



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3I55  
Title : Co-crystal structure of Mycalamide A Bound to the Large Ribosomal Subunit  
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.  
Deposited on : 2009-07-03  
Resolution : 3.11 Å(reported)

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

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

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

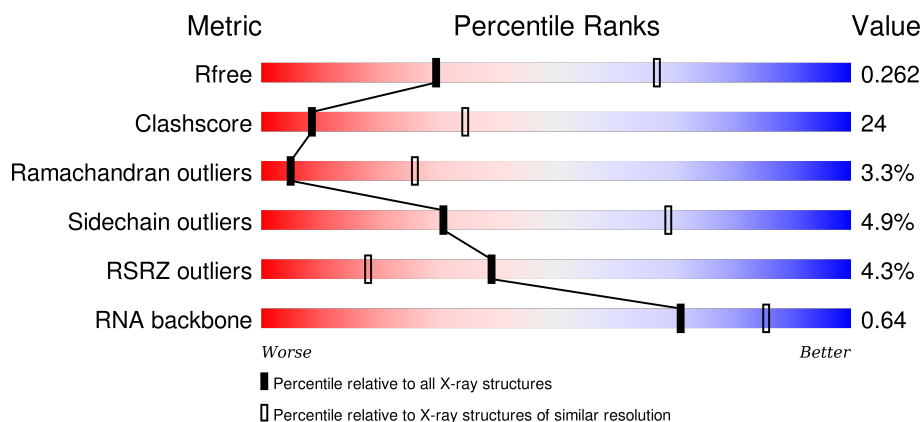
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 Å.

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



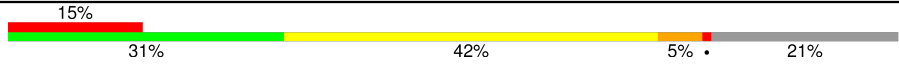

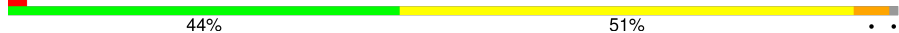




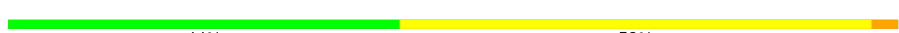







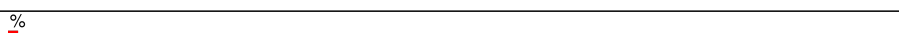
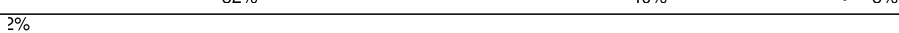





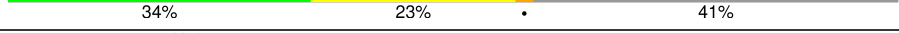


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)
RNA backbone	2183	1010 (3.54-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	0	2923	
2	A	240	
3	B	338	
4	C	246	

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	178	
7	F	120	
8	G	348	
9	H	174	
10	I	162	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	116	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	
32	4	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	5AA	4	76	-	-	X	-
33	MG	0	8043	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8076	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	Y	8086	-	-	-	X
34	K	0	8401	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8545	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	M	8539	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	Q	8540	-	-	-	X
36	CL	0	8805	-	-	-	X
37	SR	0	8904	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8962	-	-	-	X
37	SR	0	8992	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
38	MYL	0	2924	-	-	X	-
39	CD	3	8704	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99287 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 3 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

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

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 8 is a protein called 50S ribosomal protein L10E.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	160	Total	C	N	O	S	0	0	0
			1283	798	240	239	6			

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	EXPRESSION TAG	UNP P60619
Z	2	SER	-	EXPRESSION TAG	UNP P60619
Z	3	PRO	-	EXPRESSION TAG	UNP P60619
Z	4	ARG	-	EXPRESSION TAG	UNP P60619
Z	5	ALA	-	EXPRESSION TAG	UNP P60619
Z	6	ARG	-	EXPRESSION TAG	UNP P60619
Z	7	ARG	-	EXPRESSION TAG	UNP P60619
Z	8	GLU	-	EXPRESSION TAG	UNP P60619
Z	9	PRO	-	EXPRESSION TAG	UNP P60619
Z	10	ASN	-	EXPRESSION TAG	UNP P60619
Z	11	LEU	-	EXPRESSION TAG	UNP P60619
Z	12	GLU	-	EXPRESSION TAG	UNP P60619
Z	13	GLY	-	EXPRESSION TAG	UNP P60619
Z	14	LEU	-	EXPRESSION TAG	UNP P60619
Z	15	MET	-	EXPRESSION TAG	UNP P60619
Z	16	TRP	-	EXPRESSION TAG	UNP P60619
Z	17	PRO	-	EXPRESSION TAG	UNP P60619
Z	18	LEU	-	EXPRESSION TAG	UNP P60619
Z	19	GLY	-	EXPRESSION TAG	UNP P60619
Z	20	GLY	-	EXPRESSION TAG	UNP P60619
Z	21	GLN	-	EXPRESSION TAG	UNP P60619
Z	22	GLN	-	EXPRESSION TAG	UNP P60619
Z	23	THR	-	EXPRESSION TAG	UNP P60619
Z	24	THR	-	EXPRESSION TAG	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is DNA/RNA hybrid called DNA/RNA (5'-R(\*CP\*CP\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	83	Total	Mg	0	0
			83	83		
33	9	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	63	Total Na 63 63	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

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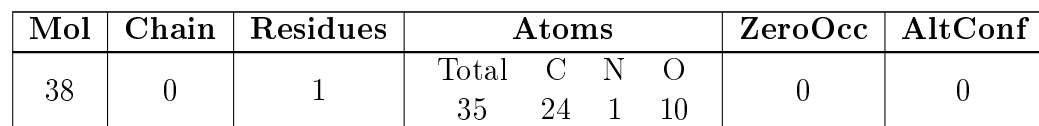
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	93	Total Sr 93 93	0	0
37	1	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	B	2	Total Sr 2 2	0	0
37	3	2	Total Sr 2 2	0	0
37	A	2	Total Sr 2 2	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	L	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	F	1	Total Sr 1 1	0	0

- Molecule 38 is MYCALAMIDE A (three-letter code: MYL) (formula: C<sub>24</sub>H<sub>41</sub>NO<sub>10</sub>).



- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39  | O     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 39  | Z     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 39  | 1     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 39  | 3     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 39  | U     | 1        | Total Cd<br>1 1 | 0       | 0       |

- | Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 40  | 0     | 5841     | Total O<br>5841 5841 | 0       | 0       |
| 40  | A     | 117      | Total O<br>117 117   | 0       | 0       |
| 40  | B     | 151      | Total O<br>151 151   | 0       | 0       |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	175	Total 175	O 175	0	0
40	D	49	Total 49	O 49	0	0
40	E	40	Total 40	O 40	0	0
40	F	29	Total 29	O 29	0	0
40	G	18	Total 18	O 18	0	0
40	H	76	Total 76	O 76	0	0
40	I	10	Total 10	O 10	0	0
40	J	57	Total 57	O 57	0	0
40	K	62	Total 62	O 62	0	0
40	L	91	Total 91	O 91	0	0
40	M	148	Total 148	O 148	0	0
40	N	61	Total 61	O 61	0	0
40	O	41	Total 41	O 41	0	0
40	P	61	Total 61	O 61	0	0
40	Q	49	Total 49	O 49	0	0
40	R	83	Total 83	O 83	0	0
40	S	37	Total 37	O 37	0	0
40	T	36	Total 36	O 36	0	0
40	U	29	Total 29	O 29	0	0
40	V	13	Total 13	O 13	0	0
40	W	67	Total 67	O 67	0	0

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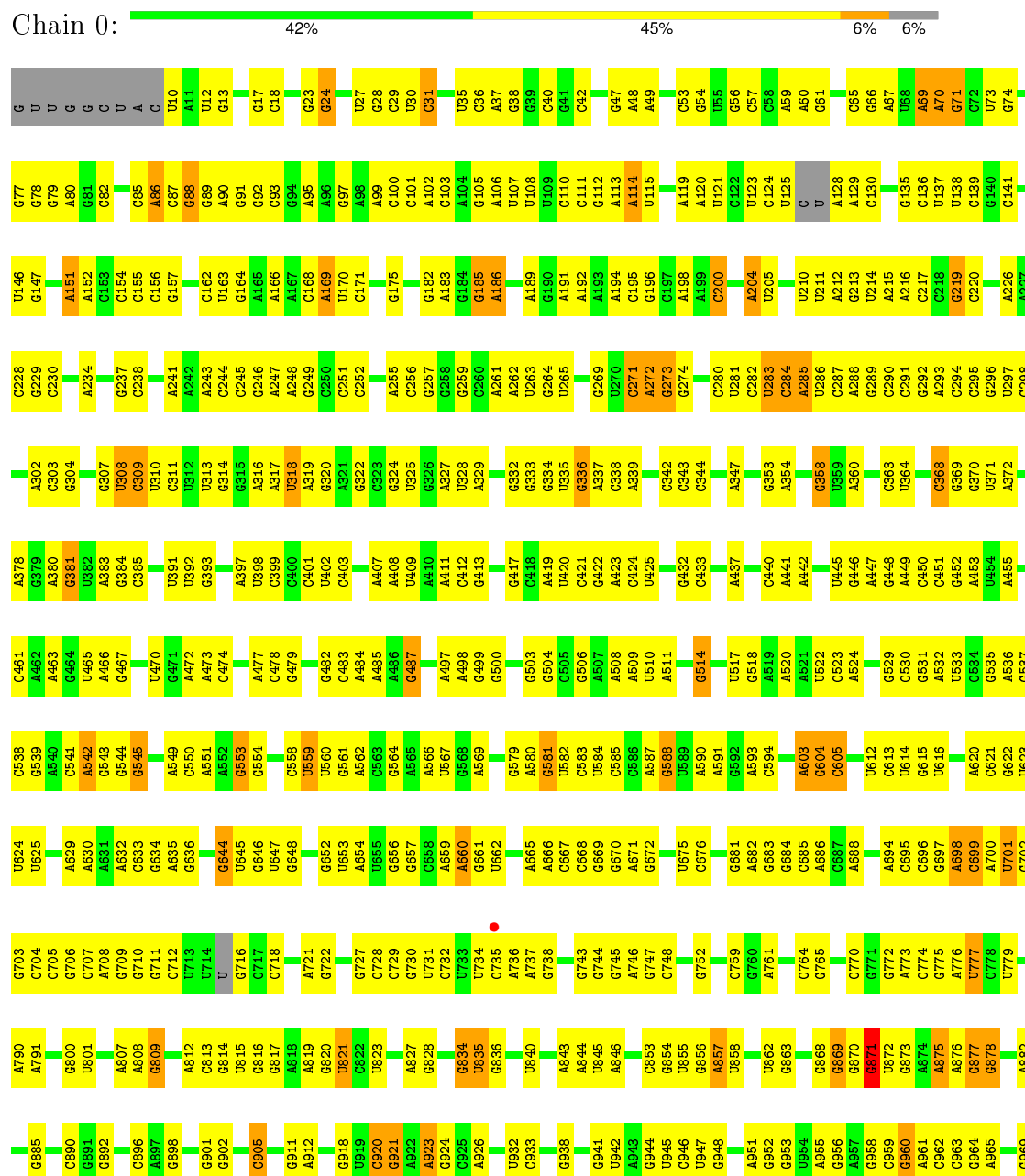
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	24	Total 24	O 24	0	0
40	Y	98	Total 98	O 98	0	0
40	Z	30	Total 30	O 30	0	0
40	1	58	Total 58	O 58	0	0
40	2	45	Total 45	O 45	0	0
40	3	70	Total 70	O 70	0	0
40	9	144	Total 144	O 144	0	0
40	4	13	Total 13	O 13	0	0



