1:A:2837:U:H2'	37:A:6811:HOH:O	2.07	0.54
4:D:148:PRO:HD2	37:D:8581:HOH:O	2.07	0.54
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.38	0.54
13:M:104:ASP:HB3	37:M:8569:HOH:O	2.08	0.54
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.42	0.54
1:A:1299:G:O6	13:M:6:ARG:HD3	2.07	0.54
1:A:951:A:C2'	1:A:952:G:H5'	2.37	0.54
4:D:63:GLU:HG3	4:D:63:GLU:O	2.07	0.54
13:M:57:VAL:HG12	13:M:57:VAL:O	2.08	0.54
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.90	0.54
23:W:39:ALA:O	23:W:41:GLU:N	2.41	0.54
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.91	0.54
1:A:2429:A:H2'	1:A:2430:A:C8	2.43	0.54
1:A:739:G:N7	37:A:7526:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.08	0.54
14:N:122:GLU:HB2	14:N:126:HIS:O	2.08	0.54
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.07	0.54
1:A:1213:C:O2'	1:A:1214:G:H5'	2.08	0.54
1:A:2121:G:C2'	1:A:2122:C:H5'	2.38	0.54
1:A:2326:U:H4'	1:A:2412:G:C4'	2.38	0.54
1:A:553:G:O4'	1:A:1325:G:H5'	2.08	0.54
1:A:738:G:H3'	37:A:7022:HOH:O	2.08	0.54
1:A:88:G:H5'	1:A:88:G:H8	1.73	0.54
3:C:132:ASP:OD1	3:C:133:ARG:N	2.40	0.54
5:E:246:ARG:NH1	37:E:8369:HOH:O	2.41	0.54
5:E:77:ALA:O	5:E:78:ARG:HG3	2.07	0.54
6:F:11:HIS:O	6:F:12:GLU:HB3	2.07	0.54
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.88	0.54
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.89	0.54
1:A:710:G:OP1	16:P:24:ALA:HB3	2.08	0.54
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.22	0.54
26:Z:133:HIS:HD2	37:Z:8581:HOH:O	1.91	0.54
1:A:2093:G:H5''	37:D:8526:HOH:O	2.08	0.54
1:A:2473:U:O3'	1:A:2474:A:H3'	2.08	0.54
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.89	0.54
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.89	0.54
6:F:136:ARG:HD2	6:F:155:HIS:O	2.07	0.54
7:G:11:VAL:CG1	7:G:12:ASP:N	2.70	0.54
1:A:1452:G:H1'	35:A:8503:CL:CL	2.45	0.54
1:A:1862:C:H1'	37:A:7198:HOH:O	2.06	0.54
1:A:2777:G:O2'	1:A:2778:A:H5'	2.07	0.54
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.73	0.54
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	1.89	0.54
26:Z:185:VAL:HA	37:Z:8563:HOH:O	2.06	0.54
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.08	0.53
1:A:2781:U:H2'	1:A:2782:G:H5'	1.89	0.53
10:J:127:GLY:O	10:J:128:ALA:CB	2.56	0.53
10:J:144:GLU:HA	10:J:144:GLU:OE1	2.08	0.53
12:L:55:VAL:HG12	12:L:56:SER:H	1.72	0.53
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.28	0.53
1:A:128:A:H3'	1:A:128:A:C8	2.42	0.53
1:A:2105:C:H2'	1:A:2106:C:C6	2.43	0.53
1:A:2459:G:P	30:4:64:LYS:HB2	2.48	0.53
1:A:2073:G:OP2	1:A:2490:A:H5'	2.08	0.53
2:B:3055:U:H4'	2:B:3056:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ASN:HB3	4:D:64:GLY:H	1.73	0.53
1:A:338:C:H4'	5:E:174:ILE:HD11	1.88	0.53
13:M:143:THR:HG22	13:M:144:ASP:H	1.73	0.53
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.23	0.53
22:V:47:ARG:HG3	37:V:4381:HOH:O	2.07	0.53
1:A:694:A:H2'	1:A:695:C:H5'	1.90	0.53
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.44	0.53
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.08	0.53
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.77	0.53
8:H:46:GLU:N	37:H:3461:HOH:O	2.41	0.53
14:N:149:TRP:O	14:N:152:ARG:HG2	2.08	0.53
1:A:392:U:C5'	14:N:193:LYS:HB3	2.38	0.53
15:O:182:GLY:O	15:O:183:ASP:O	2.26	0.53
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.33	0.53
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.89	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.08	0.53
4:D:258:GLY:N	4:D:260:HIS:CE1	2.76	0.53
37:A:7438:HOH:O	5:E:188:ARG:CD	2.56	0.53
8:H:19:ALA:O	8:H:22:VAL:HG22	2.08	0.53
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.37	0.53
10:J:136:VAL:CG2	37:J:8343:HOH:O	2.48	0.53
13:M:73:VAL:HG23	13:M:74:THR:H	1.72	0.53
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.90	0.53
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.91	0.53
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.22	0.53
27:1:13:ARG:NH1	37:1:8420:HOH:O	2.42	0.53
1:A:1205:U:C2'	1:A:1206:U:C5'	2.86	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.08	0.53
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.21	0.53
8:H:101:ALA:HA	37:H:5413:HOH:O	2.09	0.53
15:O:86:LEU:O	15:O:90:LEU:HG	2.08	0.53
1:A:2122:C:P	37:A:6550:HOH:O	2.48	0.53
37:A:7001:HOH:O	3:C:211:LYS:HG2	2.07	0.53
3:C:2:ARG:NH1	37:C:8514:HOH:O	2.23	0.53
4:D:1:PRO:O	4:D:2:GLN:HB2	2.08	0.53
10:J:39:GLY:O	10:J:41:THR:N	2.42	0.53
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.53
1:A:2064:U:H5'	1:A:2652:U:H4'	1.88	0.53
1:A:2524:G:H21	1:A:2526:C:N4	2.06	0.53
1:A:281:U:O2'	1:A:282:C:H5'	2.09	0.53
3:C:192:VAL:CG1	3:C:192:VAL:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.90	0.53
14:N:39:ARG:NE	37:N:8627:HOH:O	2.41	0.53
15:O:163:PHE:HA	37:O:8519:HOH:O	2.08	0.53
24:X:38:THR:HB	37:X:5390:HOH:O	2.08	0.53
1:A:175:G:H2'	14:N:192:ALA:HB3	1.89	0.53
1:A:1819:G:H2'	1:A:1820:G:C5'	2.39	0.53
1:A:1882:C:O2'	1:A:2012:U:OP2	2.24	0.53
1:A:2587:U:H2'	1:A:2589:U:H5''	1.90	0.53
6:F:10:PHE:CG	6:F:11:HIS:N	2.77	0.53
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.24	0.53
14:N:154:ARG:CD	37:N:8645:HOH:O	2.55	0.53
14:N:38:VAL:O	14:N:63:VAL:HG13	2.09	0.53
15:O:180:LEU:O	15:O:181:ASP:HB3	2.08	0.53
24:X:38:THR:HG22	24:X:39:ASP:N	2.24	0.53
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.44	0.53
37:A:9933:HOH:O	25:Y:23:HIS:HD2	1.92	0.53
1:A:1189:A:H1'	1:A:1209:C:O4'	2.08	0.53
2:B:3028:U:H2'	2:B:3029:C:C6	2.44	0.53
4:D:27:ASN:HD22	4:D:27:ASN:H	1.56	0.53
10:J:71:TYR:C	10:J:73:GLN:N	2.61	0.53
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.73	0.53
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.08	0.53
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.38	0.53
24:X:3:ALA:O	24:X:54:PHE:HA	2.09	0.53
1:A:1353:C:P	37:A:4654:HOH:O	2.65	0.53
1:A:2758:G:H2'	1:A:2759:C:C6	2.44	0.53
1:A:825:U:H5''	1:A:826:U:OP1	2.09	0.53
37:A:6215:HOH:O	3:C:22:ARG:HG2	2.08	0.53
5:E:214:THR:HG23	37:E:8435:HOH:O	2.08	0.53
6:F:50:VAL:O	6:F:71:ALA:HA	2.09	0.53
8:H:99:THR:O	8:H:100:ASP:HB2	2.08	0.53
9:I:23:ILE:O	9:I:27:ILE:HG13	2.09	0.53
22:V:52:THR:HG22	22:V:54:THR:HB	1.91	0.53
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.41	0.53
1:A:95:A:H5''	1:A:97:G:O4'	2.09	0.52
1:A:449:A:N7	5:E:43:LYS:HG2	2.24	0.52
6:F:154:LYS:H	6:F:154:LYS:CD	2.15	0.52
21:U:111:ARG:HB3	21:U:119:ALA:HB2	1.91	0.52
21:U:69:LYS:O	21:U:71:VAL:HG23	2.09	0.52
22:V:33:SER:O	22:V:37:GLU:HG3	2.08	0.52
1:A:2506:A:H1'	37:A:6027:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.52
1:A:2768:A:O2'	1:A:2769:C:H5'	2.09	0.52
1:A:2781:U:C2'	1:A:2782:G:H5'	2.39	0.52
1:A:371:U:H2'	1:A:372:A:H8	1.74	0.52
1:A:380:A:H5''	14:N:48:ARG:NH2	2.25	0.52
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.41	0.52
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.58	0.52
24:X:90:TYR:N	24:X:90:TYR:CD1	2.76	0.52
1:A:2594:C:O2'	1:A:2595:U:H5'	2.10	0.52
1:A:259:G:H21	14:N:58:GLN:NE2	2.06	0.52
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.91	0.52
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.08	0.52
15:O:152:GLU:C	15:O:154:LEU:H	2.10	0.52
15:O:37:ARG:HD3	35:O:8507:CL:CL	2.46	0.52
1:A:1173:A:H2'	37:A:4326:HOH:O	2.09	0.52
1:A:29:C:O2'	1:A:30:U:H5'	2.10	0.52
4:D:7:ARG:NH1	4:D:7:ARG:HG2	2.21	0.52
1:A:244:C:OP2	8:H:38:LYS:HE3	2.10	0.52
11:K:19:MET:HE1	11:K:132:LEU:HD11	1.90	0.52
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.10	0.52
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.91	0.52
26:Z:122:ARG:NH2	37:Z:8538:HOH:O	2.43	0.52
1:A:1189:A:H1'	1:A:1209:C:C1'	2.39	0.52
1:A:1659:A:H2'	1:A:1660:G:O4'	2.09	0.52
1:A:1878:G:O2'	1:A:1879:U:C6	2.60	0.52
1:A:407:A:H2'	1:A:408:A:C8	2.45	0.52
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.90	0.52
6:F:99:ASP:HB3	6:F:103:ASN:H	1.74	0.52
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.39	0.52
7:G:7:ILE:HG22	7:G:45:ASP:O	2.10	0.52
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.90	0.52
15:O:64:SER:C	15:O:66:LEU:H	2.13	0.52
24:X:122:ARG:CG	24:X:122:ARG:HH11	2.19	0.52
24:X:88:THR:CG2	24:X:89:ASP:H	2.18	0.52
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.90	0.52
30:4:3:MET:O	30:4:90:PHE:HA	2.09	0.52
1:A:2361:A:H2'	1:A:2362:A:C8	2.45	0.52
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.24	0.52
1:A:538:C:H5''	1:A:539:G:C8	2.44	0.52
1:A:60:A:C2	1:A:61:G:C8	2.98	0.52
3:C:128:LEU:HG	37:C:8577:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.90	0.52
16:P:39:THR:O	16:P:115:ARG:NH2	2.43	0.52
26:Z:144:ARG:NE	37:Z:8610:HOH:O	2.41	0.52
27:1:58:GLY:HA3	37:1:8438:HOH:O	2.09	0.52
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.10	0.52
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.49	0.52
7:G:11:VAL:HG12	7:G:12:ASP:H	1.74	0.52
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.08	0.52
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.58	0.52
1:A:962:C:C1'	15:O:5:ARG:NH1	2.67	0.52
22:V:13:ILE:HG12	22:V:32:CYS:HB2	1.91	0.52
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.25	0.52
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.40	0.52
1:A:2256:G:H2'	1:A:2257:G:H5'	1.92	0.52
1:A:2421:G:H4'	37:A:4753:HOH:O	2.10	0.52
2:B:3041:C:C6	6:F:50:VAL:HG21	2.45	0.52
37:A:5497:HOH:O	4:D:298:LYS:HD3	2.10	0.52
4:D:41:PHE:CB	4:D:190:MET:HE3	2.40	0.52
7:G:11:VAL:HG13	7:G:23:GLU:O	2.09	0.52
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.09	0.52
1:A:1119:G:H8	11:K:52:GLN:NE2	2.06	0.52
15:O:154:LEU:HG	15:O:155:GLU:N	2.24	0.52
37:A:3762:HOH:O	22:V:17:THR:CG2	2.57	0.52
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.09	0.52
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.52
28:2:10:LYS:HG3	37:2:2979:HOH:O	2.09	0.52
1:A:1497:G:H4'	1:A:1627:G:O2'	2.09	0.52
1:A:283:U:H5''	1:A:284:C:OP2	2.10	0.52
4:D:125:GLU:O	4:D:129:ARG:HG3	2.09	0.52
10:J:139:ASP:H	10:J:140:PRO:HD3	1.72	0.52
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.69	0.52
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.24	0.52
1:A:136:C:H2'	1:A:137:U:O4'	2.09	0.52
1:A:2474:A:C6	31:A:9001:BLS:H133	2.45	0.52
1:A:2769:C:C2'	1:A:2770:G:H5'	2.40	0.52
1:A:344:C:H2'	1:A:345:G:O4'	2.10	0.52
1:A:461:C:H2'	37:A:3986:HOH:O	2.10	0.52
3:C:179:MET:HG2	3:C:186:TRP:HB2	1.91	0.52
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.24	0.52
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.92	0.52
25:Y:9:VAL:HG22	25:Y:88:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:A:N3	1:A:1818:C:H2'	2.24	0.51
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.51
1:A:681:G:N3	1:A:681:G:H5'	2.25	0.51
1:A:797:A:O4'	27:1:10:ARG:N	2.42	0.51
4:D:16:ARG:NH1	37:D:8616:HOH:O	2.42	0.51
4:D:62:ARG:HG2	4:D:65:MET:HE1	1.91	0.51
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.92	0.51
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.92	0.51
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.40	0.51
37:A:6167:HOH:O	29:3:44:ARG:HG2	2.10	0.51
1:A:156:C:H5''	14:N:171:ARG:CD	2.30	0.51
1:A:1788:U:C2	1:A:1805:G:N2	2.78	0.51
1:A:2010:A:C2'	37:A:5931:HOH:O	2.58	0.51
1:A:2894:C:O2'	1:A:2895:C:H5'	2.09	0.51
2:B:3007:G:H4'	15:O:55:ASP:OD2	2.10	0.51
3:C:199:HIS:HD2	3:C:201:PHE:N	2.01	0.51
5:E:133:ARG:HD2	37:E:8410:HOH:O	2.09	0.51
6:F:170:TYR:O	6:F:171:ASP:HB3	2.09	0.51
15:O:67:ALA:C	15:O:69:TYR:H	2.13	0.51
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.89	0.51
1:A:1249:U:H2'	1:A:1250:C:C6	2.45	0.51
1:A:1393:A:H2'	1:A:1394:C:C6	2.46	0.51
1:A:1681:G:H5''	1:A:1682:A:H5'	1.91	0.51
1:A:2015:A:H2'	1:A:2016:U:O4'	2.09	0.51
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.92	0.51
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.93	0.51
4:D:74:ILE:HG13	37:D:8605:HOH:O	2.10	0.51
1:A:1352:A:N1	5:E:48:SER:HB3	2.25	0.51
10:J:150:LYS:CE	37:J:8379:HOH:O	2.57	0.51
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.41	0.51
1:A:1127:C:C5	1:A:1128:U:C4	2.98	0.51
1:A:1527:A:H1'	1:A:1528:A:C8	2.45	0.51
1:A:2467:A:H3'	37:A:5435:HOH:O	2.10	0.51
1:A:2793:A:N3	37:A:4471:HOH:O	2.34	0.51
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.41	0.51
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.92	0.51
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.45	0.51
19:S:106:GLY:HA2	19:S:109:MET:CE	2.40	0.51
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.93	0.51
1:A:245:C:H2'	1:A:246:G:H5'	1.91	0.51
4:D:280:VAL:CG1	4:D:334:SER:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:ASN:ND2	6:F:134:LEU:H	2.07	0.51
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.40	0.51
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.41	0.51
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.40	0.51
14:N:69:LYS:O	14:N:73:ARG:CZ	2.59	0.51
24:X:126:ASP:HB3	24:X:135:GLY:O	2.10	0.51
26:Z:144:ARG:CZ	37:Z:8610:HOH:O	2.59	0.51
1:A:1701:A:H5''	1:A:1702:U:H3'	1.93	0.51
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.51
1:A:737:A:H2'	1:A:738:G:O4'	2.10	0.51
2:B:3055:U:H4'	2:B:3056:A:H8	1.75	0.51
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.93	0.51
5:E:104:ASP:O	5:E:108:GLN:HG3	2.11	0.51
6:F:58:VAL:HG12	6:F:59:GLY:N	2.26	0.51
8:H:28:ALA:CB	8:H:99:THR:HG23	2.40	0.51
7:G:34:TRP:O	11:K:127:ILE:HD11	2.09	0.51
12:L:125:ALA:C	12:L:127:ALA:H	2.13	0.51
17:Q:115:SER:O	17:Q:117:SER:N	2.44	0.51
19:S:132:ARG:NH1	37:S:8559:HOH:O	2.43	0.51
1:A:1329:A:C2	37:A:4659:HOH:O	2.54	0.51
1:A:1810:C:OP1	22:V:44:ARG:NE	2.28	0.51
1:A:2359:G:H3'	37:A:5666:HOH:O	2.10	0.51
1:A:2649:A:H8	1:A:2649:A:H5'	1.75	0.51
2:B:3020:G:H3'	37:B:8436:HOH:O	2.09	0.51
37:A:9549:HOH:O	4:D:267:LYS:HD3	2.09	0.51
5:E:150:THR:HA	5:E:203:ALA:O	2.10	0.51
7:G:15:GLN:HG2	7:G:19:ASP:O	2.11	0.51
10:J:62:GLU:O	10:J:66:VAL:HG23	2.11	0.51
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.92	0.51
14:N:108:LYS:HE3	37:N:8617:HOH:O	2.10	0.51
1:A:2787:C:H5	37:A:4609:HOH:O	1.93	0.51
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.92	0.51
1:A:447:A:O2'	1:A:448:G:H5'	2.11	0.51
1:A:539:G:H2'	1:A:540:A:C8	2.46	0.51
1:A:922:A:N7	1:A:2281:C:H5'	2.25	0.51
3:C:173:GLY:O	3:C:177:HIS:CD2	2.64	0.51
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.11	0.51
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.76	0.51
11:K:107:ASN:HD22	11:K:107:ASN:C	2.14	0.51
14:N:184:ARG:HB2	14:N:184:ARG:CZ	2.40	0.51
1:A:2365:G:H4'	18:R:45:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.92	0.51
30:4:57:GLY:HA2	37:4:8527:HOH:O	2.10	0.51
2:B:3078:G:N2	2:B:3103:A:OP2	2.41	0.51
3:C:18:ALA:O	3:C:20:SER:N	2.41	0.51
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.93	0.51
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.93	0.51
1:A:1130:U:H5'	37:A:7658:HOH:O	2.10	0.51
1:A:2326:U:H4'	1:A:2412:G:H4'	1.93	0.51
1:A:814:G:H4'	37:A:3114:HOH:O	2.11	0.51
4:D:248:ARG:O	4:D:251:VAL:HG13	2.11	0.51
13:M:133:VAL:HB	37:M:8562:HOH:O	2.09	0.51
13:M:143:THR:CG2	13:M:144:ASP:H	2.24	0.51
14:N:37:VAL:CG2	14:N:108:LYS:HG3	2.40	0.51
21:U:38:ARG:NH1	37:U:6217:HOH:O	2.44	0.51
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.24	0.51
1:A:1666:C:C2'	1:A:1667:A:H5'	2.39	0.50
1:A:2323:G:H5'	37:A:6995:HOH:O	2.11	0.50
1:A:2781:U:H2'	1:A:2782:G:C5'	2.41	0.50
2:B:3023:U:C3'	2:B:3024:U:H5''	2.42	0.50
4:D:36:PRO:CA	4:D:168:GLY:HA3	2.39	0.50
4:D:2:GLN:NE2	37:D:8620:HOH:O	2.45	0.50
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.75	0.50
5:E:76:ARG:HG2	5:E:78:ARG:NH1	2.25	0.50
8:H:91:VAL:CG1	8:H:92:GLY:N	2.72	0.50
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.27	0.50
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.26	0.50
14:N:137:ASP:HA	14:N:142:LYS:HE3	1.93	0.50
15:O:22:GLN:HG2	15:O:26:LEU:HD22	1.93	0.50
24:X:80:ASP:O	24:X:84:VAL:HG23	2.11	0.50
1:A:1014:A:H2'	1:A:1015:C:H5'	1.92	0.50
37:A:5058:HOH:O	4:D:216:LYS:HA	2.12	0.50
7:G:7:ILE:HD11	7:G:11:VAL:O	2.11	0.50
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.58	0.50
37:A:9586:HOH:O	14:N:165:SER:HB3	2.11	0.50
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.26	0.50
27:1:46:LYS:HE2	37:1:8438:HOH:O	2.11	0.50
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.93	0.50
1:A:2724:U:H2'	1:A:2725:G:O4'	2.11	0.50
1:A:2815:G:N7	11:K:80:LYS:NZ	2.59	0.50
1:A:401:C:H5'	37:A:5769:HOH:O	2.11	0.50
6:F:163:VAL:HA	37:F:6326:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.11	0.50
15:O:67:ALA:HA	15:O:71:TRP:H	1.75	0.50
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.40	0.50
1:A:1669:A:H2'	1:A:1670:G:C8	2.46	0.50
1:A:2329:C:O2'	1:A:2330:U:H5'	2.11	0.50
1:A:2563:U:H2'	1:A:2565:C:O5'	2.12	0.50
1:A:646:G:H2'	1:A:647:U:C6	2.46	0.50
5:E:118:THR:HG23	37:E:8305:HOH:O	2.10	0.50
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.11	0.50