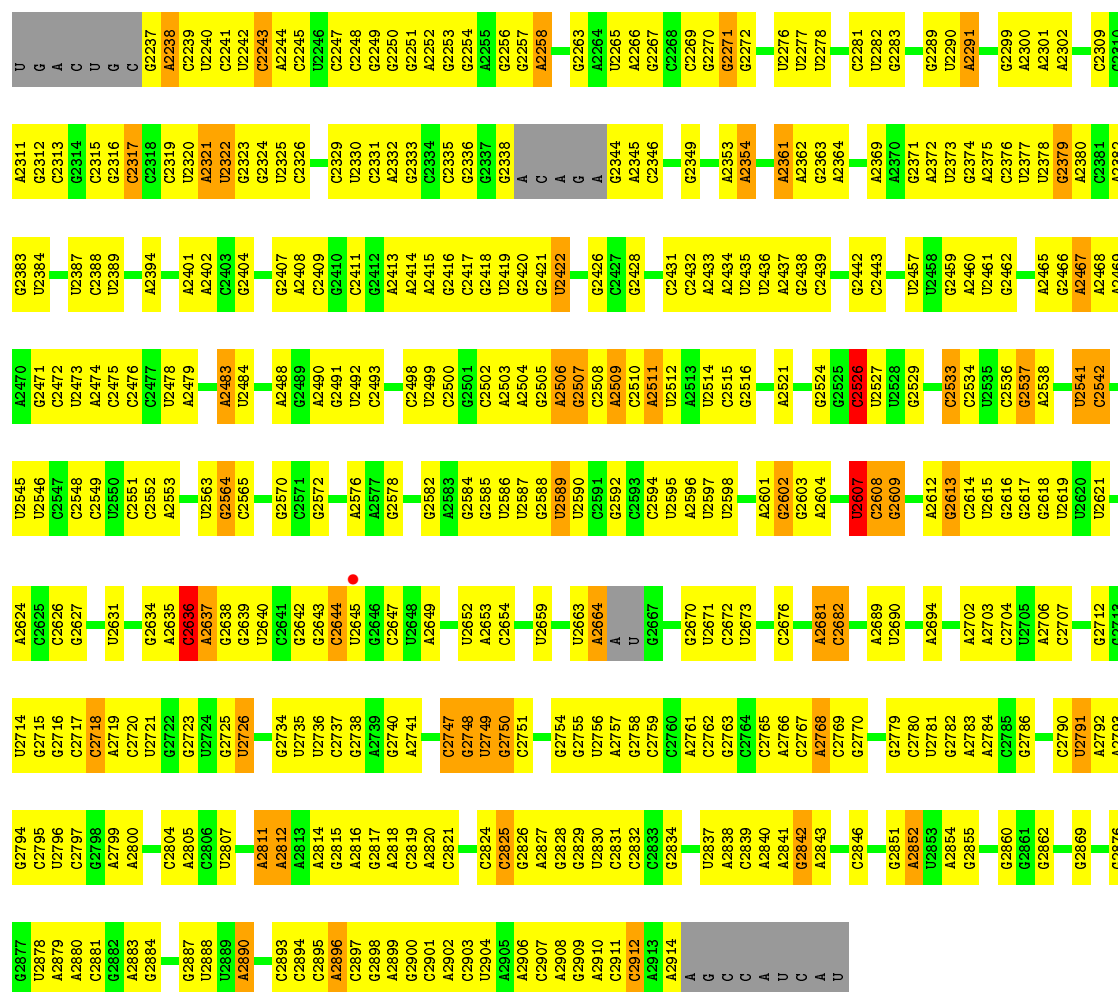
### 3 Residue-property plots

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

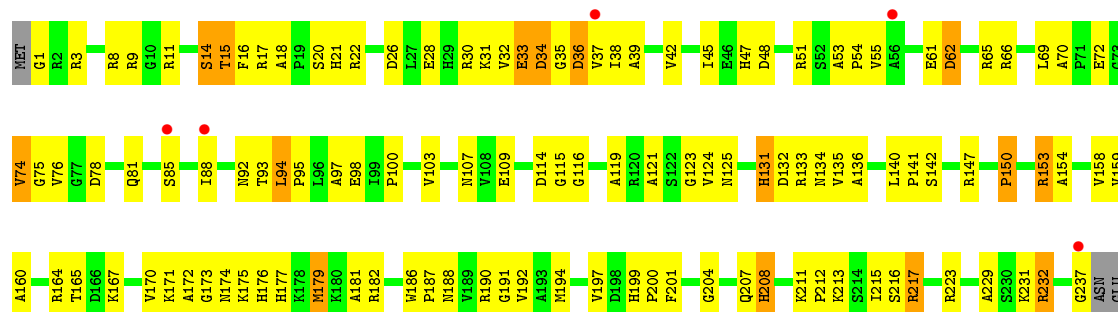
#### • Molecule 1: 23S ribosomal RNA



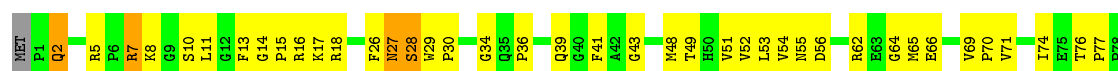


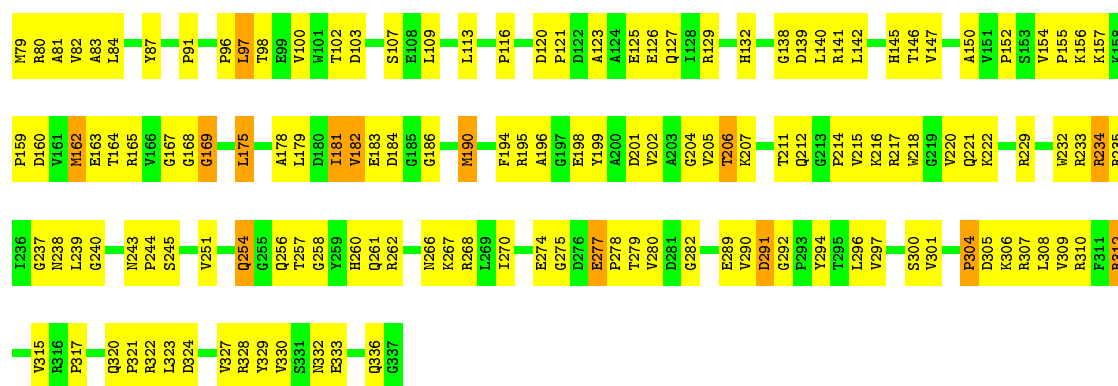


- Molecule 2: 50S ribosomal protein L2P



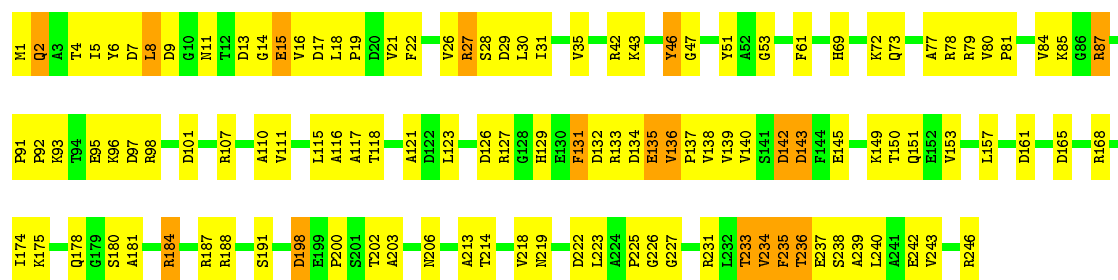
- Molecule 3: 50S ribosomal protein L3P





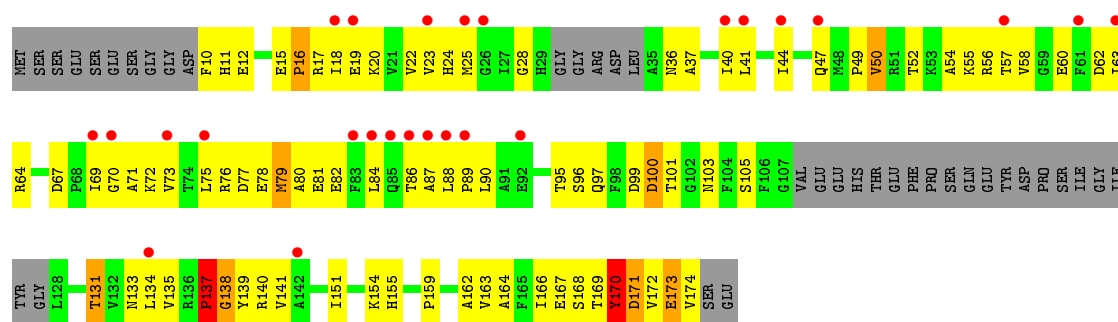
• Molecule 4: 50S ribosomal protein L4P

Chain C: 52% 41% 7%



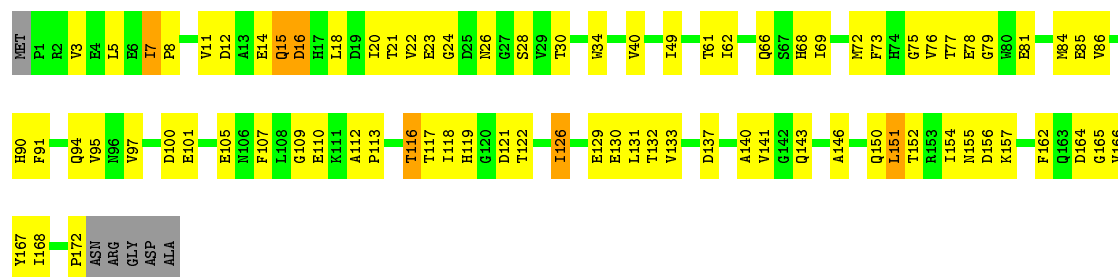
• Molecule 5: 50S ribosomal protein L5P

Chain D: 15% 31% 42% 5% 21%

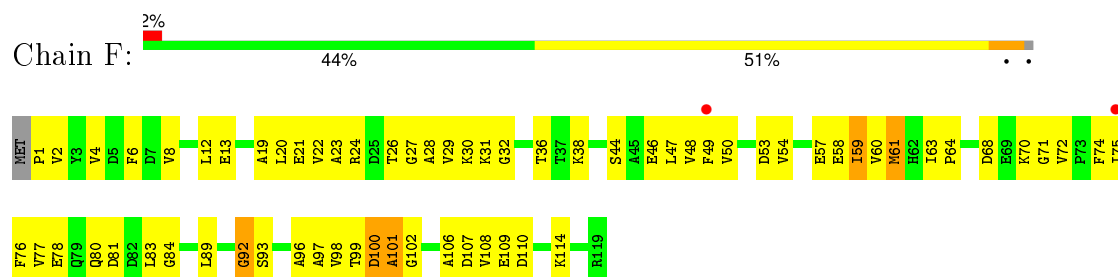


• Molecule 6: 50S ribosomal protein L6P

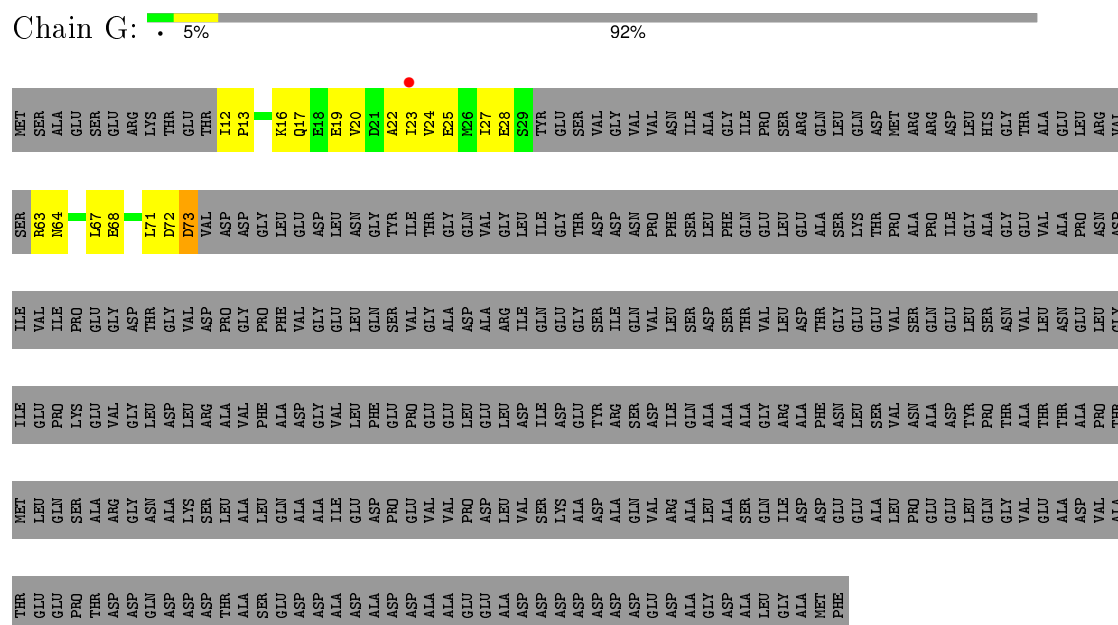
Chain E: 51% 42%



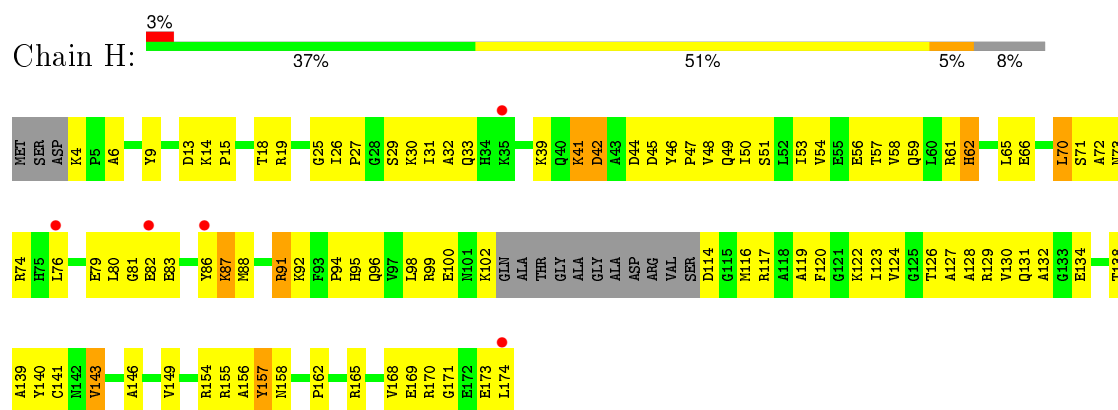
- Molecule 7: 50S ribosomal protein L7Ae