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.92	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50
1:A:1730:G:H5'	1:A:1731:C:C6	2.46	0.50
1:A:1855:G:H8	3:C:144:GLU:OE2	1.95	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.75	0.50
1:A:660:A:H4'	1:A:661:G:O5'	2.12	0.50
2:B:3049:G:O2'	2:B:3050:G:H5'	2.12	0.50
3:C:99:ILE:O	3:C:131:HIS:CE1	2.64	0.50
4:D:234:ARG:NH1	37:D:8618:HOH:O	2.38	0.50
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.94	0.50
16:P:96:VAL:HA	37:P:4258:HOH:O	2.10	0.50
19:S:33:ARG:NH1	37:S:8542:HOH:O	2.43	0.50
20:T:37:VAL:O	20:T:41:VAL:HG23	2.12	0.50
20:T:57:THR:CG2	20:T:58:MET:N	2.74	0.50
24:X:139:GLY:O	24:X:141:HIS:HD2	1.93	0.50
28:2:22:CYS:HB2	37:2:1159:HOH:O	2.12	0.50
1:A:1127:C:H2'	1:A:1128:U:H5'	1.93	0.50
1:A:1711:A:O2'	1:A:1712:A:H5'	2.12	0.50
2:B:3057:A:N6	37:B:8445:HOH:O	2.39	0.50
4:D:254:GLN:HG2	4:D:255:GLY:N	2.26	0.50
8:H:99:THR:O	8:H:99:THR:HG23	2.11	0.50
11:K:45:VAL:HG22	11:K:46:ILE:N	2.26	0.50
15:O:34:LEU:HD22	15:O:129:ILE:HD13	1.94	0.50
1:A:204:A:H2'	1:A:205:U:H5'	1.93	0.50
1:A:221:G:H2'	1:A:222:A:C8	2.46	0.50
1:A:793:A:N3	37:A:4084:HOH:O	2.35	0.50
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.11	0.50
7:G:126:ILE:HB	7:G:131:LEU:HD23	1.93	0.50
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.46	0.50
14:N:169:ARG:NH1	37:N:8574:HOH:O	2.45	0.50
24:X:88:THR:HG23	24:X:110:GLN:HB3	1.93	0.50
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:27:ASP:N	25:Y:27:ASP:OD2	2.42	0.50
29:3:18:ASN:ND2	29:3:40:ARG:H	2.07	0.50
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.73	0.50
1:A:541:C:O2'	1:A:542:A:H5''	2.12	0.50
1:A:661:G:C4	1:A:686:A:C2	3.00	0.50
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.94	0.50
6:F:169:THR:O	6:F:170:TYR:HB2	2.12	0.50
14:N:114:VAL:HB	14:N:159:THR:HG23	1.92	0.50
15:O:141:ARG:N	37:O:8568:HOH:O	2.45	0.50
15:O:67:ALA:O	15:O:69:TYR:N	2.45	0.50
30:4:65:THR:HB	30:4:83:TRP:H	1.77	0.50
1:A:1474:C:C5'	1:A:1474:C:H6	2.13	0.50
1:A:2635:A:O2'	1:A:2636:C:H5'	2.11	0.50
2:B:3107:C:H5	37:B:8438:HOH:O	1.94	0.50
4:D:275:GLY:O	4:D:291:ASP:HA	2.11	0.50
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.40	0.50
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.11	0.50
8:H:57:GLU:O	8:H:61:MET:HG3	2.11	0.50
10:J:59:ASN:N	10:J:59:ASN:ND2	2.57	0.50
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.93	0.50
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
1:A:113:A:H3'	1:A:114:A:C5'	2.42	0.49
1:A:2107:U:O2'	1:A:2108:A:H5'	2.12	0.49
1:A:2467:A:C2'	37:A:5435:HOH:O	2.45	0.49
3:C:93:THR:C	3:C:94:LEU:HD23	2.32	0.49
5:E:84:VAL:O	5:E:85:LYS:HB2	2.12	0.49
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.41	0.49
12:L:99:ASP:OD1	12:L:101:ASN:N	2.44	0.49
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.92	0.49
14:N:80:GLY:O	14:N:81:ARG:HD3	2.12	0.49
1:A:952:G:OP1	18:R:42:LYS:HE2	2.10	0.49
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.47	0.49
22:V:17:THR:HG22	22:V:18:GLY:N	2.26	0.49
1:A:119:A:H2'	1:A:120:A:H5''	1.93	0.49
1:A:371:U:H2'	1:A:372:A:C8	2.48	0.49
1:A:1874:U:P	3:C:51:ARG:HD2	2.52	0.49
5:E:187:ARG:NH2	37:E:8364:HOH:O	2.31	0.49
8:H:91:VAL:CG1	8:H:92:GLY:H	2.22	0.49
10:J:46:VAL:O	10:J:146:TRP:CH2	2.61	0.49
11:K:126:ASN:O	11:K:129:PHE:HE2	1.95	0.49
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:A:C2'	1:A:205:U:H5'	2.42	0.49
1:A:584:U:H3'	37:A:6068:HOH:O	2.12	0.49
1:A:941:G:O2'	1:A:942:U:H5'	2.12	0.49
3:C:164:ARG:HA	27:1:69:TYR:CE1	2.47	0.49
4:D:75:GLU:C	4:D:77:PRO:HD3	2.31	0.49
7:G:21:THR:HG23	7:G:30:THR:OG1	2.12	0.49
15:O:67:ALA:C	15:O:69:TYR:N	2.65	0.49
19:S:29:LYS:HB3	37:S:8531:HOH:O	2.12	0.49
1:A:2435:U:P	30:4:28:GLY:HA3	2.51	0.49
1:A:1174:A:C5	1:A:1201:C:H4'	2.47	0.49
1:A:1819:G:H2'	1:A:1820:G:C4'	2.42	0.49
5:E:236:THR:O	5:E:237:GLU:C	2.49	0.49
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.13	0.49
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.41	0.49
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.28	0.49
27:1:26:VAL:O	27:1:30:GLU:HG3	2.13	0.49
28:2:25:LYS:HG2	28:2:25:LYS:O	2.13	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.42	0.49
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.93	0.49
14:N:78:ASN:ND2	37:N:8649:HOH:O	2.41	0.49
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.78	0.49
1:A:1543:G:N1	1:A:1641:A:OP2	2.37	0.49
1:A:1834:C:H2'	1:A:1840:A:H62	1.75	0.49
1:A:240:C:O2	1:A:240:C:H2'	2.12	0.49
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.95	0.49
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.26	0.49
6:F:94:ALA:O	6:F:95:THR:O	2.30	0.49
10:J:111:MET:O	10:J:114:PRO:HD3	2.13	0.49
12:L:4:LEU:HD22	12:L:116:GLU:HB3	1.95	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.93	0.49
24:X:121:PRO:CA	24:X:153:MET:HG2	2.43	0.49
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.13	0.49
1:A:200:U:H2'	37:A:3428:HOH:O	2.12	0.49
1:A:2010:A:H2'	37:A:5931:HOH:O	2.12	0.49
4:D:32:ASP:HA	37:D:8573:HOH:O	2.12	0.49
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.93	0.49
6:F:23:VAL:CG2	6:F:23:VAL:O	2.60	0.49
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.77	0.49
13:M:73:VAL:HG23	13:M:74:THR:N	2.27	0.49
1:A:1494:A:C4	1:A:1495:C:C5	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:G:H4'	14:N:95:LYS:CE	2.43	0.49
1:A:1666:C:C2'	1:A:1667:A:C5'	2.91	0.49
2:B:3047:A:C2	2:B:3048:C:C2	3.00	0.49
6:F:62:ASP:HA	37:F:4233:HOH:O	2.13	0.49
7:G:145:ALA:HB1	7:G:168:ILE:CD1	2.43	0.49
8:H:117:GLU:C	8:H:119:ARG:H	2.16	0.49
10:J:83:PHE:CD1	10:J:134:ALA:HB2	2.48	0.49
11:K:107:ASN:HD22	11:K:109:TYR:H	1.58	0.49
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.93	0.49
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.47	0.49
1:A:2472:C:O2'	1:A:2634:G:H4'	2.12	0.49
1:A:816:G:OP1	17:Q:91:LYS:NZ	2.38	0.49
37:A:5388:HOH:O	3:C:164:ARG:NE	2.45	0.49
3:C:36:ASP:CB	3:C:83:GLY:HA3	2.43	0.49
4:D:168:GLY:N	4:D:174:ARG:HD3	2.27	0.49
17:Q:94:TRP:CZ2	17:Q:98:ILE:HG13	2.48	0.49
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.42	0.49
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.60	0.49
1:A:1162:G:H2'	37:A:6556:HOH:O	2.13	0.49
1:A:1192:A:H3'	1:A:1193:A:H5'	1.94	0.49
1:A:2761:A:C4	1:A:2763:G:C8	3.00	0.49
2:B:3025:G:H5''	2:B:3026:C:C6	2.48	0.49
9:I:27:ILE:HD12	9:I:70:ALA:HB1	1.95	0.49
10:J:141:ASN:CA	37:J:8365:HOH:O	2.55	0.49
27:1:37:HIS:O	27:1:45:LYS:HA	2.12	0.48
1:A:1535:G:H2'	1:A:1536:C:C6	2.48	0.48
1:A:168:C:O2'	1:A:169:A:H5'	2.13	0.48
1:A:1771:U:O2'	27:1:23:ARG:NH2	2.46	0.48
1:A:2115:U:H2'	1:A:2116:U:C6	2.48	0.48
1:A:2388:C:OP1	37:A:4581:HOH:O	2.19	0.48
1:A:2414:A:H2'	1:A:2415:A:C8	2.47	0.48
1:A:2526:C:O2'	1:A:2527:U:H5'	2.12	0.48
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.48
6:F:92:GLU:O	6:F:93:LEU:O	2.30	0.48
9:I:64:ASN:O	9:I:68:GLU:HG3	2.13	0.48
10:J:94:ARG:O	37:J:8333:HOH:O	2.20	0.48
26:Z:216:ARG:CD	37:Z:8568:HOH:O	2.52	0.48
27:1:46:LYS:NZ	37:1:8440:HOH:O	2.46	0.48
28:2:28:HIS:HD2	28:2:30:LYS:H	1.60	0.48
1:A:1164:U:C4'	1:A:1165:G:OP1	2.56	0.48
1:A:154:C:H2'	1:A:155:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2883:A:H2'	1:A:2884:G:O4'	2.13	0.48
1:A:818:A:O2'	27:1:13:ARG:HD3	2.13	0.48
1:A:858:U:H2'	1:A:859:C:C6	2.48	0.48
2:B:3049:G:H2'	2:B:3050:G:O4'	2.13	0.48
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.95	0.48
11:K:19:MET:HE1	11:K:132:LEU:CD1	2.43	0.48
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.43	0.48
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.33	0.48
1:A:1120:U:H5'	1:A:1121:G:OP2	2.12	0.48
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.45	0.48
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.48
1:A:1753:C:O2	4:D:229:ARG:NH2	2.44	0.48
1:A:2256:G:H2'	1:A:2257:G:C5'	2.43	0.48
1:A:2094:G:C2	1:A:2652:U:O2	2.65	0.48
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.44	0.48
5:E:185:LYS:HD3	5:E:186:TYR:CE1	2.48	0.48
6:F:86:THR:C	6:F:89:PRO:HD2	2.33	0.48
10:J:166:ASN:ND2	10:J:166:ASN:N	2.60	0.48
14:N:172:GLY:C	14:N:183:VAL:HG11	2.33	0.48
16:P:21:SER:OG	16:P:106:PRO:HB2	2.13	0.48
37:A:5998:HOH:O	18:R:50:GLY:HA2	2.13	0.48
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.12	0.48
25:Y:70:ILE:HG23	25:Y:70:ILE:O	2.13	0.48
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.49	0.48
29:3:48:ASP:O	29:3:49:GLU:HB2	2.13	0.48
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.42	0.48
1:A:2004:U:O2	1:A:2004:U:H2'	2.12	0.48
1:A:2314:G:C2'	1:A:2315:C:H5'	2.43	0.48
14:N:165:SER:HB2	37:N:8550:HOH:O	2.13	0.48
20:T:6:LYS:HB2	20:T:27:ALA:O	2.12	0.48
24:X:122:ARG:HG2	24:X:152:ALA:O	2.12	0.48
24:X:125:HIS:CD2	24:X:127:GLY:H	2.32	0.48
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	1.94	0.48
1:A:1666:C:O2'	1:A:1667:A:C5'	2.58	0.48
1:A:816:G:H5'	1:A:1598:A:H4'	1.95	0.48
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.77	0.48
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.43	0.48
4:D:119:HIS:O	4:D:121:PRO:HD3	2.12	0.48
1:A:2862:G:H4'	4:D:336:GLN:O	2.13	0.48
37:A:7438:HOH:O	5:E:188:ARG:HD2	2.14	0.48
8:H:60:VAL:O	8:H:61:MET:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:LEU:HD22	15:O:129:ILE:CD1	2.44	0.48
15:O:182:GLY:N	37:O:8569:HOH:O	2.45	0.48
16:P:26:TRP:N	37:P:3062:HOH:O	2.45	0.48
23:W:55:ARG:NE	37:W:4428:HOH:O	2.39	0.48
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.43	0.48
1:A:1279:U:H5''	37:A:9576:HOH:O	2.14	0.48
1:A:1586:G:O2'	1:A:1587:U:H5'	2.12	0.48
5:E:200:PRO:HB3	5:E:212:VAL:HG23	1.96	0.48
7:G:22:VAL:O	7:G:28:SER:HA	2.14	0.48
11:K:131:THR:HG22	11:K:133:GLY:N	2.28	0.48
11:K:39:VAL:HG13	11:K:106:GLY:O	2.13	0.48
12:L:130:MET:SD	22:V:25:ASP:O	2.71	0.48
8:H:58:GLU:CD	14:N:27:ARG:HH22	2.17	0.48
22:V:52:THR:CG2	22:V:54:THR:HB	2.43	0.48
1:A:56:G:H5''	23:W:50:ARG:HH12	1.77	0.48
24:X:122:ARG:CG	24:X:152:ALA:O	2.62	0.48
1:A:1730:G:C5'	1:A:1731:C:C6	2.96	0.48
1:A:2506:A:C1'	37:A:6027:HOH:O	2.61	0.48
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.95	0.48
1:A:1861:C:H4'	3:C:6:GLY:O	2.13	0.48
4:D:280:VAL:HG13	4:D:334:SER:HA	1.95	0.48
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.12	0.48
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.48	0.48
8:H:34:ASN:O	8:H:38:LYS:HG3	2.13	0.48
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.82	0.48
37:A:3445:HOH:O	11:K:46:ILE:HD12	2.12	0.48
12:L:75:ARG:HG2	12:L:90:PHE:CD2	2.49	0.48
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.48	0.48
27:1:30:GLU:O	27:1:33:HIS:HB3	2.14	0.48
1:A:396:U:OP2	30:4:38:ARG:NH1	2.47	0.48
1:A:1056:U:H2'	1:A:1057:A:O4'	2.14	0.48
1:A:1380:U:OP1	37:A:7859:HOH:O	2.20	0.48
1:A:2050:G:H5''	19:S:80:TYR:O	2.14	0.48
1:A:218:C:OP2	1:A:220:C:N4	2.44	0.48
1:A:426:G:H2'	1:A:427:C:O4'	2.14	0.48
37:A:6295:HOH:O	6:F:55:LYS:HB2	2.13	0.48
37:A:4066:HOH:O	8:H:31:LYS:HE3	2.12	0.48
13:M:72:ASN:HB2	37:M:8586:HOH:O	2.14	0.48
14:N:77:PHE:HD2	37:N:8527:HOH:O	1.96	0.48
18:R:32:GLU:HA	18:R:71:TYR:OH	2.14	0.48
1:A:1717:A:H5''	17:Q:54:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2019:A:H5'	37:A:4517:HOH:O	2.13	0.48
1:A:2672:C:O2'	1:A:2673:U:H5'	2.14	0.48
1:A:2896:A:N3	1:A:2896:A:H2'	2.29	0.48
1:A:951:A:O2'	1:A:952:G:H5'	2.14	0.48
2:B:3023:U:H6	2:B:3023:U:C5'	2.23	0.48
3:C:94:LEU:N	3:C:94:LEU:CD2	2.77	0.48
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.49	0.48
7:G:92:PRO:HB2	37:G:4917:HOH:O	2.13	0.48
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.43	0.48
11:K:42:GLU:O	11:K:131:THR:HG23	2.13	0.48
13:M:35:ARG:O	13:M:40:PHE:HA	2.13	0.48
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.95	0.48
24:X:48:VAL:O	24:X:48:VAL:CG1	2.60	0.48
27:1:57:CYS:O	27:1:61:GLY:N	2.45	0.48
1:A:1189:A:H1'	1:A:1209:C:H1'	1.96	0.48
1:A:1377:C:C6	1:A:1377:C:H5'	2.47	0.48
1:A:2251:G:H2'	1:A:2252:A:C8	2.49	0.48
1:A:2456:A:H5'	37:A:5670:HOH:O	2.14	0.48
1:A:2795:C:O2'	1:A:2796:U:H5'	2.13	0.48
1:A:57:C:H5''	37:A:6730:HOH:O	2.13	0.48
1:A:775:G:OP1	28:2:16:HIS:HE1	1.97	0.48
5:E:140:VAL:HG12	5:E:141:SER:N	2.29	0.48
6:F:99:ASP:HB2	6:F:103:ASN:H	1.79	0.48
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.96	0.48
10:J:14:TYR:N	10:J:91:HIS:CE1	2.80	0.48
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.49	0.48
14:N:52:LEU:HD13	14:N:116:ASN:CB	2.44	0.48
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.44	0.48
1:A:1714:C:O2'	1:A:1715:C:H5'	2.14	0.47
1:A:2353:A:H4'	1:A:2354:A:O5'	2.13	0.47
1:A:820:G:O2'	1:A:856:G:H4'	2.14	0.47
4:D:4:SER:O	4:D:5:ARG:HB2	2.14	0.47
4:D:88:GLU:O	4:D:88:GLU:HG3	2.13	0.47
5:E:162:VAL:O	5:E:162:VAL:CG1	2.62	0.47
6:F:57:THR:HG23	6:F:63:ILE:CB	2.44	0.47
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.96	0.47
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.14	0.47
12:L:66:ARG:HG2	12:L:66:ARG:HH11	1.79	0.47
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.44	0.47
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.13	0.47
19:S:82:GLU:HG3	19:S:83:LYS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:NH1	24:X:122:ARG:HG2	2.23	0.47
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.47	0.47
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.40	0.47
1:A:245:C:C2'	1:A:246:G:H5'	2.44	0.47
1:A:778:C:C4	1:A:779:U:C4	3.02	0.47
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.43	0.47
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.12	0.47
7:G:93:MET:HE1	7:G:165:GLY:N	2.29	0.47
8:H:113:ASP:O	8:H:117:GLU:HG3	2.14	0.47
9:I:12:ILE:HB	37:I:4714:HOH:O	2.12	0.47
12:L:55:VAL:CG1	12:L:56:SER:N	2.77	0.47
37:A:5917:HOH:O	17:Q:87:ARG:HG2	2.14	0.47
19:S:119:VAL:HG12	19:S:119:VAL:O	2.14	0.47
19:S:68:HIS:CD2	19:S:76:ASP:HB2	2.49	0.47
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.95	0.47
1:A:1942:A:O2'	1:A:1943:C:H5'	2.14	0.47
1:A:2408:A:H2	37:A:3081:HOH:O	1.96	0.47
1:A:644:G:H5'	1:A:644:G:N3	2.29	0.47
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.95	0.47
5:E:191:SER:OG	5:E:192:ILE:N	2.47	0.47
10:J:31:PHE:HE2	10:J:87:LYS:O	1.97	0.47
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.38	0.47
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.96	0.47
21:U:71:VAL:HG12	21:U:72:ILE:N	2.29	0.47
1:A:1589:G:N2	1:A:1605:G:H1'	2.30	0.47
1:A:2100:A:H5'	37:E:8460:HOH:O	2.14	0.47
1:A:2247:C:H5''	37:A:7323:HOH:O	2.13	0.47
1:A:2459:G:OP1	30:4:64:LYS:N	2.24	0.47
1:A:283:U:H5	1:A:284:C:N4	2.12	0.47
1:A:902:G:N7	13:M:18:HIS:CD2	2.80	0.47
1:A:949:U:O2'	18:R:40:HIS:HE1	1.97	0.47
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.29	0.47
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.97	0.47
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.50	0.47
14:N:64:ARG:NH2	37:N:8555:HOH:O	2.38	0.47
15:O:155:GLU:O	15:O:156:GLU:HG3	2.15	0.47
19:S:39:THR:CB	19:S:42:GLU:HG3	2.39	0.47
1:A:1423:C:O2'	1:A:1424:A:H5'	2.15	0.47
1:A:1506:U:H6	1:A:1506:U:H5'	1.80	0.47
1:A:251:C:O2'	1:A:252:C:H5'	2.13	0.47
1:A:282:C:H2'	1:A:283:U:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:A:H5'	21:U:54:ASP:OD2	2.13	0.47
3:C:36:ASP:HB2	3:C:83:GLY:HA3	1.96	0.47
3:C:36:ASP:HB2	3:C:84:VAL:N	2.30	0.47
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.50	0.47
7:G:20:ILE:HD12	7:G:33:LEU:CD1	2.44	0.47
7:G:69:ILE:HA	7:G:72:MET:HE2	1.97	0.47
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.45	0.47
1:A:1500:U:P	17:Q:41:ARG:HH22	2.37	0.47
22:V:52:THR:HG22	22:V:54:THR:N	2.30	0.47
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.15	0.47
5:E:51:TYR:CE2	28:2:53:LYS:HB3	2.49	0.47
1:A:1559:A:H1'	37:A:5839:HOH:O	2.13	0.47
1:A:2730:G:O2'	1:A:2731:G:H5'	2.15	0.47
1:A:566:A:H2'	1:A:567:U:O4'	2.14	0.47
1:A:948:G:O2'	1:A:949:U:H5'	2.15	0.47
7:G:11:VAL:CG1	7:G:12:ASP:H	2.28	0.47
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.95	0.47
9:I:63:ARG:O	9:I:67:LEU:HG	2.15	0.47
10:J:163:PRO:O	10:J:164:ALA:HB2	2.14	0.47
13:M:97:VAL:HG12	13:M:98:GLU:O	2.15	0.47
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.14	0.47
30:4:65:THR:O	30:4:82:GLY:HA3	2.15	0.47
1:A:1304:U:H2'	1:A:1305:C:C6	2.50	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.50	0.47
1:A:2445:U:H2'	1:A:2446:G:C8	2.50	0.47
1:A:677:C:H4'	5:E:246:ARG:NH2	2.30	0.47
5:E:34:ALA:HB3	5:E:220:THR:HG21	1.97	0.47
7:G:43:ASP:HA	37:G:5864:HOH:O	2.13	0.47
10:J:140:PRO:O	37:J:8365:HOH:O	2.20	0.47
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.27	0.47
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.68	0.47
1:A:209:G:C6	1:A:210:U:N3	2.83	0.47
1:A:2256:G:C2'	1:A:2257:G:H5'	2.45	0.47
1:A:2897:C:H2'	1:A:2898:G:H8	1.79	0.47
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.97	0.47
6:F:67:ASP:O	6:F:69:ILE:HG13	2.14	0.47
11:K:142:ASN:O	11:K:144:THR:N	2.47	0.47
15:O:25:ARG:HA	15:O:28:LYS:HG3	1.97	0.47
2:B:3028:U:H5''	15:O:40:ASN:ND2	2.29	0.47
17:Q:143:ALA:HA	37:Q:190:HOH:O	2.13	0.47
17:Q:27:ARG:HA	37:Q:172:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:30:VAL:O	18:R:30:VAL:HG12	2.15	0.47
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.14	0.47
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.79	0.47
1:A:1166:A:H61	1:A:1180:U:H3	1.61	0.47
1:A:1132:A:N6	1:A:1229:C:H2'	2.30	0.47
1:A:659:A:H5''	37:P:6799:HOH:O	2.13	0.47
3:C:6:GLY:HA3	37:C:8569:HOH:O	2.15	0.47
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.50	0.47
4:D:7:ARG:CD	4:D:9:GLY:O	2.62	0.47
15:O:43:VAL:HG13	15:O:118:ILE:HD11	1.96	0.47
15:O:171:HIS:CE1	37:O:8565:HOH:O	2.66	0.47
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.97	0.47
1:A:470:U:O2'	28:2:16:HIS:HD2	1.97	0.47
1:A:1434:A:H2'	1:A:1436:C:C5	2.49	0.47
1:A:1504:A:O2'	1:A:1506:U:OP2	2.30	0.47
1:A:2428:G:O6	1:A:2464:C:H1'	2.15	0.47
1:A:2591:C:H2'	1:A:2592:G:O4'	2.15	0.47
1:A:2681:A:H4'	1:A:2682:C:H5'	1.97	0.47
1:A:2769:C:O2'	1:A:2770:G:H5'	2.14	0.47
1:A:67:A:H5''	1:A:69:A:C8	2.50	0.47
31:A:9002:BLS:H102	31:A:9002:BLS:H132	1.84	0.47
3:C:33:GLU:H	3:C:33:GLU:CD	2.18	0.47
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.15	0.47
10:J:118:PRO:HD2	37:J:8339:HOH:O	2.13	0.47
14:N:123:ASP:OD1	14:N:123:ASP:C	2.52	0.47
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.79	0.47
27:1:59:HIS:HA	37:1:8440:HOH:O	2.14	0.47
1:A:2547:C:H2'	1:A:2548:C:H6	1.79	0.47
1:A:278:A:H2'	1:A:279:C:O4'	2.15	0.47
1:A:308:U:C4	1:A:342:C:H1'	2.49	0.47
1:A:484:A:N1	1:A:506:G:H4'	2.30	0.47
2:B:3035:C:H5''	37:B:8457:HOH:O	2.15	0.47
10:J:43:PRO:HD2	10:J:137:ASN:HA	1.96	0.47
12:L:80:ILE:HG13	12:L:80:ILE:O	2.14	0.47
14:N:125:ARG:NH1	37:N:8599:HOH:O	2.48	0.47
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.40	0.47
22:V:6:CYS:HB2	22:V:32:CYS:HB3	1.97	0.47
23:W:58:THR:O	23:W:62:GLU:HG3	2.15	0.47
27:1:46:LYS:HB2	27:1:57:CYS:HG	1.80	0.46
30:4:84:ARG:HH11	30:4:84:ARG:HG3	1.81	0.46
1:A:1014:A:H5''	2:B:3101:G:O2'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.15	0.46
1:A:420:U:H2'	1:A:421:C:C6	2.50	0.46
1:A:482:G:H4'	1:A:508:A:N1	2.31	0.46
37:A:9075:HOH:O	4:D:214:PRO:HD2	2.14	0.46
5:E:7:ASP:OD1	5:E:11:ASN:O	2.33	0.46
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.46
12:L:65:ARG:HD3	37:L:5358:HOH:O	2.15	0.46
13:M:101:ASP:C	13:M:103:ALA:H	2.18	0.46
14:N:183:VAL:HG12	14:N:184:ARG:N	2.30	0.46
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.45	0.46
17:Q:58:SER:HB3	37:Q:181:HOH:O	2.15	0.46
22:V:52:THR:HG22	22:V:54:THR:H	1.80	0.46
24:X:121:PRO:HA	24:X:153:MET:HG2	1.96	0.46
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.50	0.46
1:A:10:U:H5'	37:A:6010:HOH:O	2.15	0.46
1:A:2300:A:H4'	1:A:2301:A:O5'	2.16	0.46
1:A:1006:A:N1	1:A:2311:A:H1'	2.30	0.46
3:C:231:LYS:O	3:C:232:ARG:HB3	2.15	0.46
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.44	0.46
7:G:10:ASP:HA	37:G:3707:HOH:O	2.15	0.46
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.97	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.33	0.46
14:N:59:GLY:C	14:N:141:ILE:HD11	2.36	0.46
15:O:67:ALA:HA	15:O:71:TRP:HB3	1.97	0.46
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.14	0.46
6:F:65:GLU:HA	37:F:6752:HOH:O	2.14	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.46
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.30	0.46
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.30	0.46
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.44	0.46
20:T:38:ALA:O	20:T:42:GLU:HG3	2.15	0.46
22:V:39:ASN:ND2	22:V:44:ARG:HH11	2.13	0.46
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.46	0.46
1:A:1829:A:H61	27:1:18:TYR:CA	2.28	0.46
1:A:1878:G:C1'	37:A:6094:HOH:O	2.64	0.46
1:A:328:U:O4'	5:E:202:THR:HG22	2.15	0.46
2:B:3051:A:H5'	15:O:160:SER:HB3	1.98	0.46
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.47	0.46
9:I:64:ASN:N	9:I:64:ASN:ND2	2.62	0.46
10:J:47:GLU:HG2	10:J:133:ILE:HD12	1.96	0.46
12:L:87:ARG:CZ	37:L:4854:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:87:ARG:NE	37:L:4854:HOH:O	2.49	0.46
13:M:30:ARG:NH2	37:M:8524:HOH:O	2.31	0.46
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.62	0.46
15:O:24:LEU:O	15:O:28:LYS:HG2	2.15	0.46
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.97	0.46
25:Y:78:GLU:CG	25:Y:79:GLU:N	2.77	0.46
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.50	0.46
37:A:7565:HOH:O	27:1:31:ILE:HG13	2.16	0.46
1:A:2307:A:C2	1:A:2308:U:N3	2.84	0.46
1:A:858:U:H2'	1:A:859:C:H6	1.81	0.46
1:A:877:G:C5'	1:A:878:G:OP1	2.61	0.46
1:A:883:U:C2'	1:A:883:U:O2	2.64	0.46
1:A:920:C:H4'	1:A:921:G:C2	2.50	0.46
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.98	0.46
6:F:99:ASP:O	6:F:159:PRO:HG3	2.15	0.46
12:L:86:THR:HG22	12:L:87:ARG:N	2.30	0.46
13:M:73:VAL:HG11	13:M:118:LEU:HD21	1.97	0.46
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.46	0.46
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.81	0.46
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.30	0.46
1:A:1617:C:C4	1:A:1643:C:H4'	2.50	0.46
1:A:1730:G:C5'	1:A:1731:C:H6	2.27	0.46
6:F:35:ALA:O	6:F:37:ALA:N	2.48	0.46
6:F:59:GLY:C	6:F:61:PHE:H	2.19	0.46
7:G:84:MET:HB2	7:G:131:LEU:HB2	1.97	0.46
7:G:132:THR:HG23	7:G:132:THR:O	2.15	0.46
10:J:132:PHE:O	10:J:133:ILE:HD13	2.15	0.46
11:K:19:MET:HE1	11:K:132:LEU:HD21	1.98	0.46
1:A:2598:U:H5''	12:L:36:GLY:HA2	1.97	0.46
2:B:3008:G:O6	15:O:11:ARG:NH1	2.49	0.46
37:A:7404:HOH:O	21:U:9:LYS:HD2	2.16	0.46
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.51	0.46
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.16	0.46
1:A:2533:C:H6	1:A:2533:C:C5'	2.21	0.46
1:A:2712:G:H5'	37:L:4183:HOH:O	2.15	0.46
3:C:123:GLY:HA3	3:C:162:GLY:HA2	1.98	0.46
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.45	0.46
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.14	0.46
8:H:21:GLU:O	8:H:24:ARG:HG3	2.15	0.46
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.98	0.46
37:A:4550:HOH:O	14:N:83:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:184:ILE:HG22	15:O:185:GLU:N	2.31	0.46
15:O:43:VAL:O	15:O:43:VAL:HG12	2.16	0.46
20:T:57:THR:C	20:T:59:ASP:H	2.19	0.46
1:A:317:A:H5''	21:U:52:ARG:HD2	1.97	0.46
21:U:75:GLU:O	21:U:76:ASP:HB2	2.16	0.46
37:L:408:HOH:O	22:V:37:GLU:HB3	2.16	0.46
24:X:38:THR:HG22	24:X:39:ASP:H	1.81	0.46
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.27	0.46
27:1:41:VAL:HG12	27:1:42:CYS:N	2.31	0.46
3:C:51:ARG:NH2	3:C:69:LEU:HD13	2.31	0.46
5:E:246:ARG:NH2	37:E:8423:HOH:O	2.49	0.46
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.97	0.46
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.46	0.46
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.98	0.46
24:X:41:TYR:CD2	24:X:44:MET:HE3	2.51	0.46
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.81	0.46
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.51	0.46
1:A:1574:C:H6	1:A:1574:C:O5'	1.98	0.46
1:A:2004:U:H1'	37:A:3177:HOH:O	2.14	0.46
1:A:2462:G:N7	30:4:60:LYS:NZ	2.60	0.46
3:C:179:MET:HG2	3:C:186:TRP:CG	2.51	0.46
4:D:108:GLU:HB3	4:D:111:ARG:HD2	1.97	0.46
8:H:37:THR:O	8:H:41:GLU:HG3	2.16	0.46
11:K:51:GLU:O	11:K:55:GLU:HG3	2.16	0.46
14:N:164:THR:HG23	14:N:165:SER:H	1.78	0.46
37:A:6169:HOH:O	14:N:174:ARG:HD3	2.15	0.46
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.51	0.46
27:1:42:CYS:SG	27:1:44:PHE:CB	2.94	0.46
1:A:1562:C:O2	1:A:1562:C:H2'	2.16	0.46
1:A:2123:A:H5'	14:N:89:ASN:ND2	2.32	0.46
1:A:2432:C:C4'	37:A:9724:HOH:O	2.62	0.46
1:A:407:A:H5'	37:A:5997:HOH:O	2.15	0.46
1:A:920:C:H5'	1:A:921:G:C4	2.51	0.46
3:C:192:VAL:HG13	37:C:8558:HOH:O	2.16	0.46
4:D:7:ARG:NH1	4:D:7:ARG:CG	2.77	0.46
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.97	0.46
6:F:25:MET:HE1	6:F:37:ALA:O	2.15	0.46
7:G:16:ASP:O	7:G:17:HIS:HB2	2.16	0.46
17:Q:2:ASP:C	17:Q:2:ASP:OD1	2.54	0.46
19:S:84:ALA:O	19:S:88:PHE:HD1	1.99	0.46
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:47:ARG:CG	37:V:4381:HOH:O	2.63	0.46
1:A:1588:G:C6	1:A:1589:G:N1	2.84	0.45
1:A:2010:A:C3'	37:A:5931:HOH:O	2.63	0.45
1:A:2488:A:H2	37:A:7256:HOH:O	1.97	0.45
1:A:2720:C:O2	12:L:87:ARG:NH2	2.50	0.45
1:A:2906:A:H5'	1:A:2907:C:O4'	2.15	0.45
1:A:559:U:C6	1:A:559:U:H5'	2.43	0.45
1:A:639:A:H2'	1:A:640:G:C8	2.51	0.45
1:A:870:G:C3'	1:A:871:G:H5''	2.46	0.45
1:A:970:U:H2'	37:A:6303:HOH:O	2.14	0.45
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.99	0.45
5:E:76:ARG:HD3	37:E:8366:HOH:O	2.15	0.45
7:G:80:TRP:O	7:G:134:SER:HA	2.15	0.45
10:J:150:LYS:CB	10:J:157:ILE:HD12	2.42	0.45
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.16	0.45
14:N:89:ASN:HA	37:N:8554:HOH:O	2.15	0.45
15:O:161:GLY:O	15:O:162:ASP:C	2.54	0.45
1:A:710:G:P	16:P:24:ALA:HB3	2.56	0.45
22:V:9:CYS:O	22:V:52:THR:HG23	2.17	0.45
1:A:894:A:C2	5:E:87:ARG:NH2	2.84	0.45
6:F:159:PRO:O	6:F:163:VAL:HG23	2.16	0.45
2:B:3040:C:N4	6:F:51:ARG:HB2	2.31	0.45
6:F:81:GLU:O	6:F:85:GLN:HG3	2.16	0.45
7:G:68:HIS:O	7:G:72:MET:HG3	2.17	0.45
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.48	0.45
30:4:60:LYS:HG3	30:4:61:PRO:HD2	1.99	0.45
1:A:911:G:H5'	1:A:932:U:OP1	2.16	0.45
10:J:53:PRO:HA	10:J:125:VAL:O	2.15	0.45
11:K:19:MET:HE1	11:K:132:LEU:CD2	2.47	0.45
14:N:191:GLY:O	14:N:192:ALA:HB3	2.15	0.45
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.79	0.45
17:Q:7:LYS:HD3	17:Q:21:VAL:HG21	1.97	0.45
19:S:113:HIS:O	19:S:145:LEU:HD12	2.17	0.45
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.16	0.45
27:1:22:ILE:O	27:1:26:VAL:HG23	2.16	0.45
1:A:120:A:H2'	1:A:120:A:N3	2.31	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.16	0.45
1:A:162:C:H2'	1:A:163:U:H5'	1.98	0.45
1:A:2401:A:H5'	37:A:9481:HOH:O	2.16	0.45
1:A:397:A:P	37:A:4323:HOH:O	2.75	0.45
1:A:638:C:H2'	1:A:639:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.80	0.45
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.46	0.45
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.45
1:A:2561:C:OP1	7:G:153:ARG:NH2	2.50	0.45
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.16	0.45
11:K:19:MET:HE2	11:K:79:PHE:HA	1.98	0.45
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.81	0.45
14:N:35:PRO:CG	14:N:38:VAL:CG2	2.87	0.45
16:P:96:VAL:HG13	16:P:100:GLN:HB2	1.99	0.45
17:Q:10:ALA:O	17:Q:13:VAL:HG12	2.17	0.45
1:A:2055:A:H4'	19:S:132:ARG:NH2	2.30	0.45
19:S:39:THR:O	19:S:40:ALA:C	2.54	0.45
24:X:65:VAL:HA	24:X:68:THR:CG2	2.46	0.45
1:A:86:A:C2	29:3:25:VAL:HG13	2.51	0.45
1:A:1333:U:H2'	1:A:1334:C:H6	1.79	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
1:A:2090:G:H2'	1:A:2091:G:C8	2.51	0.45
1:A:2467:A:C3'	37:A:5435:HOH:O	2.64	0.45
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.81	0.45
1:A:731:U:H2'	1:A:732:C:C6	2.51	0.45
6:F:101:THR:O	6:F:101:THR:HG22	2.16	0.45
10:J:45:GLN:NE2	10:J:135:TRP:HE1	2.10	0.45
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.52	0.45
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.34	0.45
15:O:107:ASN:OD1	35:O:8507:CL:CL	2.71	0.45
20:T:53:ASN:ND2	37:T:2190:HOH:O	2.48	0.45
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.45
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.46	0.45
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.16	0.45
1:A:1687:C:O2	28:2:9:GLY:HA2	2.17	0.45
1:A:1269:G:H2'	1:A:1270:U:C6	2.52	0.45
1:A:128:A:H3'	1:A:128:A:H8	1.82	0.45
1:A:1525:G:H5'	1:A:1526:A:OP2	2.17	0.45
1:A:2428:G:C6	1:A:2464:C:H1'	2.51	0.45
1:A:2649:A:C8	1:A:2649:A:H5'	2.52	0.45
1:A:2900:G:H2'	1:A:2901:C:O4'	2.16	0.45
1:A:559:U:H2'	1:A:560:C:O4'	2.17	0.45
2:B:3042:C:O2	6:F:76:ARG:NH1	2.50	0.45
3:C:210:GLY:HA3	37:C:8591:HOH:O	2.17	0.45
3:C:51:ARG:NH2	37:C:8550:HOH:O	2.47	0.45
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:LEU:O	4:D:84:LEU:HD13	2.16	0.45
8:H:110:GLU:O	8:H:114:LYS:HG3	2.16	0.45
10:J:57:ARG:C	10:J:59:ASN:N	2.68	0.45
14:N:43:PRO:HG3	14:N:62:VAL:HG21	1.99	0.45
16:P:25:VAL:HG23	16:P:26:TRP:N	2.32	0.45
16:P:98:LEU:HD12	16:P:98:LEU:HA	1.84	0.45
24:X:48:VAL:O	24:X:48:VAL:HG12	2.15	0.45
25:Y:9:VAL:HG13	25:Y:88:GLU:OE1	2.17	0.45
1:A:10:U:HO2'	1:A:11:A:P	2.40	0.45
1:A:2766:A:O2'	1:A:2767:C:H5'	2.17	0.45
1:A:500:G:H21	19:S:98:ASN:HD21	1.62	0.45
1:A:820:G:C6	3:C:171:LYS:CB	2.99	0.45
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.32	0.45
15:O:154:LEU:O	15:O:155:GLU:CB	2.65	0.45
1:A:2460:A:OP1	30:4:60:LYS:HB2	2.17	0.45
1:A:1636:G:O2'	1:A:1637:A:H5'	2.16	0.45
1:A:1942:A:C3'	37:A:7325:HOH:O	2.62	0.45
1:A:2011:A:H4'	1:A:2012:U:O5'	2.17	0.45
1:A:2089:A:C2'	1:A:2090:G:H5'	2.47	0.45
1:A:2119:C:C2'	1:A:2120:U:H5'	2.47	0.45
1:A:2419:U:H5''	1:A:2420:G:C5'	2.47	0.45
1:A:2578:G:C8	1:A:2578:G:H5'	2.48	0.45
1:A:611:U:H2'	1:A:612:U:C6	2.52	0.45
1:A:716:G:H2'	1:A:717:C:O5'	2.17	0.45
1:A:816:G:C6	1:A:817:G:N1	2.85	0.45
2:B:3031:C:H2'	2:B:3032:G:O4'	2.17	0.45
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.47	0.45
6:F:84:LEU:C	6:F:86:THR:H	2.20	0.45
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.17	0.45
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.46	0.45
11:K:70:PHE:O	11:K:70:PHE:CD2	2.69	0.45
14:N:69:LYS:O	14:N:73:ARG:NH1	2.50	0.45
21:U:12:ARG:NH1	37:U:3035:HOH:O	2.49	0.45
26:Z:144:ARG:NH2	37:Z:8610:HOH:O	2.49	0.45
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.98	0.45
1:A:1517:U:C2	1:A:1670:G:N2	2.85	0.45
1:A:1996:U:O2'	1:A:1997:A:H5'	2.16	0.45
1:A:2084:C:H2'	1:A:2085:A:H8	1.82	0.45
1:A:2779:G:H21	7:G:143:GLN:HE22	1.65	0.45
1:A:2088:C:H1'	1:A:2841:A:N1	2.31	0.45
1:A:453:A:H4'	1:A:455:A:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:G:H4'	1:A:835:U:OP2	2.17	0.45
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.46	0.45
5:E:162:VAL:CG1	5:E:192:ILE:HD11	2.46	0.45
14:N:186:SER:OG	14:N:189:VAL:HG12	2.17	0.45
14:N:96:ASN:ND2	37:N:8541:HOH:O	2.46	0.45
15:O:34:LEU:HD13	15:O:47:LEU:HD21	1.99	0.45
20:T:56:ASN:O	29:3:8:LYS:HE2	2.17	0.45
30:4:38:ARG:O	30:4:42:ARG:HB2	2.17	0.45
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.52	0.45
1:A:1165:G:OP1	1:A:1165:G:H3'	2.17	0.45
1:A:1976:G:O2'	1:A:1977:U:H5'	2.17	0.45
1:A:2415:A:C2	15:O:25:ARG:HB3	2.52	0.45
1:A:244:C:O5'	1:A:244:C:H6	1.99	0.45
1:A:860:U:H2'	1:A:861:A:C8	2.52	0.45
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.98	0.45
37:A:7438:HOH:O	5:E:188:ARG:HD3	2.16	0.45
5:E:19:PRO:HG2	5:E:22:PHE:CD1	2.52	0.45
23:W:12:THR:OG1	23:W:13:PRO:HD2	2.17	0.45
20:T:10:VAL:HG11	23:W:36:ALA:HA	1.98	0.45
28:2:25:LYS:HD2	29:3:48:ASP:HA	1.99	0.44
1:A:1003:U:O2'	10:J:90:PHE:HE1	2.00	0.44
1:A:1783:A:O2'	1:A:1784:U:H5'	2.17	0.44
1:A:2362:A:H2'	1:A:2363:G:C8	2.52	0.44
1:A:2464:C:P	37:A:9918:HOH:O	2.75	0.44
1:A:2898:G:H4'	4:D:288:GLY:HA2	1.98	0.44
1:A:466:A:H2'	1:A:467:G:O4'	2.17	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.65	0.44
3:C:107:ASN:OD1	3:C:120:ARG:HD2	2.17	0.44
37:A:9110:HOH:O	5:E:103:ASN:HB3	2.16	0.44
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.99	0.44
10:J:157:ILE:CG2	10:J:158:ASN:N	2.80	0.44
14:N:134:ILE:O	14:N:136:PRO:HD3	2.17	0.44
14:N:68:ARG:CG	14:N:68:ARG:O	2.63	0.44
15:O:73:ALA:HB1	15:O:74:PRO:HD2	1.97	0.44
15:O:82:TYR:CD2	15:O:82:TYR:C	2.91	0.44
18:R:24:SER:O	37:R:2847:HOH:O	2.21	0.44
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.78	0.44
24:X:64:THR:O	24:X:68:THR:HG22	2.17	0.44
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.53	0.44
27:1:39:CYS:O	27:1:42:CYS:O	2.35	0.44
1:A:1342:C:O2'	1:A:1343:C:H5'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2468:A:H61	30:4:48:ASN:ND2	2.00	0.44
1:A:2780:C:H2'	1:A:2781:U:C6	2.52	0.44
1:A:470:U:O2'	28:2:16:HIS:CD2	2.70	0.44
1:A:514:G:O5'	1:A:514:G:H8	2.00	0.44
1:A:694:A:C2'	1:A:695:C:H5'	2.47	0.44
1:A:1884:G:O6	3:C:190:ARG:HD2	2.17	0.44
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.99	0.44
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.62	0.44
6:F:76:ARG:O	6:F:77:ASP:HB2	2.18	0.44
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.17	0.44
1:A:182:G:C4'	14:N:157:LEU:HD13	2.47	0.44
14:N:87:MET:SD	37:N:8534:HOH:O	2.61	0.44
15:O:11:ARG:O	15:O:15:GLU:HG3	2.17	0.44
17:Q:21:VAL:O	17:Q:21:VAL:HG23	2.17	0.44
20:T:10:VAL:CG1	23:W:35:ALA:O	2.65	0.44
24:X:6:GLN:CB	24:X:26:ILE:HD12	2.40	0.44
27:1:10:ARG:HG3	27:1:11:THR:N	2.33	0.44
1:A:1015:C:H2'	1:A:1016:U:C6	2.52	0.44
1:A:2405:C:P	37:A:6569:HOH:O	2.75	0.44
1:A:2437:A:H2'	1:A:2438:G:C8	2.53	0.44
1:A:1565:C:O4'	1:A:2738:G:H1'	2.17	0.44
1:A:2851:G:C2'	1:A:2852:A:H5'	2.47	0.44
1:A:401:C:P	37:A:5769:HOH:O	2.75	0.44
1:A:488:U:H2'	37:A:3992:HOH:O	2.17	0.44
1:A:489:A:C8	21:U:82:THR:HG22	2.53	0.44
1:A:960:G:N3	1:A:960:G:C2'	2.80	0.44
3:C:109:GLU:HG2	3:C:116:GLY:N	2.32	0.44
37:A:7001:HOH:O	3:C:211:LYS:CG	2.64	0.44
3:C:36:ASP:CB	3:C:85:ASP:H	2.29	0.44
4:D:238:ASN:ND2	4:D:240:GLY:H	2.07	0.44