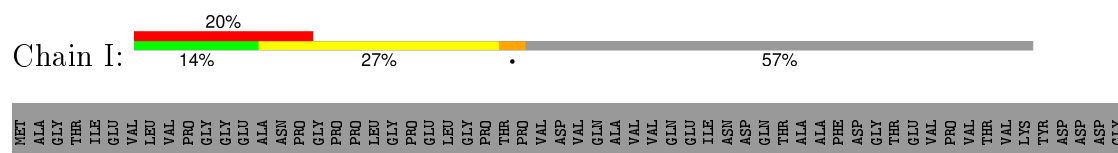
- Molecule 8: 50S ribosomal protein L10E

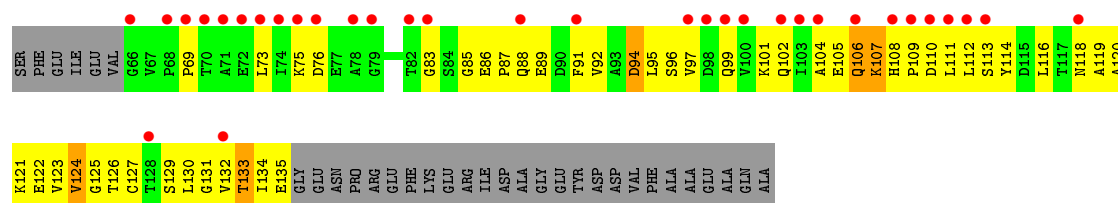


- Molecule 9: 50S ribosomal protein L10e



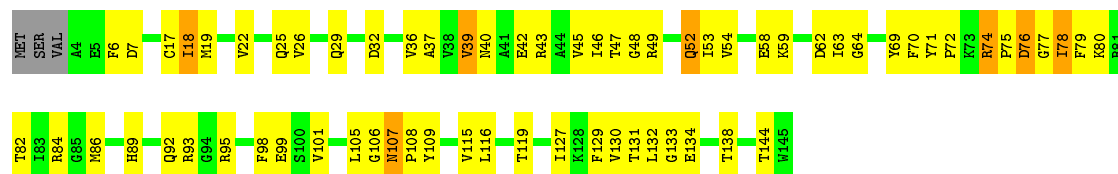
- Molecule 10: 50S ribosomal protein L11P





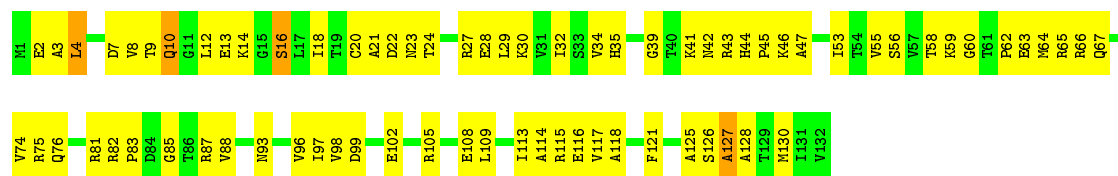
• Molecule 11: 50S ribosomal protein L13P

Chain J: 52% 41% 5%



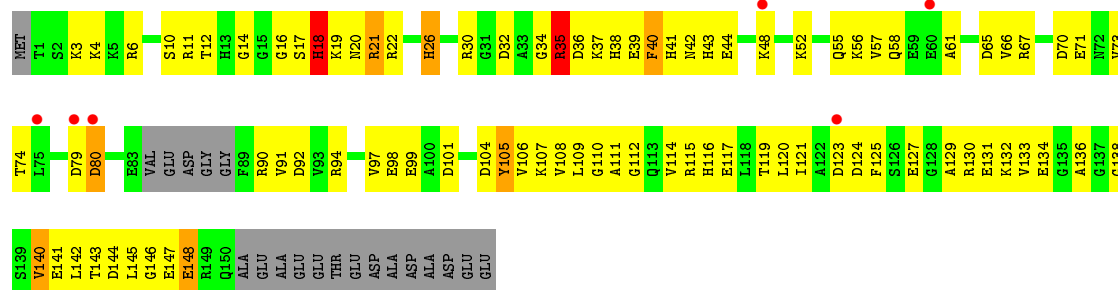
• Molecule 12: 50S ribosomal protein L14P

Chain K: 44% 53% 3%



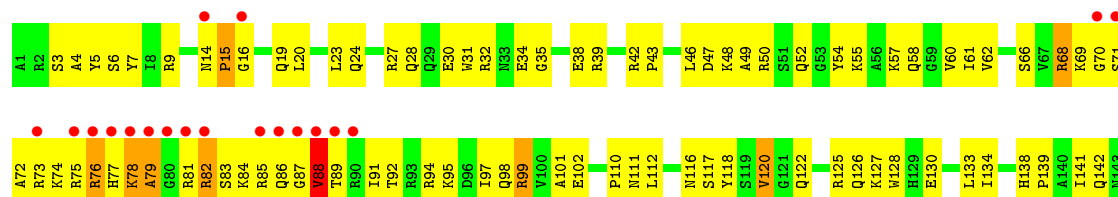
• Molecule 13: 50S ribosomal protein L15P

Chain L: 4% 34% 48% 12%



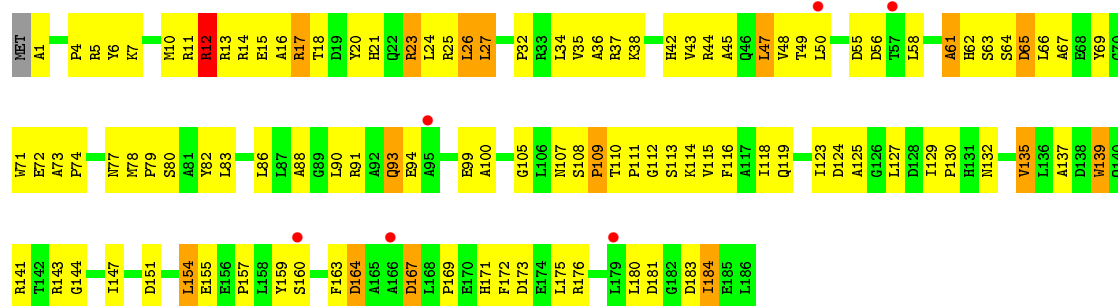
• Molecule 14: 50S ribosomal protein L15e

Chain M: 10% 42% 54% 2%

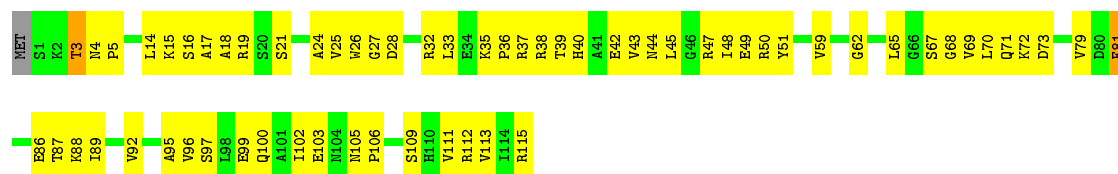




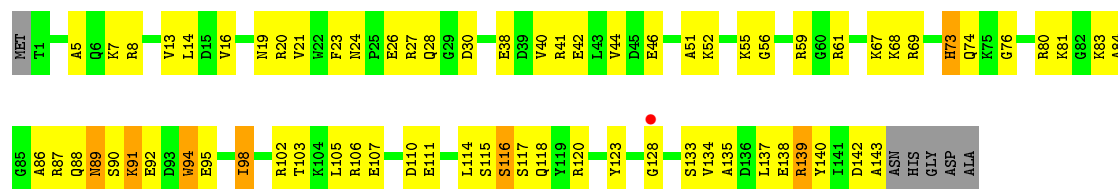
• Molecule 15: 50S ribosomal protein L18P



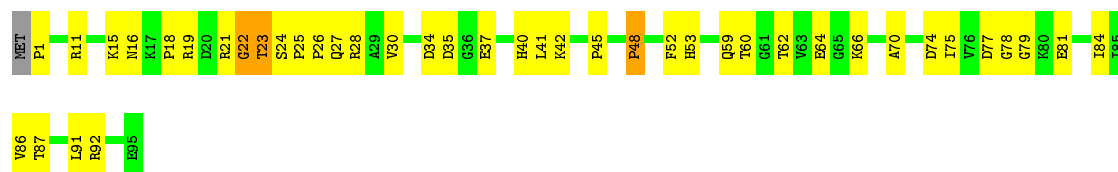
• Molecule 16: 50S ribosomal protein L18e



• Molecule 17: 50S ribosomal protein L19e

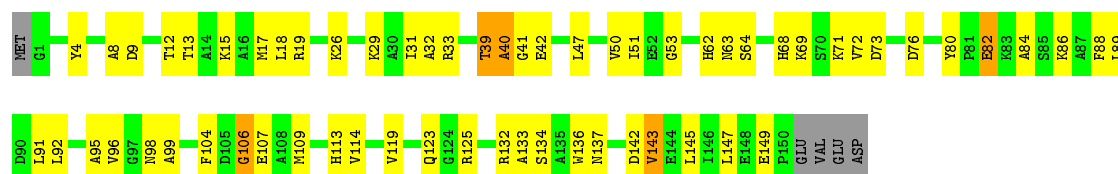


• Molecule 18: 50S ribosomal protein L21e

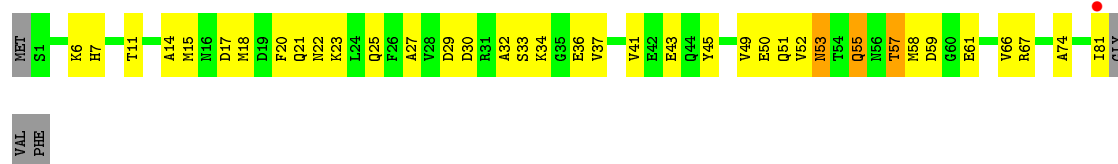


• Molecule 19: 50S ribosomal protein L22P

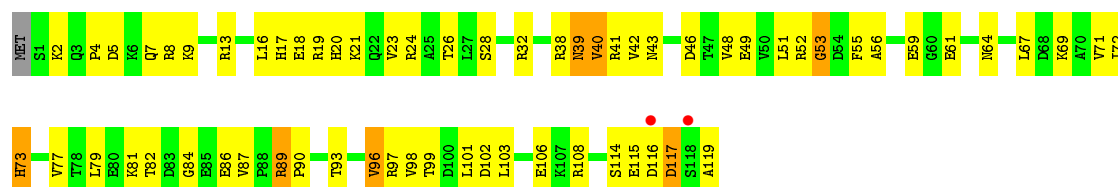




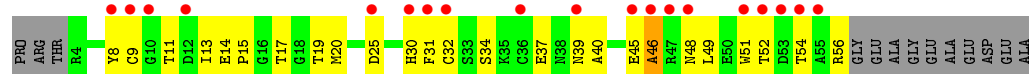
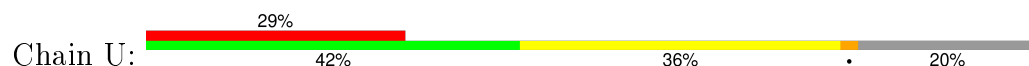
- Molecule 20: 50S ribosomal protein L23P



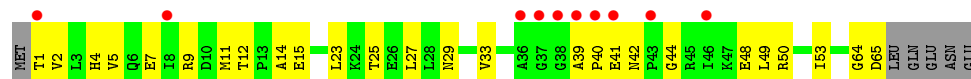
- Molecule 21: 50S ribosomal protein L24P



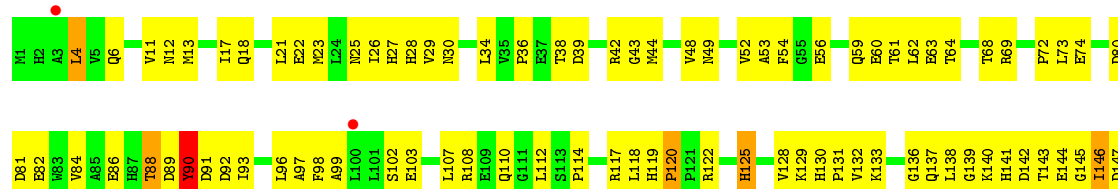
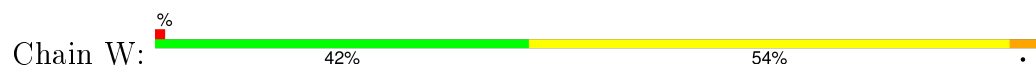
- Molecule 22: 50S ribosomal protein L24e



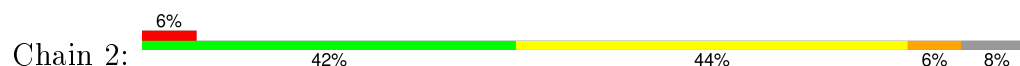
- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P