37:A:9664:HOH:O	5:E:214:THR:HB	2.17	0.44
5:E:236:THR:C	37:E:8446:HOH:O	2.56	0.44
6:F:86:THR:HG23	37:F:7477:HOH:O	2.17	0.44
7:G:5:LEU:HD21	7:G:66:GLN:HG3	1.99	0.44
11:K:6:PHE:O	11:K:8:ALA:N	2.50	0.44
13:M:104:ASP:HB2	37:M:8581:HOH:O	2.18	0.44
15:O:157:PRO:HA	37:O:8526:HOH:O	2.17	0.44
17:Q:134:VAL:O	17:Q:137:LEU:HB3	2.17	0.44
24:X:1:MET:HB2	24:X:103:GLU:HG2	2.00	0.44
24:X:122:ARG:NH2	37:X:4276:HOH:O	2.50	0.44
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:8:ARG:NH1	37:Y:2479:HOH:O	2.36	0.44
1:A:1023:C:O2'	1:A:1024:G:H5'	2.18	0.44
1:A:101:C:O2'	1:A:102:A:H5'	2.17	0.44
1:A:1200:A:H4'	37:A:7319:HOH:O	2.17	0.44
1:A:2321:A:O2'	1:A:2322:U:H3'	2.17	0.44
1:A:2064:U:H4'	1:A:2653:A:P	2.57	0.44
1:A:626:U:C4	1:A:627:G:C6	3.05	0.44
1:A:657:G:H2'	1:A:658:C:C6	2.52	0.44
5:E:154:VAL:O	5:E:158:GLU:HG3	2.16	0.44
5:E:180:SER:HB2	37:E:8443:HOH:O	2.17	0.44
10:J:81:TYR:C	10:J:81:TYR:CD1	2.90	0.44
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.98	0.44
15:O:101:VAL:HG12	37:O:8531:HOH:O	2.17	0.44
22:V:38:ASN:O	22:V:42:LEU:HG	2.17	0.44
24:X:139:GLY:O	24:X:141:HIS:CD2	2.69	0.44
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.53	0.44
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.98	0.44
1:A:1066:U:H2'	1:A:1067:A:C8	2.52	0.44
1:A:1176:C:H1'	37:A:3916:HOH:O	2.18	0.44
1:A:2505:G:C2'	1:A:2506:A:H5'	2.48	0.44
1:A:288:A:H2'	1:A:289:G:C8	2.53	0.44
1:A:564:G:H1'	37:A:6285:HOH:O	2.18	0.44
5:E:107:ARG:NE	37:E:8454:HOH:O	2.37	0.44
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.35	0.44
11:K:131:THR:HG22	11:K:134:GLU:N	2.28	0.44
37:A:4808:HOH:O	11:K:47:THR:CB	2.56	0.44
14:N:184:ARG:HG3	14:N:185:PRO:HA	1.99	0.44
14:N:57:LYS:HE2	14:N:140:ALA:O	2.17	0.44
15:O:154:LEU:CG	15:O:155:GLU:H	2.28	0.44
21:U:45:GLY:C	37:U:3851:HOH:O	2.55	0.44
21:U:71:VAL:CG1	21:U:72:ILE:N	2.80	0.44
26:Z:142:SER:OG	37:Z:8610:HOH:O	2.21	0.44
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.42	0.44
1:A:1495:C:H1'	1:A:1573:A:H1'	2.00	0.44
1:A:1684:A:O2'	1:A:1685:A:H5''	2.18	0.44
1:A:303:C:H2'	1:A:304:G:O4'	2.18	0.44
1:A:314:G:N2	1:A:316:A:H3'	2.32	0.44
1:A:596:C:H2'	1:A:597:A:C8	2.53	0.44
18:R:66:LYS:HB2	18:R:70:ALA:O	2.17	0.44
24:X:11:VAL:O	24:X:12:ASN:HB2	2.18	0.44
25:Y:9:VAL:HG13	25:Y:88:GLU:CD	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:19:SER:O	29:3:36:ASN:ND2	2.51	0.44
1:A:234:A:H4'	1:A:437:A:O4'	2.17	0.44
1:A:2559:C:H4'	37:A:7234:HOH:O	2.16	0.44
1:A:137:U:OP1	1:A:259:G:O2'	2.36	0.44
1:A:2825:C:H4'	1:A:2826:G:O5'	2.17	0.44
4:D:268:ARG:NE	37:D:8607:HOH:O	2.49	0.44
9:I:20:VAL:O	9:I:24:VAL:HG23	2.18	0.44
17:Q:7:LYS:CD	17:Q:21:VAL:HG21	2.48	0.44
19:S:29:LYS:HD3	37:S:8531:HOH:O	2.17	0.44
26:Z:115:ARG:CZ	37:Z:8556:HOH:O	2.66	0.44
26:Z:189:ASN:ND2	26:Z:189:ASN:C	2.71	0.44
30:4:70:ARG:HD3	37:4:8541:HOH:O	2.17	0.44
30:4:71:CYS:SG	30:4:72:GLY:N	2.91	0.44
1:A:128:A:C8	1:A:128:A:C3'	2.99	0.44
1:A:2257:G:H4'	1:A:2259:C:C2	2.53	0.44
1:A:2413:A:H2'	1:A:2414:A:O4'	2.18	0.44
1:A:2729:C:O2'	1:A:2730:G:H5'	2.18	0.44
1:A:329:A:OP2	5:E:206:ASN:HB2	2.17	0.44
1:A:390:G:OP1	30:4:46:ILE:HG13	2.17	0.44
1:A:853:C:H2'	1:A:854:G:O4'	2.17	0.44
3:C:36:ASP:CA	3:C:83:GLY:HA3	2.48	0.44
4:D:55:ASN:HB3	4:D:64:GLY:N	2.32	0.44
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.48	0.44
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.99	0.44
13:M:121:ILE:HG12	13:M:141:GLU:HB2	1.98	0.44
13:M:140:VAL:HG23	37:M:8562:HOH:O	2.16	0.44
14:N:39:ARG:CZ	37:N:8627:HOH:O	2.64	0.44
15:O:167:ASP:O	15:O:168:LEU:HD23	2.18	0.44
15:O:58:LEU:CD1	15:O:58:LEU:N	2.80	0.44
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.53	0.44
24:X:125:HIS:HD2	24:X:127:GLY:H	1.65	0.44
1:A:111:C:H2'	1:A:112:G:O4'	2.18	0.44
1:A:1494:A:H1'	1:A:1495:C:C6	2.52	0.44
1:A:1515:A:H2'	1:A:1516:C:C6	2.53	0.44
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.44
1:A:1634:G:H2'	1:A:1635:U:C6	2.52	0.44
1:A:1746:A:N3	1:A:1748:U:C4	2.86	0.44
1:A:2505:G:H8	37:A:5613:HOH:O	2.01	0.44
1:A:2748:G:C2'	37:A:7524:HOH:O	2.46	0.44
1:A:64:G:H2'	1:A:65:C:O4'	2.18	0.44
1:A:912:A:C4	1:A:1294:A:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.83	0.44
6:F:101:THR:CG2	37:F:7400:HOH:O	2.62	0.44
6:F:173:GLU:HG3	6:F:174:VAL:N	2.33	0.44
10:J:71:TYR:O	10:J:73:GLN:N	2.51	0.44
14:N:159:THR:HA	37:N:8520:HOH:O	2.18	0.44
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.47	0.44
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.99	0.44
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.30	0.44
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.16	0.44
23:W:56:ILE:O	23:W:60:GLN:HG3	2.17	0.44
24:X:122:ARG:NH1	24:X:152:ALA:O	2.51	0.44
26:Z:117:LEU:HD12	26:Z:174:VAL:CG1	2.47	0.44
30:4:14:CYS:HB2	36:4:8404:CD:CD	1.69	0.43
1:A:47:G:N3	1:A:114:A:C2	2.86	0.43
1:A:1191:A:C3'	1:A:1192:A:H5''	2.44	0.43
1:A:2598:U:O2	1:A:2600:A:H8	2.01	0.43
2:B:3030:C:OP1	6:F:137:PRO:O	2.35	0.43
3:C:169:PHE:O	3:C:170:VAL:HB	2.18	0.43
4:D:76:THR:N	4:D:77:PRO:HD3	2.32	0.43
4:D:7:ARG:HD3	4:D:9:GLY:O	2.18	0.43
6:F:10:PHE:CD1	6:F:11:HIS:N	2.86	0.43
37:A:6876:HOH:O	7:G:157:LYS:HD3	2.17	0.43
11:K:130:VAL:CG1	11:K:131:THR:N	2.81	0.43
12:L:118:ALA:C	12:L:120:ARG:H	2.22	0.43
14:N:84:LYS:O	14:N:87:MET:HG2	2.18	0.43
1:A:21:G:H5''	19:S:1:GLY:O	2.18	0.43
1:A:12:U:H2'	1:A:13:G:H5'	1.99	0.43
1:A:219:G:O5'	1:A:220:C:H5''	2.17	0.43
1:A:2266:A:P	37:A:5834:HOH:O	2.76	0.43
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.43
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.17	0.43
7:G:108:LEU:HD11	7:G:164:ASP:HB2	2.00	0.43
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.00	0.43
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.82	0.43
13:M:125:PHE:CE1	13:M:140:VAL:HG13	2.54	0.43
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.99	0.43
1:A:588:G:O6	24:X:154:ARG:NH1	2.51	0.43
1:A:1116:U:H3	1:A:1246:A:N6	2.06	0.43
1:A:1135:G:H5'	37:A:5900:HOH:O	2.18	0.43
1:A:1159:G:P	37:A:4274:HOH:O	2.76	0.43
1:A:1188:A:C5	1:A:1189:A:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:C:H2'	1:A:1546:G:O4'	2.18	0.43
1:A:1739:G:O2'	1:A:1740:U:H5'	2.18	0.43
1:A:1805:G:H2'	1:A:1806:G:H8	1.83	0.43
1:A:2001:G:O2'	1:A:2002:C:H5'	2.18	0.43
1:A:2274:A:H1'	14:N:86:MET:SD	2.59	0.43
1:A:2443:C:H3'	37:A:3458:HOH:O	2.17	0.43
1:A:2467:A:O2'	1:A:2468:A:H2'	2.18	0.43
1:A:269:G:C2	1:A:270:U:O4	2.71	0.43
1:A:581:G:O2'	1:A:582:C:H5'	2.17	0.43
4:D:211:THR:HA	4:D:255:GLY:O	2.18	0.43
5:E:16:VAL:HG12	5:E:17:ASP:H	1.82	0.43
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.48	0.43
8:H:63:ILE:HB	8:H:64:PRO:CD	2.43	0.43
10:J:62:GLU:HA	37:J:8385:HOH:O	2.18	0.43
13:M:7:GLN:HB3	13:M:13:HIS:CE1	2.53	0.43
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.53	0.43
37:A:3746:HOH:O	21:U:9:LYS:HD3	2.17	0.43
26:Z:185:VAL:HG12	37:Z:8569:HOH:O	2.17	0.43
1:A:2613:G:O2'	1:A:2614:C:H5'	2.19	0.43
1:A:553:G:H5'	37:A:3483:HOH:O	2.18	0.43
1:A:921:G:H4'	1:A:924:G:N1	2.34	0.43
4:D:204:GLY:C	37:D:8652:HOH:O	2.56	0.43
4:D:279:THR:CG2	4:D:280:VAL:N	2.81	0.43
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.53	0.43
5:E:129:HIS:HD2	5:E:165:ASP:OD2	2.01	0.43
11:K:54:VAL:HG11	11:K:138:THR:HG21	2.00	0.43
11:K:77:GLY:O	11:K:78:ILE:C	2.57	0.43
12:L:87:ARG:NH1	37:L:4066:HOH:O	2.51	0.43
21:U:96:VAL:CG1	21:U:97:ARG:N	2.82	0.43
27:1:38:LYS:HD3	37:1:8424:HOH:O	2.17	0.43
1:A:1391:G:H2'	1:A:1392:A:H5'	2.01	0.43
1:A:2120:U:H2'	1:A:2121:G:O4'	2.19	0.43
1:A:2241:C:H2'	1:A:2242:U:C6	2.53	0.43
2:B:3031:C:H1'	37:B:8392:HOH:O	2.19	0.43
2:B:3012:C:H5'	2:B:3070:U:O4'	2.19	0.43
4:D:154:VAL:HA	4:D:155:PRO:HD3	1.85	0.43
5:E:246:ARG:CZ	37:E:8423:HOH:O	2.66	0.43
6:F:95:THR:C	6:F:97:GLN:N	2.69	0.43
7:G:18:LEU:HD13	7:G:34:TRP:CD1	2.54	0.43
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.53	0.43
15:O:37:ARG:HA	15:O:37:ARG:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4339:HOH:O	16:P:37:ARG:HG3	2.18	0.43
21:U:38:ARG:NH1	21:U:38:ARG:HG3	2.33	0.43
24:X:4:LEU:HD21	24:X:52:VAL:HG11	1.99	0.43
26:Z:163:THR:HG23	37:Z:8530:HOH:O	2.17	0.43
27:1:77:LYS:HA	27:1:80:MET:CE	2.48	0.43
1:A:165:A:H2'	1:A:166:A:OP1	2.19	0.43
1:A:289:G:O2'	1:A:290:C:H5'	2.18	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
1:A:338:C:H4'	5:E:174:ILE:HD12	2.00	0.43
2:B:3036:C:C5	2:B:3037:C:C5	3.07	0.43
5:E:178:GLN:C	5:E:180:SER:N	2.70	0.43
6:F:55:LYS:O	6:F:56:ARG:HB2	2.19	0.43
6:F:49:PRO:HA	6:F:73:VAL:HG22	2.00	0.43
7:G:162:PHE:CD1	7:G:162:PHE:N	2.86	0.43
7:G:24:GLY:HA3	7:G:76:VAL:HB	2.01	0.43
8:H:21:GLU:HA	8:H:24:ARG:HE	1.83	0.43
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.66	0.43
21:U:48:VAL:HG22	21:U:97:ARG:C	2.39	0.43
3:C:75:GLY:HA2	27:1:63:LYS:O	2.19	0.43
30:4:91:GLN:O	30:4:92:GLU:HB2	2.18	0.43
1:A:1592:G:O2'	1:A:1593:C:O5'	2.37	0.43
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.43
1:A:37:A:H2'	1:A:38:G:C8	2.53	0.43
1:A:602:A:O2'	1:A:605:C:H4'	2.18	0.43
1:A:790:A:H2'	1:A:791:A:O4'	2.19	0.43
3:C:36:ASP:O	3:C:37:VAL:C	2.56	0.43
6:F:140:ARG:O	6:F:144:ARG:HG2	2.18	0.43
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.01	0.43
10:J:84:ARG:NH2	10:J:135:TRP:CH2	2.82	0.43
15:O:43:VAL:HG11	15:O:81:ALA:HA	2.01	0.43
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.49	0.43
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.83	0.43
23:W:55:ARG:O	23:W:59:ILE:HG12	2.19	0.43
24:X:65:VAL:CA	24:X:68:THR:HG22	2.48	0.43
1:A:1119:G:N2	1:A:1246:A:H2	2.10	0.43
1:A:155:C:OP2	14:N:188:ARG:HD3	2.19	0.43
1:A:2064:U:H2'	1:A:2065:C:H6	1.83	0.43
7:G:81:GLU:HG2	7:G:134:SER:CB	2.49	0.43
10:J:84:ARG:CZ	10:J:135:TRP:CH2	3.02	0.43
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.19	0.43
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2468:A:N6	30:4:48:ASN:HD21	2.00	0.43
1:A:1624:A:H5'	1:A:1626:A:O4'	2.19	0.43
1:A:1733:A:H4'	4:D:212:GLN:HA	2.00	0.43
1:A:2428:G:N7	37:A:3770:HOH:O	2.50	0.43
1:A:2697:A:H2'	1:A:2698:G:O4'	2.18	0.43
1:A:886:A:OP2	1:A:2113:G:H5'	2.19	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.53	0.43
1:A:1852:A:H4'	3:C:230:SER:HB2	2.01	0.43
4:D:27:ASN:HB3	37:D:8628:HOH:O	2.18	0.43
7:G:133:VAL:HG12	7:G:141:VAL:HG13	2.01	0.43
12:L:101:ASN:O	12:L:102:GLU:HB2	2.19	0.43
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.49	0.43
14:N:69:LYS:HG2	14:N:127:LYS:HG3	2.01	0.43
1:A:251:C:H1'	14:N:58:GLN:HE22	1.82	0.43
2:B:3006:C:P	15:O:37:ARG:NH1	2.92	0.43
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.18	0.43
1:A:97:G:C2	21:U:107:LYS:HD2	2.53	0.43
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.65	0.43
26:Z:116:LEU:HD23	26:Z:116:LEU:HA	1.81	0.43
27:1:57:CYS:SG	27:1:59:HIS:HB3	2.58	0.43
28:2:19:CYS:SG	28:2:21:ARG:N	2.92	0.43
29:3:40:ARG:HA	29:3:45:ASN:ND2	2.33	0.43
1:A:907:A:H4'	1:A:1328:A:C2	2.54	0.43
1:A:1603:A:H5'	1:A:1605:G:C4'	2.48	0.43
1:A:1730:G:H5'	1:A:1731:C:H5	1.81	0.43
1:A:1857:A:N6	1:A:2247:C:H1'	2.34	0.43
1:A:2577:A:H5'	37:A:7738:HOH:O	2.19	0.43
2:B:3056:A:C3'	2:B:3057:A:H5''	2.49	0.43
2:B:3078:G:O2'	2:B:3079:U:P	2.77	0.43
6:F:19:GLU:O	6:F:133:ASN:HB3	2.19	0.43
14:N:94:LYS:HD2	37:N:8648:HOH:O	2.19	0.43
19:S:17:MET:CE	19:S:19:ARG:NH2	2.81	0.43
1:A:1752:G:H2'	37:A:7531:HOH:O	2.19	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	3.07	0.42
1:A:87:C:H2'	29:3:28:LYS:O	2.19	0.42
1:A:929:A:O5'	1:A:929:A:H8	2.02	0.42
4:D:14:GLY:HA2	4:D:15:PRO:C	2.38	0.42
5:E:166:ILE:CD1	5:E:207:LEU:HD13	2.49	0.42
7:G:95:VAL:O	7:G:126:ILE:HD13	2.18	0.42
10:J:113:ALA:N	10:J:114:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.31	0.42
10:J:48:LEU:CG	10:J:157:ILE:HG21	2.47	0.42
13:M:29:GLY:HA3	13:M:33:ALA:HB3	2.00	0.42
15:O:127:LEU:HA	15:O:127:LEU:HD12	1.77	0.42
15:O:19:ASP:OD1	15:O:19:ASP:C	2.57	0.42
16:P:115:ARG:NH1	37:P:6194:HOH:O	2.52	0.42
1:A:1718:G:OP2	17:Q:20:ARG:HD2	2.18	0.42
19:S:33:ARG:NH2	37:S:8531:HOH:O	2.42	0.42
23:W:42:ASN:O	23:W:44:GLY:N	2.52	0.42
25:Y:30:MET:HE1	25:Y:55:ASN:HA	2.00	0.42
1:A:1052:G:N3	1:A:1052:G:H2'	2.34	0.42
1:A:1123:A:N1	1:A:1238:C:H5'	2.34	0.42
1:A:1298:U:H2'	1:A:1299:G:C8	2.54	0.42
1:A:2478:U:O2'	1:A:2479:A:H5'	2.18	0.42
1:A:2481:G:C3'	1:A:2482:G:H5''	2.49	0.42
1:A:306:A:P	21:U:38:ARG:HH21	2.42	0.42
1:A:695:C:H2'	1:A:696:C:C6	2.53	0.42
2:B:3064:C:C2'	2:B:3065:A:H5'	2.49	0.42
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.35	0.42
1:A:474:C:O3'	5:E:73:LEU:CD2	2.67	0.42
9:I:71:LEU:C	9:I:73:ASP:H	2.22	0.42
10:J:149:ALA:C	10:J:151:MET:H	2.22	0.42
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.86	0.42
15:O:11:ARG:NH2	37:O:8520:HOH:O	2.53	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.47	0.42
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.23	0.42
23:W:11:MET:HB3	23:W:15:GLU:HB2	2.00	0.42
26:Z:144:ARG:NH1	37:Z:8575:HOH:O	2.46	0.42
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.98	0.42
1:A:1168:C:H5	37:A:7478:HOH:O	2.02	0.42
1:A:1191:A:N1	1:A:1206:U:O4	2.52	0.42
1:A:1311:G:C2	1:A:1312:G:C8	3.07	0.42
1:A:1324:G:C2	1:A:1334:C:O2	2.73	0.42
1:A:1657:A:H2'	1:A:1658:A:C8	2.54	0.42
1:A:1754:A:H2'	1:A:1755:A:O4'	2.20	0.42
1:A:2541:U:H5'	1:A:2611:G:O6	2.19	0.42
1:A:702:G:O2'	1:A:703:G:H5'	2.19	0.42
2:B:3078:G:O2'	2:B:3079:U:OP2	2.37	0.42
2:B:3092:G:H22	10:J:52:LYS:HZ3	1.67	0.42
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.94	0.42
10:J:29:ALA:HB3	10:J:65:ARG:NH1	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:VAL:HG12	11:K:26:VAL:O	2.18	0.42
13:M:146:GLY:C	13:M:148:GLU:H	2.23	0.42
37:A:3742:HOH:O	14:N:108:LYS:HD2	2.19	0.42
14:N:69:LYS:HD3	14:N:125:ARG:HA	2.01	0.42
15:O:62:HIS:O	15:O:65:ASP:OD1	2.37	0.42
23:W:1:THR:HG23	23:W:2:VAL:N	2.25	0.42
3:C:170:VAL:HG22	27:1:22:ILE:HG23	2.00	0.42
1:A:1044:C:H3'	1:A:1045:G:H5''	2.01	0.42
1:A:1189:A:N3	37:A:7667:HOH:O	2.51	0.42
1:A:1420:C:C2	1:A:1445:G:N2	2.88	0.42
1:A:1523:G:C6	1:A:1524:U:O4	2.72	0.42
1:A:1667:A:H2'	1:A:1668:U:H6	1.83	0.42
1:A:1730:G:H4'	1:A:1731:C:O5'	2.19	0.42
1:A:2820:A:H2'	1:A:2821:C:C6	2.55	0.42
1:A:88:G:H2'	1:A:89:G:C8	2.54	0.42
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.87	0.42
3:C:97:ALA:HB2	3:C:150:PRO:HB2	2.01	0.42
6:F:173:GLU:O	6:F:174:VAL:C	2.57	0.42
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.49	0.42
10:J:136:VAL:HA	37:J:8343:HOH:O	2.18	0.42
13:M:117:GLU:HG3	37:M:8566:HOH:O	2.19	0.42
1:A:1299:G:N7	13:M:6:ARG:NH1	2.68	0.42
14:N:173:LEU:HD23	14:N:183:VAL:CG1	2.48	0.42
21:U:41:ARG:O	21:U:43:ASN:ND2	2.53	0.42
21:U:55:PHE:HB2	37:U:6384:HOH:O	2.19	0.42
22:V:11:THR:HG23	37:V:6796:HOH:O	2.19	0.42
25:Y:34:ARG:NH1	25:Y:48:VAL:O	2.46	0.42
26:Z:205:ILE:O	26:Z:206:ALA:C	2.58	0.42
27:1:38:LYS:HG2	37:1:8409:HOH:O	2.19	0.42
3:C:72:GLU:OE1	27:1:72:GLU:HA	2.20	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:1562:C:H42	1:A:2738:G:H1	1.66	0.42
1:A:2842:G:H2'	1:A:2843:A:H5'	2.01	0.42
1:A:2667:G:H1'	1:A:2914:A:N3	2.33	0.42
1:A:883:U:H2'	1:A:883:U:O2	2.19	0.42
3:C:34:ASP:OD1	3:C:35:GLY:N	2.49	0.42
4:D:41:PHE:CG	4:D:190:MET:HE3	2.54	0.42
5:E:20:ASP:O	5:E:23:GLU:HB2	2.20	0.42
11:K:131:THR:HB	11:K:134:GLU:HG3	2.01	0.42
14:N:78:ASN:C	14:N:79:LYS:HG2	2.40	0.42
15:O:163:PHE:O	15:O:164:ASP:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:71:TRP:N	37:O:8538:HOH:O	2.51	0.42
19:S:114:VAL:O	19:S:114:VAL:HG13	2.19	0.42
20:T:33:SER:OG	20:T:36:GLU:HG3	2.18	0.42
25:Y:20:GLU:CG	25:Y:21:PRO:HD2	2.49	0.42
37:A:6483:HOH:O	29:3:1:GLY:HA3	2.19	0.42
1:A:1185:U:C5'	37:A:7447:HOH:O	2.65	0.42
1:A:1593:C:OP1	17:Q:117:SER:CB	2.68	0.42
1:A:187:A:H3'	1:A:188:C:H6	1.84	0.42
1:A:2634:G:O2'	1:A:2635:A:H5'	2.19	0.42
1:A:2729:C:H2'	1:A:2730:G:H8	1.84	0.42
1:A:295:C:H2'	1:A:296:G:O4'	2.20	0.42
1:A:396:U:O2'	1:A:418:C:H4'	2.19	0.42
1:A:401:C:C5'	37:A:5769:HOH:O	2.68	0.42
1:A:711:G:C2	1:A:718:C:C2	3.08	0.42
2:B:3041:C:H4'	6:F:48:MET:HB2	2.01	0.42
2:B:3091:C:H2'	2:B:3092:G:O4'	2.19	0.42
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.48	0.42
3:C:105:VAL:CG1	3:C:106:CYS:N	2.82	0.42
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.50	0.42
3:C:55:VAL:HG11	3:C:67:LEU:HD13	2.02	0.42
6:F:84:LEU:HA	6:F:87:ALA:HB3	2.02	0.42
7:G:31:ARG:CZ	37:G:5919:HOH:O	2.67	0.42
10:J:72:VAL:O	10:J:72:VAL:HG13	2.18	0.42
10:J:83:PHE:HE1	10:J:146:TRP:CZ2	2.38	0.42
1:A:1003:U:O2	10:J:90:PHE:CZ	2.73	0.42
1:A:2453:G:H4'	13:M:50:GLY:C	2.40	0.42
14:N:115:LEU:HD13	14:N:116:ASN:HB2	2.02	0.42
21:U:28:SER:O	21:U:32:ARG:HG3	2.19	0.42
27:1:32:LYS:HZ2	27:1:70:GLN:NE2	2.18	0.42
1:A:128:A:O2'	1:A:129:A:H5'	2.19	0.42
1:A:1806:G:C6	1:A:1807:U:C4	3.08	0.42
1:A:2314:G:H2'	1:A:2315:C:H5'	2.01	0.42
1:A:2588:G:H3'	1:A:2589:U:H5"	2.01	0.42
1:A:2589:U:H2'	1:A:2590:U:C6	2.55	0.42
1:A:821:U:H2'	1:A:822:C:C6	2.52	0.42
1:A:2637:A:H62	31:A:9001:BLS:H5	1.84	0.42
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.03	0.42