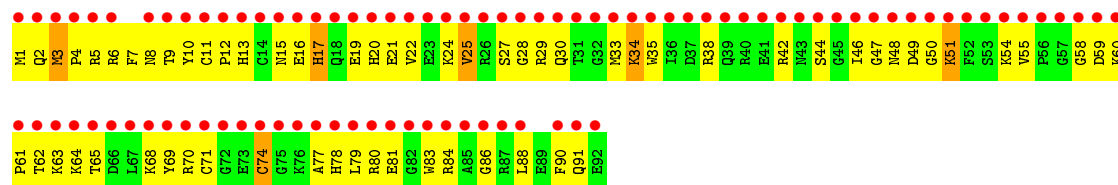




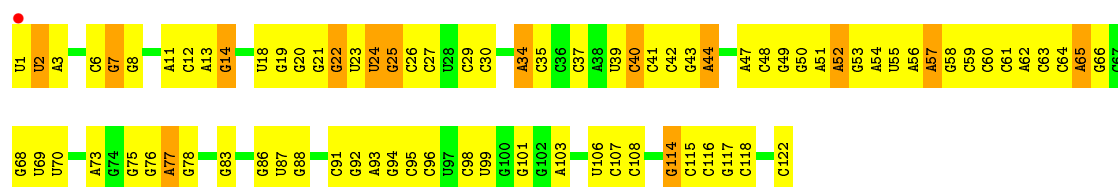




- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



- Molecule 32: DNA/RNA (5'-R(\*CP\*CP\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.32Å 299.65Å 574.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.11 85.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.98-3.11) 93.9 (85.39-2.40)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.260 0.230 , 0.262	Depositor DCC
$R_{free}$ test set	3147 reflections (1.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 92.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 667086 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	99287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, PO2, CD, 5AA, MYL, OMU, UR3, 2OP, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.42	0/65958	0.68	6/102869 (0.0%)
2	A	0.33	0/1786	0.64	0/2408
3	B	0.36	0/2690	0.64	0/3652
4	C	0.38	0/1885	0.63	0/2552
5	D	0.31	0/1111	0.56	0/1498
6	E	0.35	0/1382	0.59	0/1880
7	F	0.32	0/901	0.59	0/1224
8	G	0.31	0/241	0.49	0/324
9	H	0.31	0/1303	0.63	0/1743
10	I	0.28	0/526	0.54	0/716
11	J	0.38	0/1136	0.62	0/1530
12	K	0.36	0/1004	0.65	0/1351
13	L	0.33	0/1130	0.62	0/1509
14	M	0.36	0/1583	0.59	0/2116
15	N	0.29	0/1474	0.62	0/1999
16	O	0.33	0/874	0.61	0/1181
17	P	0.36	0/1147	0.57	0/1528
18	Q	0.35	0/749	0.65	0/1005
19	R	0.40	0/1172	0.62	0/1578
20	S	0.35	0/648	0.58	0/875
21	T	0.33	0/958	0.63	0/1289
22	U	0.31	0/417	0.55	0/562
23	V	0.30	0/502	0.57	0/675
24	W	0.37	0/1219	0.66	0/1655
25	X	0.37	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.30	0/584	0.54	0/781
28	1	0.40	0/438	0.58	0/578
29	2	0.33	0/401	0.53	0/529
30	3	0.29	0/771	0.51	0/1024
31	9	0.35	0/2904	0.69	0/4526
32	4	0.46	0/102	0.73	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.39	0/98806	0.66	6/147737 (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	0	0	12
24	W	0	1
31	9	0	1
32	4	0	1
All	All	0	15

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.22	122.09	114.00
1	0	1819	G	C5'-C4'-C3'	5.93	125.50	116.00
1	0	2726	U	N1-C1'-C2'	5.42	121.04	114.00
1	0	871	G	C5'-C4'-O4'	-5.40	102.62	109.10
1	0	1942	A	C5'-C4'-C3'	5.19	124.30	116.00
1	0	2636	C	N1-C1'-C2'	-5.14	106.34	112.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1236	A	Sidechain
1	0	1430	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	24	G	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2607	U	Sidechain
1	0	2636	C	Sidechain
1	0	2842	G	Sidechain

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Mol	Chain	Res	Type	Group
32	4	176	DA	Sidechain
31	9	94	G	Sidechain
24	W	90	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1595	1
2	A	1753	0	1766	134	0
3	B	2625	0	2533	203	0
4	C	1860	0	1813	134	0
5	D	1094	0	1085	96	0
6	E	1357	0	1266	75	0
7	F	890	0	843	63	0
8	G	240	0	231	26	0
9	H	1283	0	1292	91	0
10	I	519	0	500	56	0
11	J	1120	0	1098	81	0
12	K	994	0	1027	84	0
13	L	1118	0	1076	94	0
14	M	1559	0	1573	155	0
15	N	1445	0	1401	122	0
16	O	865	0	873	59	0
17	P	1136	0	1123	84	0
18	Q	735	0	729	42	0
19	R	1149	0	1122	73	0
20	S	641	0	605	36	0
21	T	950	0	924	73	0
22	U	410	0	368	29	0
23	V	499	0	511	32	0
24	W	1196	0	1137	102	0
25	X	654	0	653	50	0
26	Y	1130	0	1133	62	0
27	Z	573	0	535	61	0
28	1	431	0	426	41	0
29	2	396	0	413	35	0
30	3	755	0	732	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	2599	0	1325	91	0
32	4	127	0	76	37	0
33	0	83	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	63	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	93	0	0	0	0
37	1	1	0	0	0	0
37	3	2	0	0	0	0
37	9	3	0	0	0	0
37	A	2	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	0	35	0	41	22	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5841	0	0	203	0
40	1	58	0	0	4	0
40	2	45	0	0	2	0
40	3	70	0	0	6	0
40	4	13	0	0	7	0
40	9	144	0	0	7	0
40	A	117	0	0	8	0
40	B	151	0	0	16	0
40	C	175	0	0	21	0
40	D	49	0	0	6	0
40	E	40	0	0	7	0
40	F	29	0	0	5	0
40	G	18	0	0	1	0
40	H	76	0	0	11	0
40	I	10	0	0	3	0
40	J	57	0	0	2	0
40	K	62	0	0	7	0
40	L	91	0	0	12	0
40	M	148	0	0	13	0
40	N	61	0	0	8	0
40	O	41	0	0	2	0
40	P	61	0	0	3	0
40	Q	49	0	0	3	0
40	R	83	0	0	3	0
40	S	37	0	0	1	0
40	T	36	0	0	4	0
40	U	29	0	0	2	0
40	V	13	0	0	3	0
40	W	67	0	0	6	0
40	X	24	0	0	1	0
40	Y	98	0	0	5	0
40	Z	30	0	0	6	0
All	All	99287	0	60042	3609	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 24.

All (3609) 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)
40:0:4863:HOH:O	32:4:77:2OP:HB3	1.31	1.30
1:0:656:G:H5'	16:O:3:THR:HG22	1.20	1.15
1:0:871:G:C8	1:0:871:G:H5'	1.84	1.12
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.28	1.11
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.10
14:M:71:SER:HB2	14:M:92:THR:HG22	1.31	1.10
1:0:2431:C:H42	38:0:2924:MYL:HAB	1.09	1.09
1:0:871:G:H5'	1:0:871:G:H8	0.98	1.08
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.12	1.07
1:0:2717:C:H2'	1:0:2718:C:H5''	1.37	1.06
31:9:56:A:H2'	31:9:57:A:H5''	1.35	1.05
1:0:2637:A:N6	32:4:176:DA:H2'	1.70	1.05
30:3:38:ARG:HB3	30:3:42:ARG:HH12	1.19	1.05
27:Z:63:CYS:SG	27:Z:81:CYS:HB2	1.99	1.03
14:M:99:ARG:HH11	14:M:99:ARG:HG2	1.25	1.01
13:L:55:GLN:HA	13:L:58:GLN:HE21	1.25	1.01
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.43	1.00
4:C:127:ARG:NH2	4:C:225:PRO:HG2	1.77	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.43	0.99
1:0:2717:C:C2'	1:0:2718:C:H5''	1.92	0.98
1:0:2890:A:C8	22:U:56:ARG:HD2	1.99	0.98
29:2:41:HIS:H	29:2:45:ASN:HD22	1.00	0.97
1:0:2637:A:H5''	32:4:175:C:OP2	1.65	0.97
14:M:70:GLY:HA3	14:M:73:ARG:NH2	1.79	0.96
30:3:21:GLU:HG2	30:3:22:VAL:H	1.30	0.95
1:0:1242:A:H5'	11:J:82:THR:HG23	1.45	0.95
12:K:10:GLN:HE21	12:K:10:GLN:H	1.12	0.95
1:0:656:G:H5'	16:O:3:THR:CG2	1.96	0.94
15:N:141:ARG:NH2	31:9:48:C:H4'	1.83	0.94
4:C:78:ARG:HH11	4:C:78:ARG:HG3	1.30	0.94
30:3:60:LYS:HG3	30:3:61:PRO:HD2	1.50	0.94
1:0:681:G:N3	1:0:681:G:H5'	1.82	0.93
17:P:135:ALA:HB1	17:P:139:ARG:HH12	1.33	0.93
1:0:1119:G:H2'	11:J:52:GLN:NE2	1.81	0.93
1:0:2502:C:H2'	1:0:2503:A:H5'	1.51	0.93
1:0:2503:A:H5''	9:H:155:ARG:HH12	1.29	0.93
5:D:28:GLY:HA2	5:D:69:ILE:HG23	1.50	0.93
5:D:17:ARG:HH12	5:D:137:PRO:HA	1.29	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.50	0.92
15:N:17:ARG:HB3	15:N:17:ARG:HH11	1.35	0.92
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.34	0.92
9:H:72:ALA:HB2	9:H:156:ALA:HB2	1.51	0.91
1:0:823:U:H3'	40:0:3123:HOH:O	1.70	0.91
5:D:154:LYS:HD2	5:D:154:LYS:H	1.34	0.91
1:0:870:G:H2'	1:0:871:G:H5''	1.52	0.91
1:0:2506:A:HO2'	1:0:2507:G:H8	0.94	0.91
4:C:236:THR:HG22	4:C:239:ALA:H	1.36	0.90
2:A:153:ARG:HH11	2:A:153:ARG:HB2	1.33	0.90
1:0:1593:C:H5'	17:P:116:SER:O	1.71	0.90
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.17	0.89
11:J:131:THR:HB	11:J:134:GLU:HG3	1.53	0.89
12:K:10:GLN:NE2	12:K:10:GLN:H	1.71	0.89
1:0:2460:A:O4'	38:0:2924:MYL:HADB	1.72	0.89
30:3:3:MET:HG2	30:3:22:VAL:HG11	1.52	0.89
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.03	0.89
15:N:141:ARG:HH21	31:9:48:C:H4'	1.38	0.89
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.55	0.89
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.89
1:0:877:G:H5'	1:0:878:G:OP1	1.73	0.89
1:0:2468:A:H61	30:3:48:ASN:HD21	1.17	0.88
31:9:24:U:H3'	31:9:25:G:H5'	1.53	0.88
1:0:2618:G:O2'	32:4:76:5AA:H103	1.74	0.88
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.56	0.88
1:0:1205:U:H2'	1:0:1206:U:H5''	1.54	0.88
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.55	0.88
2:A:109:GLU:HG2	2:A:116:GLY:H	1.39	0.88
21:T:48:VAL:HG23	21:T:97:ARG:O	1.74	0.87
31:9:92:G:H2'	31:9:93:A:C8	2.10	0.87
1:0:381:G:H5''	40:M:2945:HOH:O	1.75	0.87
19:R:9:ASP:O	19:R:13:THR:HB	1.75	0.87
21:T:43:ASN:HD22	21:T:108:ARG:CZ	1.87	0.87
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.74	0.86
15:N:37:ARG:NH1	31:9:6:C:H5''	1.91	0.86
23:V:1:THR:HG23	23:V:2:VAL:H	1.38	0.86
12:K:39:GLY:HA2	40:K:4183:HOH:O	1.72	0.86
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.58	0.86
5:D:25:MET:HE3	5:D:37:ALA:HB1	1.57	0.85
1:0:156:C:H5''	14:M:171:ARG:HD3	1.58	0.85
17:P:115:SER:H	17:P:118:GLN:NE2	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.85
7:F:2:VAL:HG22	7:F:57:GLU:OE1	1.73	0.85
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.85
1:0:2263:G:H4'	14:M:70:GLY:HA2	1.56	0.85
1:0:2533:C:H5'	1:0:2533:C:H6	1.38	0.85
1:0:2467:A:H1'	40:0:3036:HOH:O	1.76	0.85
1:0:2578:G:H5'	1:0:2578:G:H8	1.40	0.84
14:M:97:ILE:HD12	14:M:127:LYS:HD2	1.59	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1116:U:O2'	1:0:1118:A:H2	1.57	0.84
3:B:320:GLN:HE21	3:B:321:PRO:HD2	1.42	0.84
1:0:2319:C:H3'	30:3:1:MET:N	1.92	0.84
1:0:735:C:H2'	1:0:736:A:O4'	1.78	0.84
31:9:14:G:H5'	31:9:14:G:H8	1.42	0.84
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.84
7:F:84:GLY:HA3	7:F:92:GLY:HA2	1.60	0.84
1:0:541:C:H2'	1:0:542:A:H5''	1.59	0.83
1:0:1835:U:H5	1:0:1840:A:N7	1.76	0.83
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.60	0.83
3:B:36:PRO:HA	3:B:168:GLY:HA3	1.58	0.83
31:9:56:A:C2'	31:9:57:A:H5''	2.07	0.83
1:0:1701:A:H5'	40:0:5659:HOH:O	1.77	0.83
1:0:506:G:H22	1:0:509:A:C5'	1.91	0.83
32:4:176:DA:OP1	40:4:334:HOH:O	1.94	0.83
5:D:57:THR:HG23	5:D:63:ILE:HA	1.61	0.83
1:0:1667:A:H8	1:0:1667:A:H5'	1.43	0.83
1:0:819:A:H5'	27:Z:37:ARG:HD3	1.59	0.83
3:B:62:ARG:HA	3:B:65:MET:HE2	1.58	0.83
6:E:116:THR:HG22	6:E:151:LEU:HD22	1.61	0.83
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.58	0.83
30:3:38:ARG:HB3	30:3:42:ARG:NH1	1.93	0.82
1:0:2503:A:H5''	9:H:155:ARG:NH1	1.94	0.82
11:J:39:VAL:HG22	11:J:106:GLY:O	1.79	0.82
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.59	0.82
31:9:29:C:H2'	31:9:30:C:H5'	1.61	0.82
15:N:37:ARG:HH12	31:9:6:C:H5''	1.44	0.82
1:0:2502:C:C2'	1:0:2503:A:H5'	2.09	0.81
20:S:51:GLN:HE21	20:S:53:ASN:HD21	1.25	0.81
26:Y:235:GLU:CD	26:Y:235:GLU:H	1.83	0.81
1:0:92:G:H4'	23:V:44:GLY:HA3	1.60	0.81
3:B:258:GLY:H	3:B:260:HIS:CE1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:162:MET:CE	3:B:310:ARG:HD3	2.10	0.81
1:O:200:C:H2'	40:O:7904:HOH:O	1.79	0.81
10:I:91:PHE:HD2	10:I:131:GLY:HA2	1.45	0.81
5:D:18:ILE:HG12	5:D:134:LEU:CD2	2.11	0.81
1:O:2419:U:H5''	1:O:2420:G:H5'	1.62	0.81
4:C:96:LYS:HB3	4:C:98:ARG:HH12	1.46	0.81
16:O:49:GLU:OE1	16:O:72:LYS:HG3	1.80	0.81
2:A:97:ALA:HA	2:A:131:HIS:NE2	1.95	0.81
20:S:11:THR:H	20:S:14:ALA:HB3	1.46	0.81
40:O:7291:HOH:O	3:B:211:THR:HG21	1.81	0.81
1:O:1160:G:H5'	1:O:1161:A:C5'	2.09	0.81
7:F:63:ILE:HB	7:F:64:PRO:HD3	1.62	0.80
19:R:99:ALA:HB1	19:R:109:MET:CE	2.11	0.80
21:T:9:LYS:HE3	21:T:13:ARG:NH1	1.96	0.80
1:O:506:G:H22	1:O:509:A:H5'	1.46	0.80
14:M:83:SER:HB2	30:3:47:GLY:HA2	1.64	0.80
1:O:2846:C:H4'	3:B:156:LYS:HB3	1.63	0.80
1:O:2431:C:N4	38:0:2924:MYL:HAB	1.93	0.80
38:0:2924:MYL:OAJ	38:0:2924:MYL:HBG	1.82	0.80
1:O:2637:A:C5'	32:4:175:C:OP2	2.29	0.80
11:J:74:ARG:HB3	11:J:74:ARG:HH11	1.47	0.80
1:O:1834:C:H2'	1:O:1840:A:N6	1.97	0.80
3:B:162:MET:HE2	3:B:310:ARG:HD3	1.62	0.80
32:4:75:C:C2'	40:4:6378:HOH:O	2.30	0.79
14:M:69:LYS:HG2	14:M:70:GLY:H	1.47	0.79
1:O:541:C:C2'	1:O:542:A:H5''	2.12	0.79
30:3:25:VAL:HG13	30:3:68:LYS:HE3	1.64	0.79
1:O:1446:U:H2'	20:S:55:GLN:NE2	1.97	0.79
1:O:870:G:C2'	1:O:871:G:H5''	2.12	0.79
1:O:1205:U:H2'	1:O:1206:U:C5'	2.12	0.79
7:F:29:VAL:HG12	7:F:98:VAL:HA	1.65	0.79
12:K:74:VAL:HG13	12:K:113:ILE:HG23	1.64	0.79
14:M:164:THR:HG22	14:M:166:ALA:N	1.97	0.79
17:P:103:THR:HA	17:P:106:ARG:NH1	1.98	0.79
1:O:710:G:OP1	16:O:24:ALA:HB3	1.83	0.79
1:O:871:G:C5'	1:O:871:G:H8	1.88	0.79
14:M:77:HIS:HE1	14:M:86:GLN:HE21	1.30	0.79
2:A:100:PRO:HG2	2:A:103:VAL:HG21	1.65	0.79
1:O:31:C:H4'	40:O:7242:HOH:O	1.82	0.78
1:O:2073:G:H5''	40:O:8371:HOH:O	1.83	0.78
1:O:380:A:OP2	14:M:9:ARG:HD2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:275:GLY:O	3:B:291:ASP:HA	1.83	0.78
3:B:62:ARG:HA	3:B:65:MET:CE	2.14	0.78
14:M:164:THR:HG22	14:M:166:ALA:H	1.47	0.78
2:A:88:ILE:HD13	2:A:100:PRO:HD3	1.62	0.78
1:0:420:U:H2'	1:0:421:C:H6	1.48	0.78
3:B:212:GLN:HB2	3:B:257:THR:HG21	1.64	0.78
1:0:2541:U:H4'	1:0:2542:C:OP1	1.84	0.78
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.66	0.78
1:0:2263:G:H4'	14:M:70:GLY:CA	2.14	0.77
1:0:558:C:C2'	1:0:559:U:H5''	2.13	0.77
1:0:100:C:H5'	21:T:16:LEU:HD12	1.65	0.77
1:0:2431:C:H42	38:0:2924:MYL:CAB	1.93	0.77
17:P:135:ALA:HB1	17:P:139:ARG:NH1	2.00	0.77
16:O:47:ARG:HG3	16:O:47:ARG:HH11	1.48	0.77
5:D:58:VAL:HB	5:D:62:ASP:HB3	1.63	0.77
12:K:28:GLU:OE2	12:K:58:THR:HG21	1.85	0.77
15:N:86:LEU:O	15:N:90:LEU:HG	1.84	0.77
1:0:2382:A:H4'	30:3:12:PRO:HD3	1.66	0.77
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.67	0.77
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.50	0.77
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.49	0.77
1:0:1666:C:O2'	1:0:1667:A:H5''	1.84	0.77
1:0:1372:A:H3'	40:0:6923:HOH:O	1.85	0.77
16:O:32:ARG:HD3	16:O:32:ARG:O	1.83	0.77
17:P:55:LYS:HG2	17:P:56:GLY:N	2.00	0.76
19:R:39:THR:HB	19:R:42:GLU:HG3	1.66	0.76
7:F:27:GLY:HA3	7:F:101:ALA:O	1.85	0.76
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.50	0.76
21:T:9:LYS:HE3	21:T:13:ARG:CZ	2.15	0.76