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.54	0.42
20:T:8:PRO:HD2	23:W:32:ALA:HA	2.02	0.42
25:Y:20:GLU:CD	25:Y:21:PRO:HD2	2.39	0.42
1:A:1015:C:H6	1:A:1015:C:O5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:U:H2'	1:A:1219:U:C6	2.55	0.42
1:A:1609:C:H2'	1:A:1610:G:H8	1.84	0.42
1:A:1983:C:H6	1:A:1983:C:O5'	2.03	0.42
1:A:422:G:C6	1:A:2446:G:C6	3.07	0.42
1:A:2782:G:O6	1:A:2790:C:H5''	2.19	0.42
1:A:764:C:H2'	1:A:765:G:O4'	2.20	0.42
2:B:3065:A:O2'	2:B:3066:G:P	2.77	0.42
2:B:3107:C:H2'	2:B:3108:C:C6	2.54	0.42
3:C:191:GLY:HA2	3:C:194:MET:HE1	2.00	0.42
4:D:185:GLY:HA2	37:D:8633:HOH:O	2.20	0.42
4:D:24:PRO:HG2	4:D:204:GLY:HA2	2.01	0.42
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.80	0.42
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.85	0.42
7:G:32:ARG:O	7:G:33:LEU:HD23	2.19	0.42
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.20	0.42
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.83	0.42
16:P:41:ALA:N	37:P:3240:HOH:O	2.52	0.42
17:Q:109:ARG:NH1	17:Q:119:TYR:CE2	2.87	0.42
18:R:16:ASN:HA	18:R:16:ASN:HD22	1.64	0.42
19:S:9:ASP:HA	19:S:10:PRO:HD2	1.89	0.42
24:X:151:GLU:O	24:X:154:ARG:HB3	2.19	0.42
28:2:17:THR:N	28:2:27:TYR:O	2.46	0.42
1:A:101:C:H2'	1:A:102:A:H8	1.85	0.42
1:A:1158:G:O2'	1:A:1159:G:H5'	2.20	0.42
1:A:155:C:O2'	1:A:156:C:H5'	2.20	0.42
1:A:2408:A:O2'	30:4:16:GLU:HA	2.18	0.42
3:C:36:ASP:HB2	3:C:85:ASP:H	1.85	0.42
4:D:277:GLU:N	4:D:278:PRO:HD2	2.35	0.42
5:E:214:THR:O	5:E:214:THR:HG22	2.20	0.42
7:G:35:TYR:HA	11:K:127:ILE:HD12	2.02	0.42
15:O:114:LYS:O	15:O:118:ILE:HG13	2.20	0.42
16:P:59:VAL:HG23	16:P:111:VAL:HG23	2.01	0.42
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.84	0.42
27:1:33:HIS:HE1	27:1:49:ARG:NE	2.18	0.42
1:A:1057:A:C6	1:A:1058:A:C6	3.08	0.42
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.42
1:A:2016:U:H6	1:A:2016:U:O5'	2.02	0.42
1:A:2404:G:OP1	18:R:69:ASP:N	2.47	0.42
1:A:2478:U:H2'	1:A:2479:A:C8	2.55	0.42
1:A:65:C:O2'	1:A:66:G:H5'	2.20	0.42
11:K:79:PHE:O	11:K:83:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:A:C5'	14:N:157:LEU:HD12	2.49	0.42
15:O:138:ASP:O	15:O:140:GLN:N	2.51	0.42
1:A:2403:C:O2	18:R:67:GLN:NE2	2.53	0.42
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.53	0.42
23:W:39:ALA:C	23:W:41:GLU:N	2.73	0.42
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.19	0.42
28:2:2:GLY:O	28:2:6:PRO:HG2	2.20	0.41
1:A:1684:A:C1'	29:3:43:ARG:HH22	2.26	0.41
1:A:1125:U:H2'	1:A:1126:C:H5'	2.02	0.41
1:A:1268:C:H2'	1:A:1269:G:H8	1.84	0.41
1:A:2004:U:H2'	1:A:2005:G:OP1	2.19	0.41
1:A:2073:G:C6	1:A:2607:U:C2	3.07	0.41
1:A:236:A:H2'	1:A:236:A:O5'	2.19	0.41
1:A:2781:U:O2'	1:A:2782:G:H5'	2.20	0.41
1:A:2812:A:C2	1:A:2814:A:N6	2.77	0.41
1:A:496:G:C6	1:A:498:A:C6	3.08	0.41
2:B:3003:A:H2	2:B:3021:G:N3	2.18	0.41
3:C:35:GLY:O	3:C:36:ASP:CB	2.61	0.41
5:E:102:LEU:HD12	37:E:8316:HOH:O	2.19	0.41
5:E:127:ARG:HD2	5:E:229:PRO:O	2.19	0.41
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.50	0.41
10:J:26:LYS:HD2	10:J:28:ILE:HB	2.02	0.41
11:K:79:PHE:HB3	11:K:103:VAL:HG11	2.02	0.41
11:K:39:VAL:HG11	11:K:107:ASN:HB2	2.01	0.41
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.02	0.41
16:P:44:ASN:HA	16:P:65:LEU:O	2.20	0.41
24:X:21:LEU:HB3	24:X:26:ILE:CG1	2.50	0.41
27:1:56:MET:HA	27:1:62:TYR:O	2.20	0.41
29:3:49:GLU:CD	37:3:719:HOH:O	2.57	0.41
1:A:1269:G:H2'	1:A:1270:U:H6	1.85	0.41
1:A:202:U:O2'	1:A:203:G:H5'	2.20	0.41
1:A:542:A:H1'	37:A:4652:HOH:O	2.20	0.41
2:B:3105:A:H2'	2:B:3106:C:O4'	2.20	0.41
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.34	0.41
5:E:166:ILE:HD11	5:E:207:LEU:HD13	2.02	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
10:J:113:ALA:N	10:J:114:PRO:HD3	2.34	0.41
12:L:98:VAL:HG22	12:L:102:GLU:C	2.40	0.41
1:A:154:C:H3'	14:N:188:ARG:NH1	2.34	0.41
21:U:19:ARG:NH1	21:U:68:ASP:O	2.53	0.41
23:W:55:ARG:CZ	37:W:4428:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:15:ASN:ND2	37:4:8552:HOH:O	2.52	0.41
1:A:1616:A:H5''	1:A:1617:C:OP1	2.20	0.41
1:A:1878:G:C4'	37:A:6094:HOH:O	2.69	0.41
1:A:1947:G:N2	1:A:1966:U:C2	2.88	0.41
1:A:2434:A:H2'	1:A:2435:U:H6	1.85	0.41
1:A:2687:G:O2'	1:A:2688:U:H5'	2.20	0.41
1:A:854:G:C8	37:A:3964:HOH:O	2.71	0.41
4:D:60:SER:C	4:D:62:ARG:H	2.22	0.41
4:D:91:PRO:O	11:K:144:THR:HG21	2.20	0.41
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.92	0.41
5:E:142:ASP:OD2	5:E:238:SER:OG	2.34	0.41
6:F:168:SER:O	6:F:168:SER:OG	2.35	0.41
6:F:15:GLU:HA	6:F:16:PRO:HD3	1.87	0.41
6:F:35:ALA:C	6:F:37:ALA:N	2.74	0.41
7:G:154:ILE:HG13	7:G:156:ASP:OD1	2.19	0.41
1:A:171:C:OP2	14:N:84:LYS:HG3	2.20	0.41
15:O:34:LEU:HA	15:O:47:LEU:CD2	2.51	0.41
16:P:26:TRP:HA	16:P:26:TRP:HE3	1.84	0.41
24:X:75:GLY:HA3	37:X:5763:HOH:O	2.21	0.41
1:A:1225:C:H4'	37:A:9386:HOH:O	2.19	0.41
1:A:1973:A:H8	1:A:1973:A:H5'	1.84	0.41
1:A:2064:U:H2'	1:A:2065:C:C6	2.56	0.41
1:A:2079:G:H2'	1:A:2080:G:O4'	2.21	0.41
1:A:2084:C:H2'	1:A:2085:A:C8	2.55	0.41
1:A:2255:A:H2'	1:A:2256:G:O4'	2.20	0.41
1:A:2289:G:C2	1:A:2309:C:N4	2.89	0.41
1:A:2415:A:N3	15:O:26:LEU:HD13	2.36	0.41
1:A:319:A:H4'	1:A:338:C:C4	2.55	0.41
5:E:153:VAL:O	5:E:157:LEU:HG	2.20	0.41
5:E:39:GLN:NE2	37:E:8465:HOH:O	2.53	0.41
18:R:21:ARG:NH2	37:R:5853:HOH:O	2.19	0.41
19:S:35:ILE:O	19:S:38:LYS:HB2	2.21	0.41
26:Z:101:GLY:HA3	37:Z:8560:HOH:O	2.19	0.41
1:A:1422:U:H2'	1:A:1423:C:H6	1.83	0.41
1:A:1682:A:H5''	37:A:9445:HOH:O	2.20	0.41
1:A:2265:U:H2'	1:A:2266:A:C8	2.56	0.41
1:A:1815:A:H4'	1:A:2751:C:O4'	2.21	0.41
1:A:400:C:O3'	37:A:5769:HOH:O	2.20	0.41
1:A:876:A:N3	1:A:876:A:H2'	2.35	0.41
5:E:13:ASP:OD1	5:E:13:ASP:O	2.38	0.41
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:GLU:C	6:F:62:ASP:N	2.73	0.41
7:G:11:VAL:HG11	7:G:22:VAL:HG13	2.02	0.41
8:H:32:GLY:N	37:H:3111:HOH:O	2.52	0.41
9:I:12:ILE:O	9:I:13:PRO:C	2.57	0.41
37:A:9880:HOH:O	11:K:46:ILE:HA	2.21	0.41
14:N:87:MET:H	14:N:87:MET:HG3	1.42	0.41
15:O:108:SER:HA	15:O:109:PRO:HD3	1.80	0.41
15:O:164:ASP:OD1	15:O:164:ASP:C	2.59	0.41
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.55	0.41
24:X:13:MET:O	24:X:14:HIS:C	2.59	0.41
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.35	0.41
30:4:34:LYS:N	30:4:34:LYS:HD2	2.36	0.41
1:A:1412:U:O4	1:A:1681:G:H2'	2.21	0.41
1:A:1733:A:C6	1:A:1734:C:C2	3.08	0.41
1:A:2346:C:H4'	6:F:52:THR:HG22	2.03	0.41
1:A:331:A:C6	1:A:332:G:C4	3.08	0.41
1:A:37:A:H2'	1:A:38:G:H8	1.86	0.41
1:A:382:U:C5	1:A:406:G:N2	2.88	0.41
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.41
1:A:963:C:H6	1:A:963:C:O5'	2.04	0.41
2:B:3025:G:C8	2:B:3026:C:H5'	2.56	0.41
2:B:3026:C:P	37:B:8442:HOH:O	2.78	0.41
3:C:36:ASP:O	3:C:38:ILE:N	2.53	0.41
6:F:128:LEU:N	37:F:3349:HOH:O	2.53	0.41
14:N:47:ASP:CG	14:N:48:ARG:N	2.73	0.41
15:O:175:LEU:HA	15:O:175:LEU:HD12	1.86	0.41
16:P:113:VAL:O	16:P:114:ILE:HD13	2.20	0.41
16:P:63:LYS:HG3	16:P:80:ASP:O	2.21	0.41
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.03	0.41
25:Y:43:VAL:HG12	25:Y:47:ALA:HB3	2.01	0.41
1:A:1162:G:H2'	1:A:1162:G:N3	2.35	0.41
1:A:1164:U:N3	1:A:1192:A:H2	2.10	0.41
1:A:1778:A:H2'	1:A:1779:A:H5'	2.02	0.41
1:A:1850:U:H2'	1:A:1851:G:H8	1.85	0.41
1:A:2262:C:H6	1:A:2262:C:O5'	2.04	0.41
1:A:2356:A:H2'	1:A:2357:G:O4'	2.20	0.41
1:A:2815:G:OP2	11:K:99:GLU:HG2	2.21	0.41
1:A:305:A:C5	1:A:329:A:C2	3.09	0.41
1:A:947:U:O2'	1:A:948:G:H5'	2.21	0.41
2:B:3031:C:O2'	2:B:3032:G:H5'	2.20	0.41
8:H:22:VAL:CG2	8:H:104:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:LYS:CD	10:J:28:ILE:HB	2.51	0.41
14:N:68:ARG:HG2	14:N:68:ARG:O	2.17	0.41
16:P:25:VAL:HG23	16:P:26:TRP:H	1.85	0.41
19:S:39:THR:HG22	19:S:41:GLY:N	2.36	0.41
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.66	0.41
27:1:61:GLY:HA3	37:1:8425:HOH:O	2.20	0.41
28:2:25:LYS:HG3	29:3:49:GLU:H	1.85	0.41
30:4:48:ASN:ND2	30:4:50:GLY:H	2.19	0.41
1:A:135:G:OP1	14:N:39:ARG:NH1	2.52	0.41
1:A:1407:A:O2'	1:A:1408:U:H3'	2.21	0.41
1:A:1641:A:C2'	1:A:1642:A:H5'	2.50	0.41
1:A:1675:C:O2'	1:A:1676:G:H5'	2.21	0.41
1:A:2102:G:N2	1:A:2103:A:C6	2.89	0.41
1:A:2656:G:C2'	1:A:2657:G:H5'	2.50	0.41
1:A:383:A:OP2	37:A:9758:HOH:O	2.22	0.41
1:A:585:C:H6	37:A:6068:HOH:O	2.03	0.41
1:A:657:G:H2'	1:A:658:C:H6	1.85	0.41
3:C:99:ILE:O	3:C:131:HIS:HE1	2.03	0.41
5:E:3:ALA:HA	37:E:8450:HOH:O	2.20	0.41
9:I:63:ARG:N	37:I:2569:HOH:O	2.54	0.41
10:J:95:GLU:HB3	10:J:119:VAL:HG11	2.03	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.89	0.41
13:M:61:ALA:HA	37:M:8569:HOH:O	2.21	0.41
14:N:164:THR:HB	37:N:8520:HOH:O	2.20	0.41
14:N:86:MET:CE	14:N:86:MET:CG	2.95	0.41
21:U:41:ARG:HG2	21:U:41:ARG:NH1	2.36	0.41
21:U:96:VAL:HG13	21:U:97:ARG:N	2.35	0.41
24:X:131:PRO:O	24:X:136:GLY:N	2.50	0.41
24:X:6:GLN:HA	24:X:52:VAL:HG23	2.02	0.41
1:A:1041:U:H4'	1:A:1295:G:H5'	2.03	0.41
1:A:134:U:O2	1:A:145:A:C2	2.73	0.41
1:A:1637:A:H2'	1:A:1638:U:C6	2.56	0.41
1:A:1762:C:O2'	1:A:1763:C:H5'	2.21	0.41
1:A:2293:G:C5	1:A:2294:C:C5	3.09	0.41
1:A:2407:G:O2'	1:A:2408:A:H5'	2.21	0.41
1:A:2529:G:O2'	1:A:2530:C:H5'	2.20	0.41
1:A:2791:U:H4'	1:A:2792:A:OP1	2.21	0.41
1:A:2821:C:H4'	4:D:116:PRO:CB	2.51	0.41
1:A:333:G:O2'	1:A:334:G:H5'	2.21	0.41
1:A:945:U:H2'	1:A:946:C:C6	2.56	0.41
3:C:130:THR:HG22	3:C:131:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.20	0.41
3:C:212:PRO:HB2	37:C:8562:HOH:O	2.21	0.41
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.53	0.41
14:N:61:ILE:N	14:N:61:ILE:CD1	2.82	0.41
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.36	0.41
15:O:15:GLU:HB2	15:O:17:ARG:HG3	2.02	0.41
17:Q:115:SER:C	17:Q:117:SER:N	2.74	0.41
17:Q:16:VAL:HG12	17:Q:20:ARG:HB2	2.02	0.41
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.21	0.41
24:X:107:LEU:O	24:X:112:LEU:HB2	2.21	0.41
24:X:119:HIS:CD2	24:X:120:PRO:HD2	2.56	0.41
1:A:1025:C:H5'	24:X:23:MET:O	2.20	0.41
1:A:1044:C:H5''	37:A:9025:HOH:O	2.20	0.41
1:A:1060:C:H2'	1:A:1061:C:H6	1.86	0.41
1:A:1182:C:H1'	1:A:1192:A:C8	2.53	0.41
1:A:1236:A:H2'	1:A:1237:U:O4'	2.21	0.41
1:A:1242:A:OP2	11:K:60:ARG:NH2	2.49	0.41
1:A:1588:G:C6	1:A:1589:G:C6	3.09	0.41
1:A:2061:C:H2'	1:A:2062:A:O4'	2.21	0.41
1:A:2434:A:O3'	30:4:28:GLY:CA	2.68	0.41
1:A:2718:C:C6	1:A:2718:C:H5'	2.52	0.41
3:C:110:SER:N	3:C:114:ASP:OD2	2.54	0.41
4:D:79:MET:HE1	37:D:8625:HOH:O	2.20	0.41
5:E:16:VAL:CG1	5:E:17:ASP:N	2.82	0.41
5:E:25:PRO:HD2	37:E:8427:HOH:O	2.21	0.41
1:A:447:A:O2'	5:E:44:GLN:OE1	2.29	0.41
6:F:170:TYR:N	6:F:170:TYR:CD1	2.89	0.41
6:F:59:GLY:O	6:F:61:PHE:N	2.44	0.41
8:H:1:PRO:H3	8:H:4:VAL:CG2	2.34	0.41
10:J:129:ASN:N	10:J:129:ASN:HD22	2.17	0.41
15:O:110:THR:HA	15:O:111:PRO:HD3	1.93	0.41
15:O:159:TYR:CE2	15:O:163:PHE:HE2	2.37	0.41
23:W:27:LEU:CA	23:W:49:LEU:HD13	2.51	0.41
37:A:7652:HOH:O	26:Z:172:THR:HB	2.20	0.41
1:A:1175:G:H1'	1:A:1193:A:H2'	2.03	0.41
1:A:130:C:O2'	1:A:131:A:N7	2.52	0.41
1:A:1463:A:H2'	1:A:1464:U:C6	2.56	0.41
1:A:177:A:H2'	1:A:178:U:O4'	2.21	0.41
1:A:1804:A:H2'	1:A:1805:G:C8	2.56	0.41
1:A:1943:C:O4'	3:C:212:PRO:HA	2.20	0.41
1:A:195:C:H2'	1:A:196:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:C:H2'	1:A:292:G:O4'	2.21	0.41
1:A:603:A:H4'	1:A:604:G:O5'	2.20	0.41
4:D:16:ARG:NE	37:D:8553:HOH:O	2.33	0.41
7:G:101:GLU:OE2	7:G:115:ARG:HD3	2.21	0.41
13:M:77:ALA:HB3	37:M:8533:HOH:O	2.20	0.41
37:A:7204:HOH:O	14:N:13:LYS:HE2	2.21	0.41
14:N:98:GLN:O	14:N:102:GLU:HG3	2.21	0.41
14:N:99:ARG:HD2	14:N:167:GLY:HA2	2.02	0.41
15:O:47:LEU:HA	15:O:47:LEU:HD23	1.78	0.41
17:Q:143:ALA:CA	37:Q:190:HOH:O	2.69	0.41
17:Q:24:ASN:HA	17:Q:25:PRO:HD3	1.95	0.41
20:T:73:ASP:OD1	20:T:76:GLU:HG3	2.21	0.41
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.20	0.41
24:X:38:THR:CB	37:X:5390:HOH:O	2.68	0.41
1:A:1245:C:O5'	1:A:1245:C:H6	2.04	0.40
1:A:1308:A:H5'	37:A:6908:HOH:O	2.21	0.40
1:A:2252:A:C5	1:A:2253:G:H1'	2.56	0.40
1:A:2269:C:C2'	1:A:2270:G:H5'	2.51	0.40
1:A:795:G:N3	1:A:817:G:C2	2.89	0.40
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.54	0.40
3:C:194:MET:HE3	3:C:199:HIS:HB2	2.03	0.40
4:D:144:THR:CG2	4:D:145:HIS:N	2.84	0.40
1:A:1306:U:OP1	5:E:179:GLY:HA3	2.20	0.40
5:E:1:MET:HG2	5:E:2:GLN:N	2.33	0.40
10:J:83:PHE:HD1	10:J:134:ALA:HB2	1.86	0.40
12:L:101:ASN:O	12:L:102:GLU:CB	2.69	0.40
13:M:89:PHE:CD1	13:M:89:PHE:N	2.89	0.40
15:O:116:PHE:HB2	37:O:8558:HOH:O	2.21	0.40
1:A:2353:A:O2'	15:O:7:LYS:HB3	2.21	0.40
19:S:25:PHE:CE2	19:S:29:LYS:CE	3.04	0.40
24:X:65:VAL:HG12	24:X:116:LEU:HD13	2.02	0.40
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.32	0.40
1:A:101:C:H2'	1:A:102:A:C8	2.56	0.40
1:A:2255:A:C6	1:A:2256:G:C5	3.09	0.40
1:A:2297:U:H1'	37:A:5155:HOH:O	2.22	0.40
1:A:432:G:O2'	1:A:433:C:H5'	2.21	0.40
1:A:513:A:N3	37:A:3649:HOH:O	2.36	0.40
1:A:639:A:C2	1:A:1363:G:C2	3.09	0.40
3:C:214:SER:HA	3:C:227:ASP:O	2.21	0.40
4:D:279:THR:HG22	4:D:280:VAL:N	2.35	0.40
5:E:46:TYR:CE1	5:E:92:PRO:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:ILE:CG2	7:G:45:ASP:O	2.68	0.40
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.03	0.40
10:J:30:GLN:H	10:J:65:ARG:NH1	2.19	0.40
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.50	0.40
23:W:45:ARG:C	23:W:47:LYS:N	2.75	0.40
1:A:622:G:P	26:Z:148:GLY:HA3	2.61	0.40
27:1:46:LYS:O	27:1:57:CYS:HA	2.21	0.40
29:3:30:ASP:O	29:3:31:GLU:HB2	2.20	0.40
1:A:120:A:H5'	28:2:20:ARG:HH21	1.86	0.40
1:A:165:A:C2'	1:A:166:A:OP1	2.70	0.40
1:A:2453:G:H5'	37:M:8546:HOH:O	2.21	0.40
1:A:812:A:H2'	1:A:813:C:C6	2.56	0.40
4:D:53:LEU:HD11	4:D:327:VAL:HG22	2.03	0.40
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.85	0.40
7:G:9:GLU:HG3	7:G:10:ASP:N	2.36	0.40
7:G:156:ASP:OD2	7:G:157:LYS:NZ	2.43	0.40
9:I:69:ARG:NH1	37:I:3513:HOH:O	2.54	0.40
14:N:23:LEU:O	14:N:26:HIS:HB2	2.21	0.40
8:H:38:LYS:NZ	14:N:3:SER:HA	2.36	0.40
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.55	0.40
1:A:2123:A:P	14:N:89:ASN:HD22	2.45	0.40
1:A:1307:A:H2'	1:A:1308:A:C8	2.56	0.40
1:A:1331:A:OP2	26:Z:142:SER:OG	2.28	0.40
1:A:133:U:H5'	1:A:1465:A:OP1	2.21	0.40
1:A:164:G:C6	1:A:165:A:C5	3.08	0.40
1:A:1825:U:O2'	1:A:1826:C:H5'	2.21	0.40
1:A:185:G:H4'	1:A:186:A:H4'	2.03	0.40
1:A:383:A:C2	1:A:407:A:C4	3.09	0.40
1:A:485:A:O2'	1:A:487:G:H5'	2.22	0.40
1:A:777:U:H4'	1:A:777:U:OP2	2.22	0.40
4:D:258:GLY:H	4:D:260:HIS:HE1	1.63	0.40
4:D:53:LEU:HD21	4:D:270:ILE:HD12	2.04	0.40
4:D:277:GLU:N	4:D:278:PRO:CD	2.84	0.40
5:E:93:LYS:O	5:E:98:ARG:NH2	2.54	0.40
8:H:58:GLU:CA	8:H:61:MET:HG3	2.49	0.40
14:N:58:GLN:HG3	37:N:8609:HOH:O	2.20	0.40
17:Q:38:GLU:OE1	17:Q:41:ARG:NH1	2.54	0.40
20:T:58:MET:SD	29:3:8:LYS:HE3	2.61	0.40
23:W:27:LEU:HA	23:W:49:LEU:HD13	2.03	0.40
1:A:1328:A:C8	26:Z:169:ARG:HD3	2.56	0.40
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:18:ASN:HD22	29:3:18:ASN:HA	1.58	0.40
29:3:44:ARG:HD3	29:3:44:ARG:HA	1.98	0.40
1:A:1041:U:H2'	1:A:1042:U:H5'	2.02	0.40
1:A:1211:G:O2'	1:A:1212:C:H5'	2.21	0.40
1:A:1246:A:H8	1:A:1246:A:H5'	1.87	0.40
1:A:1972:U:C2'	1:A:1973:A:H5'	2.49	0.40
1:A:2415:A:H2'	1:A:2416:G:H5'	2.03	0.40
1:A:2819:C:H2'	1:A:2820:A:C8	2.57	0.40
1:A:2909:G:O2'	1:A:2910:A:H5'	2.22	0.40
1:A:391:U:OP2	14:N:84:LYS:NZ	2.50	0.40
1:A:514:G:OP1	1:A:514:G:H2'	2.21	0.40
1:A:553:G:P	26:Z:204:ARG:NH2	2.92	0.40
1:A:696:C:O2'	1:A:697:G:H5'	2.22	0.40
3:C:186:TRP:CG	3:C:187:PRO:HA	2.57	0.40
6:F:41:LEU:O	6:F:44:ILE:HG22	2.21	0.40
13:M:145:LEU:O	13:M:145:LEU:HD23	2.21	0.40
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.37	0.40
16:P:96:VAL:HG12	16:P:97:SER:O	2.20	0.40
19:S:29:LYS:NZ	37:S:8539:HOH:O	2.54	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%)	204 (87%)	26 (11%)	5 (2%)	7	31
4	D	335/337 (99%)	305 (91%)	23 (7%)	7 (2%)	7	31
5	E	244/246 (99%)	225 (92%)	18 (7%)	1 (0%)	34	71
6	F	134/176 (76%)	97 (72%)	27 (20%)	10 (8%)	1	4
7	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	37
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	4	20
11	K	140/145 (97%)	129 (92%)	8 (6%)	3 (2%)	7	31
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	10	40
13	M	141/164 (86%)	121 (86%)	19 (14%)	1 (1%)	22	59
14	N	192/194 (99%)	172 (90%)	19 (10%)	1 (0%)	29	66
15	O	184/186 (99%)	166 (90%)	10 (5%)	8 (4%)	2	14
16	P	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
17	Q	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	22	59
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	48
19	S	148/154 (96%)	141 (95%)	7 (5%)	0	100	100
20	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
21	U	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	17	53
22	V	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	21
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	59
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	5	26
26	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	5	24
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6	30
All	All	3633/4235 (86%)	3323 (92%)	252 (7%)	58 (2%)	9	38

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA

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Mol	Chain	Res	Type
10	J	162	SER
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
3	C	34	ASP
3	C	132	ASP
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	20	LYS
6	F	36	ASN
10	J	164	ALA
11	K	5	GLU
11	K	7	ASP
11	K	143	LYS
15	O	162	ASP
15	O	167	ASP
23	W	43	PRO
27	1	81	LYS
30	4	57	GLY
4	D	184	ASP
5	E	8	LEU
6	F	171	ASP
10	J	40	PRO
10	J	138	PRO
12	L	119	GLN
14	N	140	ALA
15	O	68	GLU
15	O	181	ASP
17	Q	116	SER
24	X	77	ALA
25	Y	77	PHE
30	4	56	PRO
6	F	61	PHE
8	H	64	PRO
3	C	37	VAL
3	C	62	ASP
3	C	119	ALA
4	D	2	GLN
4	D	107	SER
4	D	185	GLY

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Mol	Chain	Res	Type
10	J	72	VAL
12	L	126	SER
21	U	53	GLY
25	Y	87	ALA
6	F	170	TYR
15	O	155	GLU
23	W	40	PRO
27	1	41	VAL
7	G	44	GLY
18	R	18	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	167 (93%)	12 (7%)	16	47
4	D	282/282 (100%)	261 (93%)	21 (7%)	13	42
5	E	193/193 (100%)	179 (93%)	14 (7%)	14	43
6	F	117/147 (80%)	107 (92%)	10 (8%)	10	36
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	77
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	29
11	K	118/121 (98%)	107 (91%)	11 (9%)	9	32
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	76
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	69
14	N	166/166 (100%)	157 (95%)	9 (5%)	22	56
15	O	149/149 (100%)	144 (97%)	5 (3%)	37	72
16	P	93/93 (100%)	90 (97%)	3 (3%)	39	73
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	76
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	102 (97%)	3 (3%)	42	75
22	V	44/52 (85%)	42 (96%)	2 (4%)	27	63
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	82
24	X	130/130 (100%)	121 (93%)	9 (7%)	15	46
25	Y	66/73 (90%)	61 (92%)	5 (8%)	13	41
26	Z	120/195 (62%)	113 (94%)	7 (6%)	20	53
27	1	56/56 (100%)	50 (89%)	6 (11%)	6	25
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
30	4	79/79 (100%)	74 (94%)	5 (6%)	18	49
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	22	57

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

Mol	Chain	Res	Type
3	C	3	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

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Mol	Chain	Res	Type
4	D	162	MET
4	D	190	MET
4	D	195	ARG
4	D	234	ARG
4	D	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	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	67	GLN
5	E	94	THR
5	E	101	ASP
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	50	VAL
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	54	ASP
7	G	102	VAL
7	G	164	ASP
8	H	12	LEU
10	J	1	LYS

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Mol	Chain	Res	Type
10	J	30	GLN
10	J	59	ASN
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	94	ARG
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN
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	48	ARG
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	127	LEU
15	O	128	ASP
15	O	152	GLU

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Mol	Chain	Res	Type
15	O	163	PHE
16	P	3	THR
16	P	28	ASP
16	P	111	VAL
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	132	ARG
21	U	39	ASN
21	U	48	VAL
21	U	73	HIS
22	V	9	CYS
22	V	32	CYS
23	W	65	ASP
24	X	4	LEU
24	X	35	VAL
24	X	42	ARG
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	44	ASP
25	Y	52	PRO
25	Y	72	VAL
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	186	ARG
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL

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Mol	Chain	Res	Type
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	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	177	HIS
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	221	GLN
4	D	238	ASN
4	D	256	GLN
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	85	GLN
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	143	GLN
9	I	17	GLN
9	I	64	ASN
10	J	35	ASN
10	J	55	GLN
10	J	58	HIS

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Mol	Chain	Res	Type
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
11	K	126	ASN
12	L	10	GLN
13	M	18	HIS
13	M	41	HIS
13	M	42	ASN
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	153	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
20	T	9	HIS
20	T	53	ASN
21	U	39	ASN
21	U	73	HIS
22	V	39	ASN
23	W	60	GLN
24	X	12	ASN
24	X	27	HIS
24	X	28	HIS
24	X	87	HIS

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Mol	Chain	Res	Type
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
27	1	70	GLN
28	2	8	GLN
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	30	GLN
30	4	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	243 (8%)	36 (1%)
2	B	121/122 (99%)	18 (14%)	6 (4%)
All	All	2868/3044 (94%)	261 (9%)	42 (1%)

All (261) 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

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Mol	Chain	Res	Type
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	219	G
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	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

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Mol	Chain	Res	Type
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	705	C
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
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	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

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Mol	Chain	Res	Type
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1162	G
1	A	1164	U
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	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1331	A
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	1485	A
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	1564	C

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Mol	Chain	Res	Type
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
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	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	1979	G
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2006	C
1	A	2008	U
1	A	2011	A
1	A	2012	U

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Mol	Chain	Res	Type
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	2101	A
1	A	2102	G
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	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2466	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

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Mol	Chain	Res	Type
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
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	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	2914	A
2	B	3002	U
2	B	3003	A
2	B	3004	G
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	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 (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1685	A
1	A	1692	C
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	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	2761	A
1	A	2791	U
2	B	3002	U
2	B	3003	A
2	B	3023	U
2	B	3024	U
2	B	3065	A
2	B	3103	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 235 ligands modelled in this entry, 233 are monoatomic - leaving 2 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	BLS	A	9002	-	25,31,31	1.95	7 (28%)	23,43,43	2.33	7 (30%)
31	BLS	A	9001	-	25,31,31	3.02	11 (44%)	23,43,43	2.95	8 (34%)