1:0:1189:A:H3'	40:0:7609:HOH:O	1.85	0.76
15:N:110:THR:HB	15:N:113:SER:OG	1.86	0.76
5:D:103:ASN:ND2	5:D:133:ASN:HA	2.01	0.76
14:M:99:ARG:CG	14:M:99:ARG:HH11	1.98	0.76
1:0:420:U:H2'	1:0:421:C:C6	2.20	0.76
12:K:23:ASN:HD21	12:K:108:GLU:H	1.33	0.76
1:0:1213:C:O2'	1:0:1214:G:H5'	1.86	0.76
9:H:62:HIS:HA	9:H:65:LEU:HD23	1.66	0.76
3:B:162:MET:HE1	3:B:308:LEU:HD21	1.67	0.76
3:B:195:ARG:HG2	3:B:323:LEU:HD22	1.68	0.76
2:A:217:ARG:HG2	2:A:229:ALA:HB2	1.66	0.76
11:J:26:VAL:HG13	11:J:36:VAL:HG11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:98:VAL:HG11	21:T:101:LEU:HD23	1.66	0.75
1:O:399:C:H5'	14:M:179:GLY:O	1.86	0.75
3:B:36:PRO:HG3	3:B:169:GLY:H	1.51	0.75
9:H:168:VAL:HG13	40:H:4963:HOH:O	1.86	0.75
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.67	0.75
19:R:99:ALA:HB1	19:R:109:MET:HE3	1.69	0.75
6:E:101:GLU:HB3	6:E:117:THR:HA	1.69	0.75
1:O:1759:A:N3	1:O:1818:C:H2'	2.01	0.75
1:O:204:A:H2'	1:O:205:U:H5'	1.69	0.75
1:O:2320:U:H5	30:3:1:MET:HE3	1.52	0.75
1:O:2420:G:O2'	1:O:2421:G:H5'	1.86	0.75
24:W:4:LEU:HD13	24:W:52:VAL:HG21	1.67	0.75
14:M:70:GLY:HA3	14:M:73:ARG:HH22	1.52	0.74
12:K:10:GLN:N	12:K:10:GLN:HE21	1.85	0.74
38:O:2924:MYL:HAZ	38:O:2924:MYL:HABB	1.68	0.74
1:O:1166:A:H61	1:O:1180:U:H3	1.32	0.74
15:N:169:PRO:O	15:N:172:PHE:HB3	1.88	0.74
1:O:1641:A:H2'	1:O:1642:A:H5'	1.68	0.74
15:N:38:LYS:HE2	15:N:107:ASN:ND2	2.02	0.74
16:O:73:ASP:HA	16:O:92:VAL:O	1.87	0.74
13:L:90:ARG:HA	13:L:119:THR:HB	1.69	0.74
7:F:58:GLU:CD	14:M:27:ARG:HH22	1.91	0.74
1:O:545:G:H8	1:O:545:G:H5'	1.52	0.74
1:O:282:C:H1'	1:O:368:C:N4	2.03	0.74
1:O:1528:A:H2'	1:O:1529:G:O4'	1.88	0.74
13:L:138:GLY:HA3	40:L:4360:HOH:O	1.87	0.74
14:M:68:ARG:NH2	14:M:73:ARG:HD3	2.03	0.74
3:B:18:ARG:HG3	3:B:256:GLN:HG3	1.68	0.74
7:F:61:MET:HB3	14:M:19:GLN:OE1	1.88	0.73
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.69	0.73
1:O:1679:C:H5'	40:O:3948:HOH:O	1.87	0.73
25:X:30:MET:HE1	25:X:55:ASN:HA	1.70	0.73
1:O:1300:G:H1'	40:O:3448:HOH:O	1.88	0.73
1:O:2055:A:H4'	19:R:132:ARG:NH2	2.02	0.73
1:O:2251:G:H2'	1:O:2252:A:C8	2.24	0.73
1:O:1116:U:H3	1:O:1246:A:H62	1.35	0.73
31:9:24:U:H3'	31:9:25:G:C5'	2.18	0.73
1:O:156:C:H5''	14:M:171:ARG:CD	2.18	0.73
1:O:2121:G:H21	14:M:86:GLN:HE22	1.35	0.73
1:O:2506:A:O2'	1:O:2507:G:H8	1.70	0.72
1:O:1603:A:H5'	1:O:1605:G:O4'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:45:VAL:HG23	11:J:130:VAL:O	1.89	0.72
29:2:41:HIS:N	29:2:45:ASN:HD22	1.82	0.72
1:0:1183:C:N4	1:0:1184:C:H41	1.86	0.72
1:0:2588:OMG:O6	32:4:75:C:N4	2.15	0.72
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.71	0.72
6:E:84:MET:HG2	6:E:168:ILE:HA	1.69	0.72
9:H:61:ARG:HH11	9:H:61:ARG:HG3	1.54	0.72
8:G:16:LYS:O	8:G:20:VAL:HG23	1.89	0.72
32:4:175:C:OP1	40:4:334:HOH:O	2.07	0.72
2:A:192:VAL:HG11	2:A:208:HIS:N	2.05	0.72
5:D:105:SER:HB2	5:D:131:THR:HG23	1.72	0.72
5:D:41:LEU:HA	5:D:44:ILE:HG22	1.70	0.72
1:0:2816:A:H5'	1:0:2817:G:H5'	1.69	0.72
1:0:1130:U:H5'	40:0:7596:HOH:O	1.90	0.72
3:B:84:LEU:HD23	3:B:142:LEU:HD23	1.71	0.72
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.71	0.72
40:0:8828:HOH:O	2:A:200:PRO:HA	1.89	0.72
15:N:11:ARG:HD3	31:9:114:G:O6	1.88	0.72
14:M:72:ALA:HB3	14:M:91:ILE:O	1.89	0.72
6:E:7:ILE:HG13	6:E:11:VAL:HB	1.72	0.72
1:0:447:A:OP1	21:T:2:LYS:HG2	1.90	0.72
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.70	0.72
1:0:2618:G:N3	32:4:76:5AA:C2	2.53	0.71
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.04	0.71
26:Y:219:GLU:HG3	26:Y:220:GLU:N	2.05	0.71
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.72	0.71
1:0:183:A:H1'	14:M:161:ARG:NH1	2.05	0.71
27:Z:34:SER:HB2	40:Z:3188:HOH:O	1.90	0.71
4:C:1:MET:HG2	4:C:2:GLN:H	1.55	0.71
1:0:1771:U:H1'	27:Z:47:ARG:NH2	2.05	0.71
24:W:63:GLU:HG2	24:W:93:ILE:HG22	1.73	0.71
32:4:75:C:H2'	40:4:6378:HOH:O	1.88	0.71
1:0:558:C:H2'	1:0:559:U:H5''	1.72	0.71
22:U:34:SER:HA	22:U:37:GLU:HB2	1.72	0.71
1:0:926:A:H4'	13:L:39:GLU:HG2	1.71	0.71
4:C:236:THR:HA	40:C:6502:HOH:O	1.90	0.71
1:0:2533:C:C6	1:0:2533:C:H5'	2.24	0.71
1:0:2618:G:N3	32:4:76:5AA:H2	2.06	0.71
4:C:129:HIS:CE1	4:C:231:ARG:HA	2.26	0.71
21:T:41:ARG:HG2	21:T:41:ARG:HH11	1.55	0.71
4:C:236:THR:CG2	4:C:239:ALA:H	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:H2'	1:0:542:A:C5'	2.20	0.71
28:1:5:THR:N	28:1:6:PRO:HD2	2.05	0.71
3:B:27:ASN:H	3:B:27:ASN:HD22	1.39	0.71
1:0:2820:A:OP1	3:B:98:THR:HG22	1.91	0.71
38:0:2924:MYL:HBD	38:0:2924:MYL:OAR	1.89	0.71
21:T:48:VAL:HG21	21:T:96:VAL:HG13	1.72	0.71
1:0:450:C:OP1	4:C:184:ARG:NH2	2.23	0.71
1:0:853:C:H3'	40:0:3276:HOH:O	1.91	0.70
24:W:151:GLU:O	24:W:154:ARG:HG3	1.91	0.70
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.21	0.70
24:W:81:ASP:OD1	24:W:92:ASP:HB2	1.90	0.70
1:0:1973:A:H2'	1:0:1974:G:O4'	1.91	0.70
1:0:2316:G:O2'	30:3:61:PRO:HG3	1.90	0.70
1:0:1118:A:H3'	1:0:1118:A:C8	2.25	0.70
24:W:141:HIS:HB2	24:W:146:ILE:HG12	1.72	0.70
11:J:107:ASN:ND2	11:J:109:TYR:H	1.89	0.70
21:T:16:LEU:HA	21:T:19:ARG:HG3	1.74	0.70
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.74	0.70
1:0:2472:C:O2'	1:0:2634:G:H4'	1.91	0.70
30:3:71:CYS:HB3	30:3:74:CYS:HB3	1.72	0.70
6:E:154:ILE:HD11	6:E:157:LYS:HB2	1.73	0.70
28:1:25:LYS:HD2	29:2:49:GLU:H	1.56	0.70
14:M:72:ALA:HB2	14:M:92:THR:HA	1.72	0.70
1:0:2320:U:H2'	30:3:2:GLN:HB2	1.74	0.70
31:9:13:A:O2'	31:9:14:G:H5''	1.91	0.70
4:C:115:LEU:HD21	4:C:243:VAL:HG22	1.72	0.70
1:0:1377:C:H6	1:0:1377:C:H5'	1.56	0.70
23:V:1:THR:HG23	23:V:2:VAL:N	2.07	0.70
1:0:1527:A:H1'	1:0:1528:A:C8	2.27	0.70
9:H:41:LYS:HE2	9:H:45:ASP:HB3	1.72	0.70
15:N:119:GLN:O	15:N:123:ILE:HG13	1.92	0.70
1:0:820:G:H3'	40:0:6474:HOH:O	1.92	0.70
1:0:2542:C:H4'	32:4:75:C:O2'	1.92	0.70
12:K:98:VAL:HG11	12:K:102:GLU:HA	1.72	0.70
25:X:79:GLU:CD	25:X:80:GLU:H	1.95	0.70
40:0:4808:HOH:O	3:B:267:LYS:HD3	1.92	0.70
1:0:2291:A:C8	1:0:2309:C:H5'	2.27	0.70
3:B:320:GLN:NE2	3:B:321:PRO:HD2	2.07	0.69
22:U:9:CYS:HA	22:U:52:THR:HG23	1.74	0.69
31:9:73:A:H61	31:9:108:C:H42	1.40	0.69
17:P:55:LYS:HG2	17:P:56:GLY:H	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:51:ALA:HA	40:Z:3188:HOH:O	1.92	0.69
1:0:69:A:H5'	1:0:69:A:H8	1.56	0.69
15:N:61:ALA:CB	15:N:88:ALA:HB2	2.21	0.69
31:9:3:A:N6	31:9:22:G:H1'	2.07	0.69
3:B:312:ARG:HD3	3:B:315:VAL:HG13	1.72	0.69
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.08	0.69
1:0:1688:G:O2'	28:1:5:THR:HG23	1.92	0.69
1:0:1474:C:H6	1:0:1474:C:H5'	1.58	0.69
30:3:24:LYS:HG3	30:3:90:PHE:CZ	2.28	0.69
31:9:54:A:O2'	31:9:55:U:H5'	1.93	0.69
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.22	0.69
1:0:1224:G:H2'	1:0:1225:C:C6	2.27	0.69
19:R:12:THR:HG22	19:R:149:GLU:OE1	1.93	0.69
18:Q:75:ILE:HG12	18:Q:84:ILE:HD12	1.74	0.69
1:0:2353:A:H1'	18:Q:21:ARG:HH12	1.56	0.69
27:Z:70:ARG:HH12	27:Z:82:SER:C	1.95	0.69
10:I:91:PHE:CD2	10:I:131:GLY:HA2	2.26	0.69
12:K:62:PRO:HG3	12:K:65:ARG:NH2	2.07	0.69
20:S:33:SER:O	20:S:37:VAL:HG23	1.93	0.69
38:0:2924:MYL:CBC	38:0:2924:MYL:OAJ	2.40	0.69
11:J:19:MET:CE	11:J:132:LEU:HD11	2.21	0.69
4:C:236:THR:HG22	4:C:239:ALA:N	2.07	0.69
3:B:162:MET:CE	3:B:308:LEU:HD21	2.21	0.69
1:0:447:A:O2'	1:0:448:G:H5'	1.92	0.69
1:0:69:A:H5'	1:0:69:A:C8	2.28	0.69
4:C:139:VAL:HG13	40:C:6251:HOH:O	1.92	0.69
10:I:95:LEU:HD23	10:I:99:GLN:OE1	1.93	0.69
1:0:902:G:N7	13:L:18:HIS:HD2	1.90	0.69
4:C:98:ARG:HG2	4:C:98:ARG:HH11	1.58	0.69
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.22	0.69
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.69
1:0:1162:G:H1'	10:I:112:LEU:HD11	1.74	0.69
1:0:721:A:H4'	16:O:51:TYR:CD1	2.28	0.69
1:0:1132:A:N6	1:0:1229:C:H2'	2.07	0.69
1:0:926:A:O2'	13:L:41:HIS:HD2	1.76	0.68
1:0:1762:C:H2'	1:0:1763:C:H6	1.57	0.68
18:Q:16:ASN:HD21	18:Q:45:PRO:HD2	1.59	0.68
1:0:533:U:H3'	40:0:8292:HOH:O	1.92	0.68
1:0:1835:U:C5	1:0:1840:A:N7	2.60	0.68
1:0:1771:U:H1'	27:Z:47:ARG:HH21	1.58	0.68
4:C:78:ARG:HG3	4:C:78:ARG:NH1	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H5'	1:0:1868:G:H5'	1.76	0.68
13:L:145:LEU:O	13:L:148:GLU:HG3	1.92	0.68
11:J:95:ARG:O	11:J:99:GLU:HG3	1.93	0.68
38:0:2924:MYL:OAJ	38:0:2924:MYL:CBG	2.42	0.68
19:R:17:MET:HE1	19:R:19:ARG:NH2	2.09	0.68
4:C:246:ARG:NH1	4:C:246:ARG:HB3	2.09	0.68
1:0:1191:A:H2'	1:0:1193:A:H5'	1.76	0.68
1:0:2717:C:H2'	1:0:2718:C:C5'	2.20	0.68
11:J:107:ASN:C	11:J:107:ASN:HD22	1.96	0.68
22:U:52:THR:HG22	22:U:54:THR:H	1.59	0.68
1:0:280:C:H2'	1:0:281:U:O4'	1.94	0.68
4:C:246:ARG:HH11	4:C:246:ARG:HB3	1.58	0.68
25:X:25:ARG:HD3	25:X:64:ALA:O	1.93	0.68
30:3:78:HIS:O	30:3:79:LEU:HD23	1.94	0.68
1:0:2460:A:H5''	30:3:59:ASP:HA	1.75	0.68
29:2:41:HIS:H	29:2:45:ASN:ND2	1.84	0.68
27:Z:54:GLU:HG2	27:Z:57:MET:CE	2.23	0.68
1:0:2769:C:H2'	1:0:2770:G:O4'	1.93	0.68
1:0:56:G:H5''	23:V:50:ARG:HH12	1.58	0.68