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	BLS	A	9002	-	-	2/17/38/38	0/2/2/2
31	BLS	A	9001	-	-	3/17/38/38	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9001	BLS	C10-C9	-8.91	1.40	1.53
31	A	9001	BLS	C4'-N6	5.72	1.54	1.46
31	A	9001	BLS	C4'-C5'	-5.18	1.44	1.53
31	A	9001	BLS	O5'-C5'	4.51	1.49	1.44
31	A	9002	BLS	C14-N14	4.33	1.41	1.29
31	A	9001	BLS	C14-N14	3.80	1.40	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9002	BLS	C10-C9	-3.37	1.48	1.53
31	A	9002	BLS	C10-C11	3.37	1.59	1.52
31	A	9002	BLS	C14-N12	-3.34	1.28	1.35
31	A	9002	BLS	C3'-C2'	3.17	1.43	1.33
31	A	9001	BLS	C8-C9	-2.90	1.49	1.53
31	A	9001	BLS	C3'-C2'	2.83	1.41	1.33
31	A	9002	BLS	O5'-C5'	2.81	1.47	1.44
31	A	9002	BLS	C11-N12	2.63	1.52	1.47
31	A	9001	BLS	C4'-C3'	2.52	1.58	1.49
31	A	9001	BLS	C11-N12	2.52	1.52	1.47
31	A	9001	BLS	C9-N9	2.38	1.54	1.46
31	A	9001	BLS	C6-N1	2.12	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9002	BLS	N15-C14-N12	7.70	127.75	118.53
31	A	9001	BLS	N15-C14-N12	7.61	127.65	118.53
31	A	9001	BLS	O7-C7-C8	6.72	131.34	121.50
31	A	9001	BLS	C4'-N6-C7	4.85	128.32	123.13
31	A	9001	BLS	O5'-C1'-C2'	-4.42	110.74	113.13
31	A	9001	BLS	C8-C7-N6	-4.12	110.93	116.33
31	A	9001	BLS	O7-C7-N6	-3.11	117.70	122.95
31	A	9002	BLS	C11-C10-C9	-2.85	109.15	114.52
31	A	9001	BLS	C2-N3-C4	2.83	119.22	116.34
31	A	9001	BLS	N12-C14-N14	-2.83	114.54	121.23
31	A	9002	BLS	C10-C11-N12	-2.67	107.86	112.15
31	A	9002	BLS	C2-N3-C4	2.42	118.79	116.34
31	A	9002	BLS	C3'-C4'-N6	-2.40	106.19	110.60
31	A	9002	BLS	N15-C14-N14	-2.33	113.18	120.44
31	A	9002	BLS	C5-C4-N3	2.24	124.31	121.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

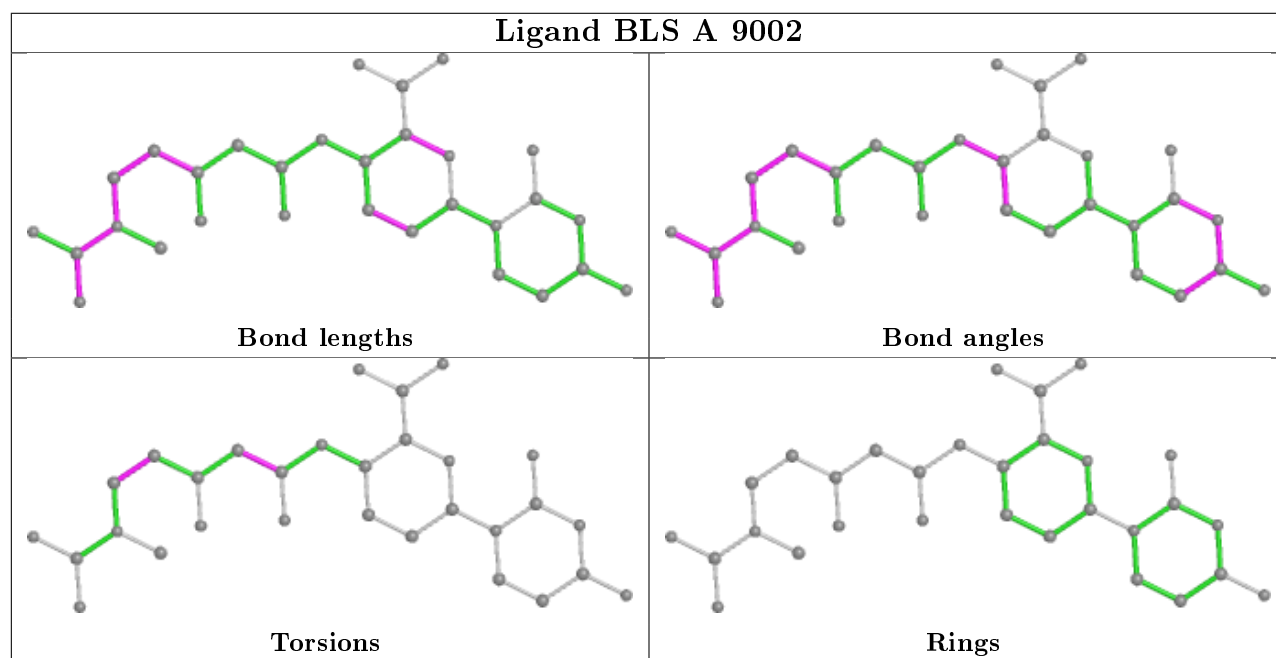
Mol	Chain	Res	Type	Atoms
31	A	9002	BLS	C9-C10-C11-N12
31	A	9001	BLS	C11-C10-C9-C8
31	A	9001	BLS	C11-C10-C9-N9
31	A	9001	BLS	O7-C7-C8-C9
31	A	9002	BLS	N6-C7-C8-C9

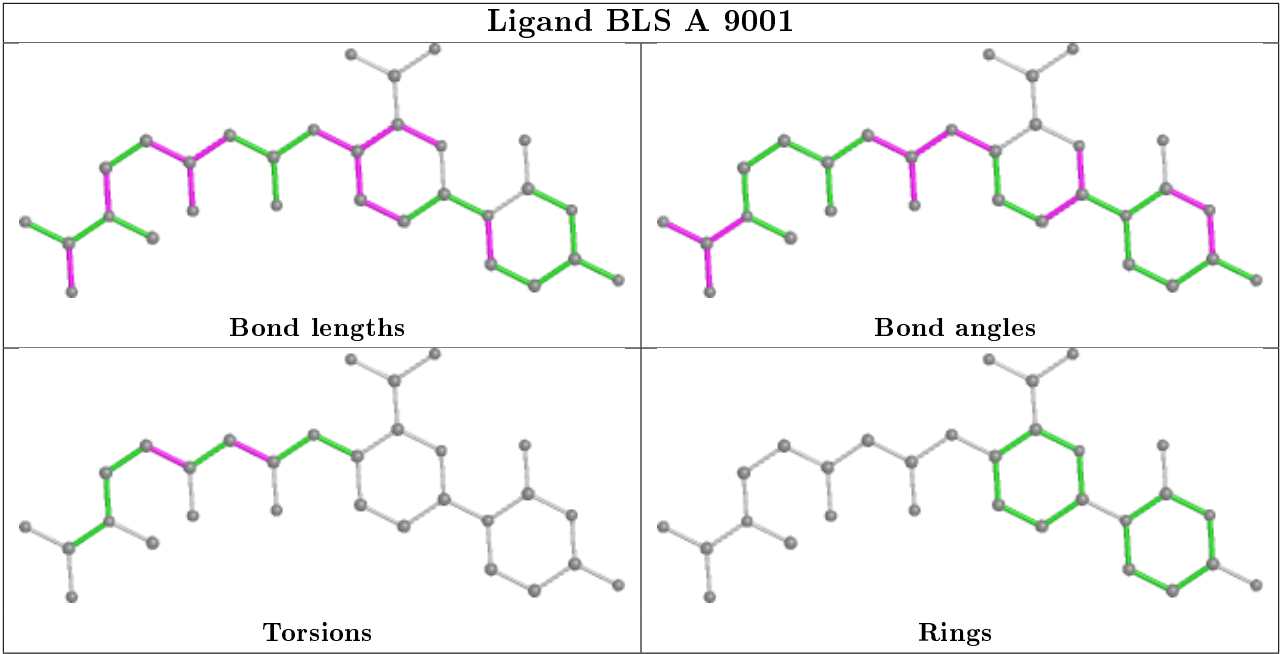
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9002	BLS	3	0
31	A	9001	BLS	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2472:C	O3'	2473:U	P	1.81

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.25	38 (1%) 75 48	14, 40, 85, 133	0
2	B	122/122 (100%)	0.06	5 (4%) 37 15	29, 58, 85, 140	0
3	C	237/239 (99%)	0.03	8 (3%) 45 19	21, 53, 85, 100	0
4	D	337/337 (100%)	-0.30	0 100 100	19, 46, 72, 82	0
5	E	246/246 (100%)	-0.36	0 100 100	16, 38, 63, 72	0
6	F	140/176 (79%)	1.37	40 (28%) 0 0	52, 92, 113, 117	0
7	G	172/177 (97%)	0.35	3 (1%) 70 41	34, 58, 80, 86	0
8	H	119/119 (100%)	0.32	3 (2%) 57 28	43, 65, 90, 99	0
9	I	29/348 (8%)	1.40	6 (20%) 1 0	64, 80, 87, 91	0
10	J	156/167 (93%)	0.13	4 (2%) 56 27	30, 48, 76, 81	0
11	K	142/145 (97%)	-0.24	0 100 100	27, 41, 62, 78	0
12	L	132/132 (100%)	-0.27	0 100 100	30, 43, 70, 75	0
13	M	145/164 (88%)	0.36	11 (7%) 13 4	20, 65, 95, 108	0
14	N	194/194 (100%)	0.07	19 (9%) 7 2	24, 40, 88, 98	0
15	O	186/186 (100%)	0.39	11 (5%) 22 7	38, 61, 99, 113	0
16	P	115/115 (100%)	-0.25	0 100 100	35, 47, 63, 66	0
17	Q	143/148 (96%)	-0.03	1 (0%) 87 68	29, 48, 66, 75	0
18	R	95/95 (100%)	-0.30	1 (1%) 80 55	30, 38, 55, 73	0
19	S	150/154 (97%)	-0.43	0 100 100	23, 35, 55, 64	0
20	T	81/84 (96%)	0.01	1 (1%) 79 53	35, 53, 74, 80	0
21	U	119/119 (100%)	0.10	1 (0%) 86 65	34, 49, 75, 89	0
22	V	53/66 (80%)	3.50	38 (71%) 0 0	80, 90, 96, 101	0
23	W	65/70 (92%)	0.71	6 (9%) 9 3	45, 68, 103, 107	0
24	X	154/154 (100%)	-0.36	0 100 100	27, 38, 57, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.17	2 (2%) 59 30	34, 48, 73, 90	0
26	Z	142/240 (59%)	-0.24	2 (1%) 75 48	20, 35, 59, 77	0
27	1	73/73 (100%)	3.66	44 (60%) 0 0	74, 94, 99, 101	0
28	2	56/56 (100%)	-0.66	0 100 100	19, 28, 34, 37	0
29	3	46/48 (95%)	0.14	3 (6%) 18 5	27, 55, 84, 97	0
30	4	92/92 (100%)	6.72	92 (100%) 0 0	87, 101, 106, 108	0
All	All	6577/7279 (90%)	0.07	339 (5%) 27 10	14, 46, 94, 140	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	15.6
30	4	62	THR	12.9
27	1	11	THR	12.3
30	4	11	CYS	11.5
30	4	39	GLN	11.1
30	4	83	TRP	11.1
30	4	38	ARG	10.9
27	1	30	GLU	10.7
27	1	12	GLY	10.6
30	4	31	THR	10.4
30	4	59	ASP	10.4
30	4	36	ILE	10.3
27	1	20	LEU	10.3
30	4	91	GLN	10.1
30	4	35	TRP	10.0
30	4	33	MET	9.7
30	4	1	MET	9.6
30	4	85	ALA	9.6
30	4	14	CYS	9.6
30	4	82	GLY	9.6
30	4	65	THR	9.5
30	4	71	CYS	9.4
27	1	31	ILE	9.2
30	4	84	ARG	9.2
30	4	34	LYS	8.9
30	4	20	HIS	8.8
30	4	15	ASN	8.6
27	1	34	LYS	8.5
27	1	26	VAL	8.5

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Mol	Chain	Res	Type	RSRZ
30	4	78	HIS	8.4
30	4	41	GLU	8.3
23	W	1	THR	8.3
30	4	27	SER	8.1
27	1	15	GLY	8.1
30	4	16	GLU	8.0
30	4	81	GLU	7.9
30	4	18	GLN	7.9
30	4	22	VAL	7.9
30	4	74	CYS	7.8
30	4	76	LYS	7.7
14	N	89	ASN	7.7
2	B	3001	U	7.7
30	4	45	GLY	7.6
30	4	77	ALA	7.4
27	1	28	ASP	7.3
30	4	44	SER	7.3
27	1	22	ILE	7.3
30	4	75	GLY	7.3
22	V	36	CYS	7.2
30	4	23	GLU	7.2
27	1	35	LYS	7.1
22	V	54	THR	7.0
30	4	13	HIS	7.0
30	4	21	GLU	6.9
27	1	32	LYS	6.9
30	4	67	LEU	6.8
30	4	68	LYS	6.8
30	4	4	PRO	6.8
30	4	32	GLY	6.8
14	N	71	SER	6.8
22	V	9	CYS	6.8
27	1	45	LYS	6.8
30	4	3	MET	6.7
30	4	56	PRO	6.7
30	4	86	GLY	6.6
27	1	16	PRO	6.6
27	1	19	GLY	6.6
22	V	48	ASN	6.4
27	1	23	ARG	6.4
14	N	70	GLY	6.4
6	F	57	THR	6.4

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Mol	Chain	Res	Type	RSRZ
30	4	60	LYS	6.4
14	N	80	GLY	6.4
27	1	44	PHE	6.3
22	V	55	ALA	6.3
22	V	6	CYS	6.3
30	4	12	PRO	6.3
27	1	33	HIS	6.2
30	4	10	TYR	6.2
22	V	52	THR	6.1
27	1	39	CYS	6.1
30	4	9	THR	6.1
30	4	2	GLN	6.1
30	4	30	GLN	6.0
30	4	8	ASN	6.0
30	4	17	HIS	5.9
30	4	63	LYS	5.8
22	V	43	GLY	5.8
30	4	47	GLY	5.8
1	A	735	C	5.7
22	V	53	ASP	5.6
30	4	43	ASN	5.6
27	1	25	ARG	5.6
27	1	21	LYS	5.6
22	V	46	ALA	5.6
22	V	39	ASN	5.5
30	4	53	SER	5.5
22	V	11	THR	5.3
30	4	49	ASP	5.3
22	V	51	TRP	5.3
30	4	6	ARG	5.3
30	4	61	PRO	5.3
30	4	42	ARG	5.3
27	1	42	CYS	5.3
30	4	40	ARG	5.1
27	1	41	VAL	5.1
27	1	58	GLY	5.1
14	N	83	SER	5.0
27	1	43	GLY	5.0
30	4	58	GLY	5.0
30	4	24	LYS	4.9
30	4	64	LYS	4.8
30	4	66	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
30	4	48	ASN	4.8
14	N	78	ASN	4.8
27	1	24	VAL	4.8
22	V	40	ALA	4.7
27	1	29	VAL	4.7
30	4	88	LEU	4.7
30	4	89	GLU	4.7
30	4	72	GLY	4.6
30	4	19	GLU	4.6
30	4	80	ARG	4.6
27	1	27	ALA	4.6
22	V	47	ARG	4.6
30	4	55	VAL	4.6
30	4	70	ARG	4.6
27	1	57	CYS	4.5
22	V	29	THR	4.5
27	1	13	ARG	4.5
30	4	90	PHE	4.4
6	F	69	ILE	4.4
14	N	81	ARG	4.4
22	V	4	ARG	4.4
14	N	72	SER	4.3
30	4	69	TYR	4.3
30	4	52	PHE	4.3
22	V	19	THR	4.3
6	F	63	ILE	4.3
30	4	26	ARG	4.3
22	V	12	ASP	4.3
22	V	49	LEU	4.2
30	4	57	GLY	4.2
27	1	18	TYR	4.2
6	F	88	LEU	4.2
22	V	13	ILE	4.2
30	4	28	GLY	4.2
30	4	25	VAL	4.1
22	V	50	GLU	4.1
30	4	51	LYS	4.0
30	4	79	LEU	4.0
2	B	3025	G	4.0
14	N	74	ARG	4.0
27	1	14	PHE	4.0
30	4	5	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1198	U	4.0
30	4	87	ARG	4.0
25	Y	88	GLU	3.9
13	M	60	GLU	3.9
1	A	1173	A	3.9
1	A	1171	A	3.8
1	A	1172	G	3.8
22	V	10	GLY	3.8
3	C	36	ASP	3.7
22	V	41	ASP	3.7
9	I	27	ILE	3.7
15	O	186	LEU	3.7
30	4	92	GLU	3.7
6	F	66	GLY	3.7
7	G	45	ASP	3.7
27	1	38	LYS	3.7
23	W	40	PRO	3.7
6	F	171	ASP	3.6
30	4	29	ARG	3.6
1	A	1177	A	3.6
15	O	160	SER	3.6
27	1	40	PRO	3.6
23	W	39	ALA	3.6
22	V	33	SER	3.6
27	1	36	LYS	3.5
30	4	73	GLU	3.5
27	1	37	HIS	3.4
15	O	179	LEU	3.4
22	V	32	CYS	3.4
1	A	2433	A	3.4
9	I	23	ILE	3.4
27	1	10	ARG	3.4
1	A	2436	U	3.3
6	F	85	GLN	3.3
22	V	5	GLU	3.3
14	N	77	PHE	3.3
1	A	2432	C	3.3
15	O	162	ASP	3.3
2	B	3002	U	3.3
3	C	37	VAL	3.3
1	A	1951	G	3.2
13	M	105	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
6	F	56	ARG	3.2
13	M	80	ASP	3.2
6	F	75	LEU	3.1
22	V	25	ASP	3.1
2	B	3023	U	3.1
6	F	27	ILE	3.1
30	4	46	ILE	3.1
1	A	1199	A	3.1
6	F	10	PHE	3.1
22	V	45	GLU	3.0
1	A	1170	U	3.0
22	V	24	LYS	3.0
15	O	184	ILE	3.0
6	F	62	ASP	3.0
1	A	2237	G	3.0
20	T	81	ILE	3.0
23	W	38	GLY	3.0
14	N	87	MET	3.0
1	A	282	C	3.0
14	N	90	ARG	3.0
6	F	26	GLY	2.9
6	F	89	PRO	2.9
14	N	82	ARG	2.9
1	A	2748	G	2.9
6	F	58	VAL	2.9
6	F	166	ILE	2.9
27	1	46	LYS	2.9
6	F	86	THR	2.8
6	F	44	ILE	2.8
8	H	106	THR	2.8
22	V	14	GLU	2.8
1	A	960	G	2.8
3	C	85	ASP	2.8
21	U	119	ALA	2.8
14	N	76	ARG	2.8
22	V	8	TYR	2.8
1	A	1169	U	2.7
14	N	73	ARG	2.7
29	3	36	ASN	2.7
14	N	88	VAL	2.7
15	O	138	ASP	2.7
1	A	1165	G	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	23	VAL	2.7
6	F	87	ALA	2.7
27	1	82	ALA	2.6
9	I	71	LEU	2.6
27	1	47	LEU	2.6
17	Q	110	ASP	2.6
6	F	102	GLY	2.6
13	M	106	VAL	2.6
6	F	134	LEU	2.6
13	M	59	GLU	2.6
30	4	54	LYS	2.6
2	B	3122	C	2.6
13	M	104	ASP	2.5
27	1	59	HIS	2.5
6	F	170	TYR	2.5
15	O	167	ASP	2.5
14	N	75	THR	2.5
6	F	18	ILE	2.5
6	F	54	ALA	2.5
6	F	67	ASP	2.5
8	H	44	SER	2.5
6	F	64	ARG	2.5
15	O	185	GLU	2.5
1	A	1175	G	2.5
22	V	56	ARG	2.5
29	3	39	ARG	2.5
27	1	17	ARG	2.5
10	J	142	VAL	2.4
1	A	2345	A	2.4
3	C	38	ILE	2.4
6	F	25	MET	2.4
22	V	23	HIS	2.4
8	H	26	THR	2.4
1	A	1948	G	2.4
27	1	53	GLY	2.4
6	F	92	GLU	2.4
25	Y	80	GLU	2.4
26	Z	235	GLU	2.4
1	A	1168	C	2.4
22	V	15	PRO	2.4
1	A	736	A	2.4
10	J	135	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	101	ASP	2.4
26	Z	108	ASP	2.3
27	1	79	VAL	2.3
1	A	1190	G	2.3
18	R	95	GLU	2.3
14	N	79	LYS	2.3
30	4	7	PHE	2.3
1	A	1950	G	2.3
9	I	68	GLU	2.3
6	F	130	VAL	2.3
9	I	26	MET	2.3
1	A	2637	A	2.3
6	F	68	PRO	2.3
1	A	1525	G	2.3
10	J	32	ASP	2.3
22	V	44	ARG	2.3
13	M	102	ASP	2.2
1	A	1163	G	2.2
15	O	67	ALA	2.2
1	A	1913	C	2.2
6	F	47	GLN	2.2
1	A	1162	G	2.2
1	A	2344	G	2.2
1	A	281	U	2.2
15	O	127	LEU	2.2
1	A	280	C	2.2
15	O	163	PHE	2.2
23	W	37	GLY	2.2
30	4	50	GLY	2.2
3	C	82	VAL	2.1
6	F	49	PRO	2.1
1	A	1181	A	2.1
6	F	90	LEU	2.1
9	I	65	THR	2.1
22	V	31	PHE	2.1
13	M	73	VAL	2.1
7	G	108	LEU	2.1
3	C	64	ASP	2.1
3	C	237	GLY	2.1
6	F	81	GLU	2.1
22	V	28	THR	2.1
10	J	83	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	61	PHE	2.1
23	W	8	ILE	2.1
1	A	2437	A	2.1
6	F	45	THR	2.1
1	A	2004	U	2.1
13	M	133	VAL	2.1
6	F	106	PHE	2.0
6	F	158	ASN	2.0
3	C	133	ARG	2.0
7	G	100	ASP	2.0
1	A	1925	G	2.0
14	N	68	ARG	2.0
29	3	49	GLU	2.0
13	M	48	LYS	2.0
1	A	1167	G	2.0
6	F	172	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8329	1/1	0.36	0.30	61,61,61,61	0
34	NA	S	8386	1/1	0.45	0.68	77,77,77,77	0
35	CL	4	8504	1/1	0.53	0.74	116,116,116,116	0
36	CD	V	8401	1/1	0.56	0.49	199,199,199,199	0
34	NA	T	8312	1/1	0.58	0.32	39,39,39,39	0
32	MG	B	8095	1/1	0.58	0.12	64,64,64,64	0
36	CD	4	8404	1/1	0.58	0.64	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	M	8510	1/1	0.64	0.25	69,69,69,69	0
34	NA	A	8301	1/1	0.67	0.28	27,27,27,27	0
34	NA	A	8363	1/1	0.69	0.54	44,44,44,44	0
34	NA	A	8385	1/1	0.71	0.35	45,45,45,45	0
34	NA	A	8384	1/1	0.72	0.35	65,65,65,65	0
34	NA	A	8382	1/1	0.73	0.43	73,73,73,73	0
34	NA	B	8383	1/1	0.73	0.53	66,66,66,66	0
32	MG	1	8105	1/1	0.74	0.33	53,53,53,53	0
34	NA	A	8371	1/1	0.74	0.35	41,41,41,41	0
32	MG	A	8049	1/1	0.75	0.38	57,57,57,57	0
34	NA	B	8351	1/1	0.78	0.15	42,42,42,42	0
32	MG	A	8046	1/1	0.78	0.14	44,44,44,44	0
32	MG	A	8102	1/1	0.78	1.44	112,112,112,112	0
34	NA	A	8377	1/1	0.79	0.57	60,60,60,60	0
32	MG	A	8092	1/1	0.79	0.32	84,84,84,84	0
36	CD	1	8403	1/1	0.79	0.29	186,186,186,186	0
34	NA	A	8366	1/1	0.80	0.20	34,34,34,34	0
34	NA	S	8337	1/1	0.80	0.12	39,39,39,39	0
32	MG	A	8076	1/1	0.80	0.14	73,73,73,73	0
36	CD	P	8405	1/1	0.81	0.08	114,114,114,114	0
32	MG	A	8064	1/1	0.82	0.20	21,21,21,21	0
31	BLS	A	9002	30/30	0.82	0.38	73,83,98,98	0
32	MG	A	8114	1/1	0.83	0.49	104,104,104,104	0
32	MG	U	8073	1/1	0.83	0.13	35,35,35,35	0
32	MG	A	8055	1/1	0.83	0.12	84,84,84,84	0
32	MG	A	8115	1/1	0.83	0.09	45,45,45,45	0
34	NA	A	8318	1/1	0.84	0.22	32,32,32,32	0
35	CL	K	8502	1/1	0.84	0.18	57,57,57,57	0
32	MG	A	8093	1/1	0.85	0.15	43,43,43,43	0
34	NA	A	8328	1/1	0.85	0.42	38,38,38,38	0
32	MG	A	8085	1/1	0.85	0.11	83,83,83,83	0
34	NA	A	8357	1/1	0.85	0.06	46,46,46,46	0
34	NA	A	8368	1/1	0.85	0.15	46,46,46,46	0
32	MG	A	8001	1/1	0.86	0.08	26,26,26,26	0
34	NA	A	8331	1/1	0.86	0.25	69,69,69,69	0
34	NA	A	8356	1/1	0.86	0.92	44,44,44,44	0
32	MG	A	8088	1/1	0.86	0.14	31,31,31,31	0
33	K	A	8203	1/1	0.87	0.33	79,79,79,79	0
34	NA	A	8355	1/1	0.87	0.54	80,80,80,80	0
35	CL	A	8511	1/1	0.87	0.35	48,48,48,48	0
35	CL	C	8509	1/1	0.87	0.36	86,86,86,86	0
32	MG	A	8111	1/1	0.87	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	K	A	8202	1/1	0.87	0.41	91,91,91,91	0
34	NA	A	8372	1/1	0.87	0.45	59,59,59,59	0
34	NA	A	8364	1/1	0.87	0.26	43,43,43,43	0
34	NA	K	8346	1/1	0.88	0.13	32,32,32,32	0
32	MG	A	8053	1/1	0.88	0.16	40,40,40,40	0
32	MG	4	8078	1/1	0.88	0.34	87,87,87,87	0
34	NA	A	8326	1/1	0.88	0.19	34,34,34,34	0
32	MG	A	8087	1/1	0.88	0.10	36,36,36,36	0
34	NA	A	8335	1/1	0.89	0.33	53,53,53,53	0
35	CL	K	8501	1/1	0.89	0.30	58,58,58,58	0
33	K	A	8201	1/1	0.89	0.26	52,52,52,52	0
34	NA	A	8334	1/1	0.89	0.12	43,43,43,43	0
34	NA	A	8341	1/1	0.89	0.09	39,39,39,39	0
34	NA	A	8360	1/1	0.89	0.61	75,75,75,75	0
34	NA	A	8332	1/1	0.90	0.28	58,58,58,58	0
35	CL	A	8505	1/1	0.90	0.17	52,52,52,52	0
32	MG	A	8112	1/1	0.90	0.10	39,39,39,39	0
34	NA	A	8327	1/1	0.90	0.15	23,23,23,23	0
34	NA	A	8340	1/1	0.90	0.27	43,43,43,43	0
34	NA	A	8303	1/1	0.90	0.22	34,34,34,34	0
34	NA	A	8307	1/1	0.90	0.28	42,42,42,42	0
35	CL	A	8522	1/1	0.90	0.32	69,69,69,69	0
32	MG	A	8047	1/1	0.90	0.27	48,48,48,48	0
34	NA	A	8310	1/1	0.90	0.33	23,23,23,23	0
34	NA	A	8352	1/1	0.90	0.27	42,42,42,42	0
34	NA	A	8313	1/1	0.91	0.13	53,53,53,53	0
34	NA	A	8358	1/1	0.91	0.47	80,80,80,80	0
34	NA	R	8348	1/1	0.91	0.14	41,41,41,41	0
34	NA	A	8369	1/1	0.91	0.31	78,78,78,78	0
34	NA	A	8302	1/1	0.91	0.17	30,30,30,30	0
32	MG	A	8051	1/1	0.91	0.10	60,60,60,60	0
34	NA	E	8304	1/1	0.91	0.13	27,27,27,27	0
32	MG	A	8108	1/1	0.91	0.06	66,66,66,66	0
32	MG	A	8103	1/1	0.91	0.33	58,58,58,58	0
32	MG	A	8096	1/1	0.91	0.11	60,60,60,60	0
32	MG	A	8097	1/1	0.92	0.17	33,33,33,33	0
34	NA	A	8381	1/1	0.92	0.27	59,59,59,59	0
34	NA	A	8375	1/1	0.92	0.23	51,51,51,51	0
35	CL	Z	8520	1/1	0.92	0.17	27,27,27,27	0
34	NA	A	8305	1/1	0.92	0.14	24,24,24,24	0
35	CL	A	8515	1/1	0.92	0.28	66,66,66,66	0
35	CL	N	8518	1/1	0.92	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8045	1/1	0.92	0.10	50,50,50,50	0
32	MG	A	8104	1/1	0.92	0.45	55,55,55,55	0
34	NA	A	8361	1/1	0.92	0.25	50,50,50,50	0
34	NA	A	8354	1/1	0.92	0.38	36,36,36,36	0
34	NA	M	8380	1/1	0.92	0.23	62,62,62,62	0
34	NA	A	8362	1/1	0.93	0.19	68,68,68,68	0
32	MG	A	8048	1/1	0.93	0.08	30,30,30,30	0
32	MG	A	8070	1/1	0.93	0.40	47,47,47,47	0
32	MG	A	8018	1/1	0.93	0.10	37,37,37,37	0
34	NA	A	8316	1/1	0.93	0.15	34,34,34,34	0
34	NA	C	8345	1/1	0.93	0.17	40,40,40,40	0
34	NA	A	8311	1/1	0.93	0.12	39,39,39,39	0
32	MG	A	8099	1/1	0.93	0.20	46,46,46,46	0
32	MG	A	8071	1/1	0.93	0.04	75,75,75,75	0
32	MG	A	8101	1/1	0.93	0.13	40,40,40,40	0
34	NA	A	8374	1/1	0.93	0.49	49,49,49,49	0
35	CL	A	8503	1/1	0.93	0.25	49,49,49,49	0
32	MG	A	8059	1/1	0.93	0.08	37,37,37,37	0
32	MG	A	8072	1/1	0.94	0.09	43,43,43,43	0
34	NA	A	8373	1/1	0.94	0.30	42,42,42,42	0
32	MG	A	8032	1/1	0.94	0.07	33,33,33,33	0
32	MG	A	8003	1/1	0.94	0.10	20,20,20,20	0
34	NA	A	8323	1/1	0.94	0.16	46,46,46,46	0
34	NA	A	8325	1/1	0.94	0.14	42,42,42,42	0
35	CL	K	8516	1/1	0.94	0.34	44,44,44,44	0
32	MG	A	8057	1/1	0.94	0.10	33,33,33,33	0
34	NA	A	8324	1/1	0.94	0.16	35,35,35,35	0
32	MG	A	8089	1/1	0.94	0.17	66,66,66,66	0
32	MG	A	8030	1/1	0.94	0.08	25,25,25,25	0
32	MG	A	8014	1/1	0.94	0.08	23,23,23,23	0
32	MG	A	8041	1/1	0.94	0.20	54,54,54,54	0
34	NA	A	8308	1/1	0.94	0.20	51,51,51,51	0
32	MG	A	8024	1/1	0.94	0.60	38,38,38,38	0
32	MG	A	8091	1/1	0.94	0.07	51,51,51,51	0
34	NA	J	8322	1/1	0.94	0.28	43,43,43,43	0
34	NA	A	8315	1/1	0.94	0.16	32,32,32,32	0
34	NA	A	8370	1/1	0.94	0.27	56,56,56,56	0
34	NA	A	8367	1/1	0.94	0.14	55,55,55,55	0
34	NA	A	8353	1/1	0.94	0.10	38,38,38,38	0
31	BLS	A	9001	30/30	0.95	0.21	26,37,43,45	0
35	CL	A	8517	1/1	0.95	0.23	54,54,54,54	0
35	CL	O	8507	1/1	0.95	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8080	1/1	0.95	0.08	32,32,32,32	0
32	MG	A	8050	1/1	0.95	0.10	76,76,76,76	0
32	MG	A	8040	1/1	0.95	0.10	86,86,86,86	0
32	MG	A	8084	1/1	0.95	0.08	56,56,56,56	0
34	NA	A	8319	1/1	0.95	0.08	46,46,46,46	0
34	NA	A	8321	1/1	0.95	0.26	52,52,52,52	0
32	MG	A	8113	1/1	0.95	0.10	24,24,24,24	0
32	MG	L	8069	1/1	0.95	0.06	48,48,48,48	0
34	NA	A	8333	1/1	0.95	0.10	27,27,27,27	0
35	CL	D	8519	1/1	0.95	0.29	49,49,49,49	0
35	CL	K	8521	1/1	0.95	0.14	46,46,46,46	0
32	MG	A	8090	1/1	0.95	0.28	90,90,90,90	0
34	NA	A	8330	1/1	0.95	0.18	21,21,21,21	0
32	MG	A	8082	1/1	0.95	0.09	40,40,40,40	0
32	MG	A	8116	1/1	0.95	0.15	71,71,71,71	0
35	CL	A	8512	1/1	0.95	0.18	33,33,33,33	0
32	MG	A	8075	1/1	0.95	0.10	44,44,44,44	0
34	NA	A	8344	1/1	0.95	0.07	20,20,20,20	0
32	MG	A	8037	1/1	0.95	0.06	31,31,31,31	0
34	NA	A	8378	1/1	0.95	0.34	42,42,42,42	0
34	NA	A	8306	1/1	0.95	0.42	31,31,31,31	0
32	MG	A	8061	1/1	0.96	0.09	35,35,35,35	0
34	NA	A	8314	1/1	0.96	0.17	36,36,36,36	0
34	NA	A	8349	1/1	0.96	0.15	47,47,47,47	0
34	NA	A	8365	1/1	0.96	0.16	31,31,31,31	0
32	MG	A	8044	1/1	0.96	0.17	36,36,36,36	0
32	MG	A	8010	1/1	0.96	0.08	21,21,21,21	0
34	NA	A	8359	1/1	0.96	0.28	47,47,47,47	0
32	MG	A	8004	1/1	0.96	0.05	27,27,27,27	0
34	NA	J	8309	1/1	0.96	0.13	32,32,32,32	0
32	MG	A	8054	1/1	0.96	0.07	32,32,32,32	0
32	MG	A	8035	1/1	0.96	0.04	37,37,37,37	0
32	MG	A	8058	1/1	0.96	0.08	25,25,25,25	0
34	NA	A	8379	1/1	0.96	0.14	46,46,46,46	0
35	CL	A	8514	1/1	0.96	0.17	44,44,44,44	0
34	NA	A	8339	1/1	0.96	0.15	11,11,11,11	0
34	NA	S	8338	1/1	0.96	0.09	44,44,44,44	0
32	MG	A	8060	1/1	0.96	0.13	26,26,26,26	0
32	MG	A	8066	1/1	0.96	0.11	83,83,83,83	0
32	MG	A	8068	1/1	0.96	0.14	47,47,47,47	0
32	MG	A	8022	1/1	0.96	0.05	33,33,33,33	0
34	NA	A	8317	1/1	0.96	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	N	8347	1/1	0.97	0.06	18,18,18,18	0
32	MG	A	8098	1/1	0.97	0.15	25,25,25,25	0
35	CL	S	8506	1/1	0.97	0.12	38,38,38,38	0
32	MG	C	8065	1/1	0.97	0.11	61,61,61,61	0
32	MG	A	8034	1/1	0.97	0.04	28,28,28,28	0
32	MG	A	8033	1/1	0.97	0.08	17,17,17,17	0
32	MG	A	8031	1/1	0.97	0.05	22,22,22,22	0
32	MG	A	8013	1/1	0.97	0.12	41,41,41,41	0
32	MG	A	8043	1/1	0.97	0.12	32,32,32,32	0
32	MG	A	8006	1/1	0.97	0.08	33,33,33,33	0
32	MG	A	8081	1/1	0.97	0.11	41,41,41,41	0
34	NA	A	8336	1/1	0.97	0.16	31,31,31,31	0
34	NA	U	8343	1/1	0.97	0.06	18,18,18,18	0
32	MG	A	8042	1/1	0.97	0.14	34,34,34,34	0
32	MG	A	8008	1/1	0.97	0.09	26,26,26,26	0
32	MG	A	8106	1/1	0.97	0.25	61,61,61,61	0
35	CL	A	8513	1/1	0.97	0.10	47,47,47,47	0
32	MG	A	8062	1/1	0.97	0.12	54,54,54,54	0
32	MG	A	8023	1/1	0.97	0.07	29,29,29,29	0
32	MG	A	8029	1/1	0.97	0.06	16,16,16,16	0
32	MG	A	8056	1/1	0.97	0.11	40,40,40,40	0
34	NA	A	8342	1/1	0.97	0.15	30,30,30,30	0
32	MG	A	8100	1/1	0.97	0.09	73,73,73,73	0
32	MG	A	8083	1/1	0.97	0.07	39,39,39,39	0
32	MG	A	8027	1/1	0.97	0.07	36,36,36,36	0
32	MG	A	8117	1/1	0.97	0.06	29,29,29,29	0
32	MG	A	8107	1/1	0.97	0.05	32,32,32,32	0
32	MG	A	8028	1/1	0.97	0.05	26,26,26,26	0
32	MG	A	8007	1/1	0.98	0.05	17,17,17,17	0
32	MG	A	8016	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8039	1/1	0.98	0.04	42,42,42,42	0
32	MG	A	8017	1/1	0.98	0.05	21,21,21,21	0
32	MG	A	8005	1/1	0.98	0.06	28,28,28,28	0
32	MG	A	8063	1/1	0.98	0.08	54,54,54,54	0
32	MG	A	8074	1/1	0.98	0.06	29,29,29,29	0
32	MG	A	8036	1/1	0.98	0.06	32,32,32,32	0
32	MG	A	8079	1/1	0.98	0.08	21,21,21,21	0
32	MG	A	8052	1/1	0.98	0.08	42,42,42,42	0
32	MG	A	8019	1/1	0.98	0.06	27,27,27,27	0
34	NA	A	8376	1/1	0.98	0.06	45,45,45,45	0
35	CL	P	8508	1/1	0.98	0.37	80,80,80,80	0
34	NA	A	8320	1/1	0.98	0.12	21,21,21,21	0

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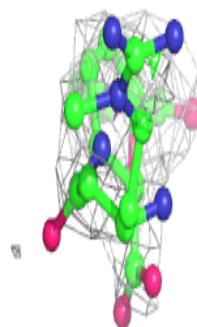
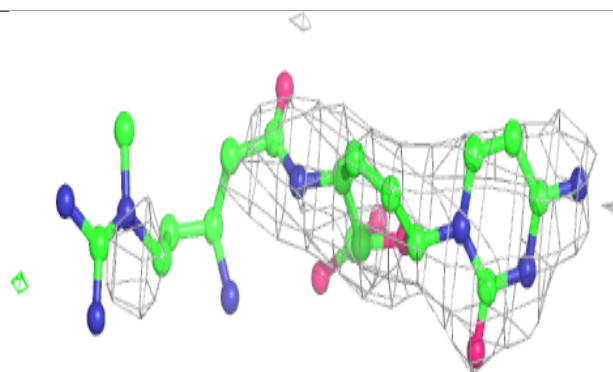
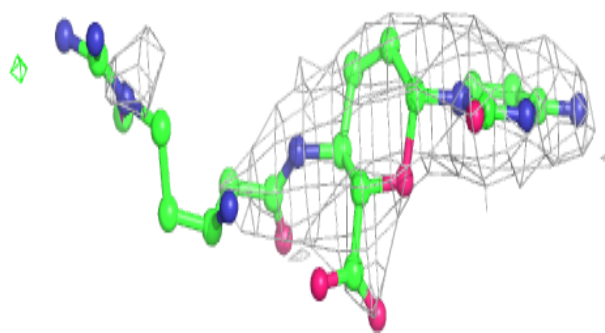
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8067	1/1	0.98	0.13	52,52,52,52	0
32	MG	A	8015	1/1	0.98	0.06	36,36,36,36	0
32	MG	A	8038	1/1	0.98	0.06	24,24,24,24	0
32	MG	A	8094	1/1	0.98	0.12	57,57,57,57	0
32	MG	A	8020	1/1	0.99	0.04	23,23,23,23	0
32	MG	A	8077	1/1	0.99	0.04	30,30,30,30	0
32	MG	A	8026	1/1	0.99	0.03	13,13,13,13	0
32	MG	Z	8109	1/1	0.99	0.09	26,26,26,26	0
36	CD	2	8402	1/1	0.99	0.05	50,50,50,50	0
32	MG	A	8086	1/1	0.99	0.11	36,36,36,36	0
34	NA	A	8350	1/1	0.99	0.15	31,31,31,31	0
32	MG	A	8002	1/1	0.99	0.06	24,24,24,24	0
32	MG	A	8110	1/1	0.99	0.11	22,22,22,22	0
32	MG	A	8009	1/1	0.99	0.04	22,22,22,22	0
32	MG	A	8021	1/1	0.99	0.06	17,17,17,17	0
32	MG	A	8012	1/1	0.99	0.07	42,42,42,42	0
32	MG	A	8025	1/1	0.99	0.03	34,34,34,34	0
32	MG	A	8011	1/1	1.00	0.08	18,18,18,18	0

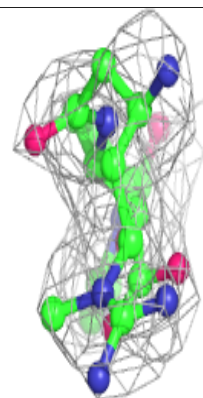
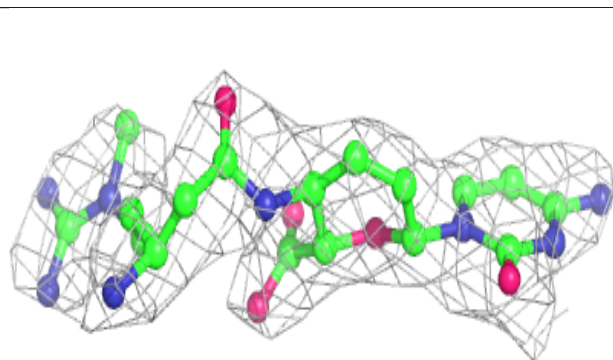
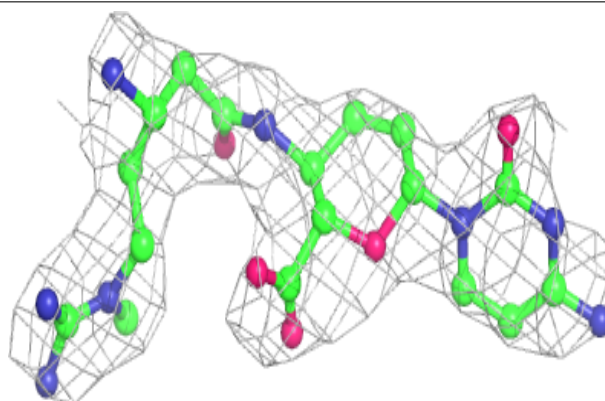
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BLS A 9002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BLS A 9001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.