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.68
1:0:42:C:H1'	40:0:3438:HOH:O	1.94	0.68
24:W:52:VAL:HG22	24:W:53:ALA:N	2.09	0.67
24:W:110:GLN:HA	24:W:110:GLN:NE2	2.09	0.67
1:0:2005:G:H3'	1:0:2005:G:OP2	1.93	0.67
29:2:35:ARG:HD3	29:2:37:HIS:NE2	2.08	0.67
1:0:2904:U:H4'	25:X:8:ARG:NH1	2.08	0.67
2:A:30:ARG:HG2	2:A:31:LYS:N	2.09	0.67
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.76	0.67
1:0:877:G:H3'	40:0:6671:HOH:O	1.94	0.67
21:T:26:THR:HG23	21:T:97:ARG:HG3	1.75	0.67
14:M:81:ARG:NH1	14:M:81:ARG:HB2	2.10	0.67
18:Q:21:ARG:HG2	18:Q:22:GLY:H	1.59	0.67
2:A:51:ARG:NH2	2:A:53:ALA:HB3	2.08	0.67
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.42	0.67
24:W:64:THR:O	24:W:68:THR:HG22	1.94	0.67
14:M:91:ILE:HG21	40:M:533:HOH:O	1.95	0.67
1:0:1206:U:H5'	1:0:1206:U:H6	1.60	0.67
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.75	0.67
1:0:656:G:C5'	16:O:3:THR:HG22	2.12	0.67
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.29	0.67
31:9:12:C:H5'	31:9:70:U:O4'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:30:PRO:HB2	3:B:39:GLN:NE2	2.08	0.67
1:0:2435:U:O2'	30:3:68:LYS:HE2	1.95	0.67
1:0:2491:G:H5'	40:0:4195:HOH:O	1.94	0.67
1:0:1375:A:C2'	1:0:1376:G:H5'	2.24	0.67
1:0:1375:A:H2'	1:0:1376:G:H5'	1.77	0.67
1:0:1119:G:H22	1:0:1246:A:H2	1.42	0.67
10:I:91:PHE:HA	10:I:131:GLY:CA	2.25	0.67
21:T:98:VAL:HG11	21:T:101:LEU:CD2	2.25	0.67
2:A:192:VAL:HB	40:A:4780:HOH:O	1.94	0.67
1:0:1500:U:P	17:P:41:ARG:HH22	2.18	0.67
9:H:102:LYS:HD3	9:H:122:LYS:HD3	1.77	0.67
13:L:30:ARG:HH11	13:L:30:ARG:HG3	1.60	0.67
1:0:1244:U:OP1	11:J:18:ILE:HD13	1.95	0.66
4:C:127:ARG:HH21	4:C:225:PRO:HG2	1.59	0.66
26:Y:189:ASN:HD22	26:Y:189:ASN:C	1.99	0.66
1:0:559:U:H2'	1:0:560:U:O4'	1.94	0.66
1:0:1118:A:H3'	1:0:1118:A:H8	1.60	0.66
30:3:11:CYS:HB2	30:3:20:HIS:NE2	2.10	0.66
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.61	0.66
1:0:558:C:O2'	1:0:559:U:H5''	1.95	0.66
15:N:62:HIS:HB3	15:N:65:ASP:OD1	1.95	0.66
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.77	0.66
17:P:105:LEU:HD21	17:P:137:LEU:HD21	1.77	0.66
1:0:136:C:H2'	1:0:137:U:O4'	1.94	0.66
1:0:559:U:H6	1:0:559:U:H5'	1.60	0.66
29:2:36:ASN:H	29:2:39:ARG:NH2	1.93	0.66
1:0:2578:G:C8	1:0:2578:G:H5'	2.29	0.66
1:0:951:A:H5''	18:Q:42:LYS:HD3	1.75	0.66
6:E:20:ILE:HD11	6:E:40:VAL:HG11	1.77	0.66
4:C:26:VAL:HG22	4:C:117:ALA:HB2	1.77	0.66
2:A:33:GLU:H	2:A:33:GLU:CD	1.99	0.66
1:0:2768:A:O2'	1:0:2769:C:H5'	1.95	0.66
1:0:1939:U:H5''	2:A:237:GLY:O	1.94	0.66
10:I:120:ALA:O	10:I:124:VAL:HG23	1.95	0.66
1:0:297:U:H2'	1:0:298:C:C6	2.31	0.66
14:M:84:LYS:HD3	40:M:674:HOH:O	1.96	0.66
14:M:77:HIS:CE1	14:M:86:GLN:HE21	2.13	0.66
4:C:218:VAL:HG12	40:C:5065:HOH:O	1.95	0.66
1:0:1624:A:H4'	1:0:1626:A:H5''	1.77	0.66
1:0:2716:G:H5'	3:B:262:ARG:HG3	1.78	0.66
1:0:2460:A:H4'	30:3:58:GLY:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1209:C:H2'	1:0:1210:G:H8	1.60	0.66
1:0:2716:G:H5''	3:B:206:THR:HG21	1.76	0.66
3:B:5:ARG:HD2	3:B:8:LYS:HE2	1.78	0.66
1:0:2526:C:O2'	1:0:2527:U:H5'	1.96	0.66
1:0:1942:A:H2'	1:0:1943:C:H6	1.60	0.66
15:N:113:SER:HB2	40:N:6448:HOH:O	1.95	0.66
1:0:282:C:O2'	1:0:283:U:H5'	1.95	0.66
1:0:2253:G:H2'	1:0:2254:G:H8	1.61	0.66
27:Z:101:LYS:HA	27:Z:104:ARG:NH1	2.10	0.66
1:0:10:U:H6	1:0:10:U:H3'	1.61	0.66
13:L:79:ASP:HB3	40:L:4967:HOH:O	1.95	0.66
14:M:74:LYS:HD3	14:M:91:ILE:HD11	1.76	0.66
1:0:281:U:H2'	1:0:282:C:O4'	1.96	0.66
1:0:2338:G:H1'	5:D:105:SER:OG	1.95	0.66
14:M:74:LYS:HG3	40:M:3198:HOH:O	1.95	0.65
11:J:39:VAL:CG2	11:J:107:ASN:HA	2.27	0.65
13:L:65:ASP:HA	13:L:109:LEU:O	1.96	0.65
1:0:2694:A:H4'	6:E:91:PHE:HE1	1.60	0.65
1:0:1589:G:H22	1:0:1605:G:H1'	1.61	0.65
1:0:371:U:H2'	1:0:372:A:H8	1.61	0.65
1:0:12:U:H2'	1:0:13:G:H5'	1.78	0.65
38:0:2924:MYL:HACB	38:0:2924:MYL:HANA	1.78	0.65
21:T:40:VAL:HG23	21:T:119:ALA:OXT	1.96	0.65
1:0:1118:A:H8	1:0:1119:G:H5''	1.61	0.65
1:0:2510:C:H42	1:0:2564:G:H22	1.44	0.65
2:A:153:ARG:CB	2:A:153:ARG:HH11	2.07	0.65
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.37	0.65
12:K:87:ARG:HB2	22:U:19:THR:HG23	1.78	0.65
20:S:33:SER:OG	20:S:36:GLU:HG3	1.96	0.65
1:0:10:U:O4	1:0:531:G:H2'	1.96	0.65
3:B:41:PHE:CD1	3:B:79:MET:HE2	2.32	0.65
40:0:4078:HOH:O	28:1:1:THR:HA	1.96	0.65
1:0:558:C:H2'	1:0:559:U:C5'	2.26	0.65
13:L:80:ASP:HB2	13:L:90:ARG:O	1.97	0.65
4:C:77:ALA:O	4:C:78:ARG:HG3	1.97	0.65
1:0:1182:C:HO2'	1:0:1183:C:H5	1.44	0.65
1:0:1446:U:H2'	20:S:55:GLN:HE22	1.60	0.65
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.79	0.65
1:0:657:G:OP1	4:C:27:ARG:NH2	2.28	0.65
23:V:64:GLY:O	23:V:65:ASP:HB2	1.95	0.65
1:0:1654:U:H2'	2:A:47:HIS:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:21:GLU:HG2	30:3:22:VAL:N	2.08	0.65
11:J:109:TYR:HE1	40:J:7556:HOH:O	1.80	0.65
1:0:1555:G:H4'	1:0:1630:A:H2	1.61	0.65
1:0:2114:C:O2'	1:0:2115:U:H5'	1.96	0.65
15:N:27:LEU:HD21	15:N:50:LEU:HD13	1.77	0.65
1:0:1838:U:H1'	1:0:2644:C:H5'	1.78	0.65
3:B:179:LEU:O	3:B:183:GLU:HG2	1.96	0.65
12:K:81:ARG:HD3	12:K:87:ARG:NH1	2.11	0.65
25:X:20:GLU:HG3	25:X:21:PRO:HD2	1.78	0.65
1:0:523:C:H2'	1:0:524:A:C8	2.32	0.65
1:0:1589:G:N2	1:0:1605:G:H1'	2.12	0.65
1:0:1477:C:H5'	1:0:1868:G:C5'	2.27	0.65
2:A:76:VAL:HG23	27:Z:87:LYS:O	1.97	0.65
12:K:41:LYS:HE3	40:K:7871:HOH:O	1.97	0.65
23:V:39:ALA:N	23:V:40:PRO:HD2	2.12	0.65
1:0:2748:G:H5'	40:0:7410:HOH:O	1.97	0.65
38:0:2924:MYL:HABB	38:0:2924:MYL:CAZ	2.25	0.64
14:M:81:ARG:HG2	14:M:85:ARG:O	1.97	0.64
40:0:5319:HOH:O	28:1:6:PRO:HB3	1.96	0.64
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.61	0.64
5:D:47:GLN:HE21	5:D:75:LEU:HD23	1.61	0.64
15:N:164:ASP:OD1	15:N:167:ASP:HA	1.96	0.64
1:0:706:G:HO2'	1:0:707:C:H6	1.42	0.64
14:M:69:LYS:HB2	14:M:126:GLN:N	2.12	0.64
6:E:7:ILE:HD11	6:E:11:VAL:O	1.96	0.64
1:0:182:G:H5'	40:0:4102:HOH:O	1.97	0.64
17:P:7:LYS:HD3	17:P:23:PHE:CE1	2.33	0.64
13:L:12:THR:HG21	13:L:16:GLY:O	1.96	0.64
1:0:1595:G:O2'	1:0:1596:U:H5'	1.97	0.64
7:F:21:GLU:O	7:F:24:ARG:HG3	1.97	0.64
1:0:705:C:H2'	1:0:705:C:O2	1.97	0.64
4:C:127:ARG:CZ	4:C:225:PRO:HG2	2.26	0.64
9:H:59:GLN:NE2	9:H:129:ARG:HE	1.95	0.64
24:W:132:VAL:HG21	24:W:140:LYS:O	1.97	0.64
1:0:1441:G:H1'	40:0:7717:HOH:O	1.97	0.64
3:B:205:VAL:HA	3:B:260:HIS:O	1.96	0.64
1:0:1189:A:H1'	1:0:1209:C:O4'	1.97	0.64
14:M:134:ILE:HG23	14:M:141:ILE:HD13	1.80	0.64
9:H:72:ALA:CB	9:H:156:ALA:HB2	2.27	0.64
1:0:564:G:H1'	40:0:5694:HOH:O	1.95	0.64
2:A:167:LYS:HE2	27:Z:50:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:157:G:H4'	14:M:95:LYS:HE2	1.79	0.64
32:4:76:5AA:C4	40:4:6378:HOH:O	2.45	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.71	0.64
1:0:2613:G:O2'	1:0:2614:C:H5'	1.97	0.64
1:0:2469:A:H1'	40:0:7148:HOH:O	1.96	0.64
1:0:2382:A:O2'	30:3:12:PRO:HB3	1.98	0.64
1:0:1741:U:H5'	1:0:1742:A:OP1	1.97	0.64
9:H:146:ALA:O	9:H:149:VAL:HG12	1.97	0.64
26:Y:182:PHE:HD2	26:Y:200:THR:O	1.81	0.64
1:0:1201:C:H2'	1:0:1202:A:H5'	1.80	0.64
1:0:204:A:C2'	1:0:205:U:H5'	2.27	0.64
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.28	0.64
2:A:199:HIS:CD2	2:A:201:PHE:H	2.15	0.64
12:K:28:GLU:HG2	12:K:58:THR:HB	1.80	0.64
3:B:56:ASP:HB2	3:B:322:ARG:HE	1.61	0.64
1:0:1015:C:H2'	1:0:1016:U:H6	1.61	0.64
16:O:44:ASN:OD1	16:O:65:LEU:HB2	1.98	0.64
6:E:5:LEU:HD21	6:E:66:GLN:HG3	1.80	0.64
1:0:262:A:C6	7:F:89:LEU:HD21	2.33	0.64
26:Y:234:VAL:HG12	26:Y:235:GLU:H	1.63	0.64
2:A:48:ASP:HB3	40:A:5706:HOH:O	1.96	0.64
1:0:470:U:O2'	28:1:16:HIS:HD2	1.80	0.64
1:0:1295:G:H5''	13:L:14:GLY:O	1.98	0.64
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.63
18:Q:66:LYS:HB2	18:Q:70:ALA:O	1.98	0.63
11:J:131:THR:HB	11:J:134:GLU:CG	2.26	0.63
3:B:201:ASP:HB2	3:B:312:ARG:HD2	1.80	0.63
12:K:23:ASN:HD21	12:K:108:GLU:N	1.96	0.63
9:H:42:ASP:HB2	9:H:45:ASP:OD1	1.98	0.63
1:0:65:C:O2'	1:0:66:G:H5'	1.97	0.63
1:0:482:G:H4'	1:0:508:A:N1	2.13	0.63
17:P:61:ARG:HH11	17:P:61:ARG:HB2	1.63	0.63
1:0:2618:G:O2'	32:4:76:5AA:C10	2.45	0.63
13:L:125:PHE:CZ	13:L:140:VAL:HG22	2.33	0.63
22:U:56:ARG:HG3	22:U:56:ARG:HH11	1.64	0.63
10:I:73:LEU:HD12	10:I:107:LYS:NZ	2.12	0.63
24:W:88:THR:C	24:W:90:TYR:H	2.00	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.97	0.63
27:Z:64:PRO:HB2	27:Z:86:TYR:CE2	2.34	0.63
17:P:38:GLU:HA	17:P:41:ARG:HH11	1.61	0.63
1:0:2457:U:O3'	30:3:81:GLU:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:VAL:HG21	2:A:74:VAL:CG1	2.29	0.63
1:0:1118:A:H62	1:0:1244:U:H3	1.45	0.63
4:C:165:ASP:OD2	4:C:191:SER:HB2	1.98	0.63
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.80	0.63
5:D:167:GLU:OE1	5:D:173:GLU:HB3	1.98	0.63
2:A:190:ARG:NH2	2:A:207:GLN:OE1	2.32	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63
6:E:20:ILE:CD1	6:E:40:VAL:HG11	2.29	0.63
1:0:1015:C:H2'	1:0:1016:U:C6	2.33	0.63
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.63
9:H:57:THR:HG23	9:H:131:GLN:HA	1.81	0.63
1:0:1748:U:H4'	40:0:7383:HOH:O	1.99	0.63
15:N:139:TRP:CE3	15:N:139:TRP:HA	2.34	0.63
5:D:88:LEU:HB2	5:D:89:PRO:HD3	1.80	0.63
14:M:52:GLN:OE1	14:M:116:ASN:HB3	1.96	0.63
1:0:1593:C:OP1	17:P:117:SER:HB3	1.99	0.63
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.63
1:0:1189:A:H1'	1:0:1209:C:C1'	2.28	0.63
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.80	0.63
1:0:2780:C:C1'	6:E:143:GLN:HE21	2.11	0.63
1:0:2111:G:H1'	40:0:3046:HOH:O	1.97	0.63
1:0:1234:U:N3	3:B:244:PRO:HB3	2.13	0.63
17:P:89:ASN:OD1	17:P:92:GLU:HG3	1.98	0.63
1:0:1773:G:C8	27:Z:40:ALA:HA	2.32	0.63
1:0:506:G:H22	1:0:509:A:H5''	1.63	0.62
1:0:1632:A:H2'	1:0:1633:C:H5'	1.80	0.62
1:0:821:U:H3'	40:0:8314:HOH:O	1.98	0.62
1:0:1778:A:H2'	1:0:1779:A:H5'	1.79	0.62
27:Z:70:ARG:CB	27:Z:70:ARG:HH11	2.12	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.64	0.62
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.79	0.62
6:E:95:VAL:O	6:E:126:ILE:HD12	1.99	0.62
10:I:96:SER:OG	10:I:99:GLN:HG3	1.99	0.62
17:P:134:VAL:O	17:P:137:LEU:HB3	1.99	0.62
3:B:13:PHE:O	3:B:16:ARG:HD2	1.99	0.62
38:0:2924:MYL:HBB	40:0:8226:HOH:O	1.97	0.62
30:3:4:PRO:HG2	30:3:7:PHE:HD2	1.65	0.62
1:0:588:G:O6	24:W:154:ARG:NH1	2.32	0.62
20:S:53:ASN:N	20:S:53:ASN:HD22	1.97	0.62
1:0:1972:U:H2'	1:0:1973:A:C5'	2.30	0.62
3:B:305:ASP:O	3:B:306:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:44:SER:HA	30:3:49:ASP:OD1	1.98	0.62
1:0:2426:G:H1'	40:0:5391:HOH:O	1.99	0.62
31:9:14:G:C8	31:9:14:G:H5'	2.30	0.62
24:W:80:ASP:O	24:W:84:VAL:HG23	1.99	0.62
1:0:1943:C:H4'	2:A:211:LYS:O	1.99	0.62
1:0:10:U:O4	1:0:532:A:OP2	2.17	0.62
1:0:523:C:H2'	1:0:524:A:H8	1.64	0.62
24:W:122:ARG:HG3	24:W:122:ARG:HH11	1.64	0.62
2:A:135:VAL:HG21	2:A:147:ARG:HB3	1.82	0.62
16:O:21:SER:OG	16:O:106:PRO:HB2	1.99	0.62
1:0:2413:A:N7	15:N:109:PRO:HB3	2.15	0.62
1:0:1943:C:O4'	2:A:212:PRO:HA	2.00	0.62
4:C:79:ARG:O	4:C:87:ARG:HG2	1.99	0.62
3:B:80:ARG:HB2	3:B:145:HIS:CE1	2.34	0.62
40:0:4874:HOH:O	27:Z:41:ARG:HG2	1.99	0.62
23:V:12:THR:HG22	23:V:15:GLU:CG	2.29	0.62
1:0:1224:G:H2'	1:0:1225:C:H6	1.63	0.62
2:A:75:GLY:HA2	27:Z:88:PHE:HA	1.82	0.62
6:E:101:GLU:HB2	6:E:116:THR:O	1.99	0.62
15:N:55:ASP:OD2	31:9:7:G:H4'	2.00	0.62
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.35	0.62
1:0:553:G:P	26:Y:204:ARG:HH22	2.21	0.62
6:E:81:GLU:O	6:E:172:PRO:HD3	2.00	0.62
1:0:1768:C:H2'	1:0:1769:C:O4'	2.00	0.62
30:3:24:LYS:HG3	30:3:90:PHE:HZ	1.64	0.62
7:F:50:VAL:HG13	7:F:60:VAL:HG11	1.81	0.62
27:Z:54:GLU:HB2	40:Z:3188:HOH:O	1.98	0.62
28:1:15:THR:HB	28:1:28:HIS:CD2	2.35	0.62
1:0:2837:U:H2'	40:0:6433:HOH:O	1.99	0.62
14:M:77:HIS:CE1	14:M:86:GLN:HG2	2.35	0.62
16:O:47:ARG:O	16:O:47:ARG:HG2	1.99	0.62
1:0:2521:A:OP2	9:H:6:ALA:HB3	2.00	0.62
4:C:1:MET:HG2	4:C:2:GLN:N	2.14	0.62
1:0:292:G:H2'	1:0:358:G:N2	2.15	0.62
1:0:960:G:H4'	40:0:7253:HOH:O	2.00	0.62
21:T:48:VAL:HG23	21:T:97:ARG:C	2.19	0.61
1:0:542:A:H5'	1:0:542:A:C8	2.29	0.61
1:0:90:A:H2'	1:0:91:G:O4'	2.00	0.61
10:I:126:THR:O	10:I:130:LEU:HG	2.00	0.61
1:0:1350:U:H4'	40:0:4055:HOH:O	2.00	0.61
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:819:A:C5'	27:Z:37:ARG:HD3	2.29	0.61
1:0:450:C:H4'	4:C:46:TYR:CE1	2.35	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.80	0.61
1:0:855:U:H3'	40:0:3915:HOH:O	2.00	0.61
1:0:1308:A:O4'	4:C:226:GLY:HA3	2.00	0.61
18:Q:62:THR:O	18:Q:64:GLU:HG2	1.99	0.61
2:A:186:TRP:CG	2:A:187:PRO:HA	2.35	0.61
1:0:2541:U:O2	32:4:77:2OP:HA	2.00	0.61
15:N:17:ARG:HB3	15:N:17:ARG:NH1	2.12	0.61
1:0:2511:A:H2'	1:0:2512:U:O4'	2.00	0.61
14:M:77:HIS:HD2	14:M:81:ARG:H	1.46	0.61
3:B:256:GLN:HG2	40:B:7358:HOH:O	1.99	0.61
1:0:1972:U:H2'	1:0:1973:A:H5'	1.82	0.61
1:0:2795:C:O2'	1:0:2796:U:H5'	1.99	0.61
17:P:7:LYS:HD2	17:P:21:VAL:CG2	2.30	0.61
1:0:2321:A:H4'	1:0:2322:U:OP1	2.00	0.61
5:D:17:ARG:NH1	5:D:137:PRO:HA	2.07	0.61
1:0:500:G:H21	19:R:98:ASN:HD21	1.45	0.61
4:C:131:PHE:H	4:C:131:PHE:HD2	1.48	0.61
19:R:4:TYR:CE2	19:R:15:LYS:HB3	2.34	0.61
1:0:100:C:H4'	21:T:16:LEU:HB2	1.82	0.61
19:R:39:THR:HB	19:R:42:GLU:CG	2.29	0.61
15:N:79:PRO:HG3	15:N:143:ARG:O	2.00	0.61
20:S:37:VAL:O	20:S:41:VAL:HG23	2.01	0.61
17:P:138:GLU:C	17:P:140:TYR:H	2.03	0.61
15:N:154:LEU:HG	15:N:155:GLU:H	1.65	0.61
14:M:68:ARG:HD3	14:M:68:ARG:O	2.01	0.61
11:J:107:ASN:HD22	11:J:109:TYR:H	1.45	0.61
3:B:258:GLY:H	3:B:260:HIS:HE1	1.45	0.61
7:F:99:THR:HA	40:F:3461:HOH:O	1.99	0.61
1:0:1474:C:C6	1:0:1474:C:H5'	2.36	0.61
4:C:27:ARG:NH2	16:O:4:ASN:ND2	2.48	0.61
29:2:25:VAL:O	29:2:29:THR:HG23	2.00	0.61
18:Q:26:PRO:O	18:Q:30:VAL:HG22	2.01	0.61
5:D:76:ARG:NE	31:9:44:A:O4'	2.33	0.61
1:0:603:A:H5''	1:0:604:G:OP1	2.00	0.61
40:0:5298:HOH:O	3:B:254:GLN:HG3	1.99	0.61
1:0:1205:U:C2'	1:0:1206:U:H5''	2.29	0.61
13:L:121:ILE:HG12	13:L:141:GLU:HB2	1.82	0.61
3:B:84:LEU:HD23	3:B:142:LEU:CD2	2.30	0.61
31:9:39:U:H1'	31:9:44:A:H61	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:PRO:HG2	2:A:98:GLU:HG2	1.82	0.61
1:0:1447:U:H3'	1:0:1506:U:O2	1.99	0.61
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.30	0.61
1:0:343:C:O2'	1:0:344:C:H5'	2.00	0.61
4:C:127:ARG:HD3	4:C:129:HIS:HE1	1.65	0.61
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.49	0.61
1:0:271:C:H41	1:0:378:A:H2	1.49	0.61
1:0:946:C:H2'	1:0:947:U:C6	2.36	0.61
1:0:168:C:H6	1:0:168:C:O5'	1.84	0.61
13:L:73:VAL:HG21	13:L:116:HIS:NE2	2.16	0.61
27:Z:81:CYS:SG	27:Z:83:TYR:HB3	2.41	0.61
13:L:66:VAL:HG22	13:L:111:ALA:H	1.65	0.61
23:V:49:LEU:O	23:V:53:ILE:HG13	2.01	0.61
7:F:53:ASP:OD1	7:F:80:GLN:HB2	2.00	0.61
4:C:242:GLU:HB2	40:C:3133:HOH:O	2.00	0.61
10:I:113:SER:HB2	10:I:118:ASN:HB2	1.83	0.61
11:J:6:PHE:HB3	11:J:109:TYR:OH	2.01	0.61
2:A:88:ILE:HG22	2:A:88:ILE:O	2.00	0.61
17:P:55:LYS:CG	17:P:56:GLY:H	2.14	0.61
1:0:244:C:OP2	7:F:38:LYS:HE3	2.01	0.61
19:R:47:LEU:HB2	19:R:89:LEU:HD21	1.82	0.61
3:B:140:LEU:HA	40:B:3693:HOH:O	1.99	0.61
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.00	0.60
24:W:90:TYR:CD1	24:W:90:TYR:N	2.66	0.60
3:B:41:PHE:CE1	3:B:79:MET:HG3	2.35	0.60
1:0:157:G:H4'	14:M:95:LYS:CE	2.31	0.60
1:0:2851:G:C2'	1:0:2852:A:H5'	2.31	0.60
17:P:59:ARG:HD3	40:P:5642:HOH:O	2.00	0.60
1:0:682:A:H2'	1:0:683:G:O4'	2.00	0.60
13:L:17:SER:C	13:L:19:LYS:H	2.05	0.60
30:3:55:VAL:HG22	40:3:895:HOH:O	2.01	0.60
1:0:1615:A:H5'	40:0:8791:HOH:O	2.01	0.60
5:D:135:VAL:HG21	5:D:139:TYR:CD1	2.36	0.60
1:0:2564:G:OP2	1:0:2565:C:H5''	2.02	0.60
31:9:2:U:OP2	31:9:3:A:H5'	2.01	0.60
1:0:2851:G:O2'	1:0:2852:A:H5'	2.00	0.60
2:A:8:ARG:HG2	40:A:2279:HOH:O	2.01	0.60
6:E:14:GLU:HG2	6:E:15:GLN:N	2.15	0.60
1:0:2717:C:O2'	1:0:2718:C:H5''	2.00	0.60
12:K:109:LEU:HD12	12:K:113:ILE:HD11	1.82	0.60
1:0:1641:A:H2'	1:0:1642:A:C5'	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:192:VAL:HG11	2:A:208:HIS:H	1.65	0.60
1:0:259:G:H21	14:M:58:GLN:NE2	1.99	0.60
9:H:57:THR:N	9:H:132:ALA:HB2	2.17	0.60
18:Q:64:GLU:HG3	18:Q:74:ASP:OD2	2.01	0.60
1:0:947:U:H2'	1:0:948:G:C8	2.36	0.60
1:0:727:G:H3'	1:0:728:C:H6	1.66	0.60
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.16	0.60
1:0:1682:A:O2'	1:0:1683:G:H5''	2.01	0.60
1:0:1981:A:H1'	1:0:1983:C:N4	2.16	0.60
14:M:77:HIS:CD2	14:M:81:ARG:H	2.19	0.60
1:0:1120:U:C6	1:0:1120:U:H5''	2.36	0.60
1:0:56:G:H5''	23:V:50:ARG:NH1	2.15	0.60
2:A:51:ARG:HB2	40:A:5706:HOH:O	2.01	0.60
1:0:2325:U:O2'	1:0:2411:C:H1'	2.00	0.60
1:0:2329:C:O2'	1:0:2330:U:H5'	2.01	0.60
2:A:36:ASP:O	2:A:38:ILE:N	2.33	0.60
5:D:58:VAL:CG1	5:D:60:GLU:HG2	2.31	0.60
25:X:22:ASN:HA	25:X:25:ARG:HG3	1.83	0.60
15:N:27:LEU:HD22	15:N:50:LEU:HD22	1.84	0.60
1:0:1613:C:H2'	1:0:1614:G:O4'	2.00	0.60
1:0:440:C:H2'	1:0:441:A:C8	2.37	0.60
1:0:2563:U:H2'	1:0:2565:C:O5'	2.01	0.60
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.09	0.60
28:1:25:LYS:HD2	29:2:49:GLU:N	2.16	0.60
1:0:291:C:H2'	1:0:292:G:O4'	2.02	0.60
4:C:188:ARG:HD3	40:C:2507:HOH:O	2.00	0.60
3:B:7:ARG:HG2	3:B:7:ARG:HH11	1.65	0.60
1:0:2689:A:H2'	1:0:2690:U:H5'	1.83	0.60
1:0:24:G:N2	1:0:518:G:H1'	2.15	0.60
1:0:2542:C:H1'	40:4:6378:HOH:O	2.01	0.60
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.60
1:0:1733:A:H4'	3:B:212:GLN:HA	1.84	0.60
12:K:88:VAL:HG22	22:U:20:MET:HB3	1.82	0.60
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.37	0.60
24:W:59:GLN:HE22	24:W:98:PHE:N	1.98	0.60
4:C:145:GLU:OE1	4:C:198:ASP:HB2	2.02	0.60
19:R:72:VAL:HG12	19:R:73:ASP:N	2.16	0.60
5:D:154:LYS:CD	5:D:154:LYS:H	2.10	0.60
2:A:153:ARG:NH1	2:A:153:ARG:HB2	2.11	0.60
11:J:74:ARG:NH1	11:J:76:ASP:HB2	2.17	0.60
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:O2'	1:0:1208:C:H2'	2.02	0.60
1:0:1654:U:H2'	2:A:47:HIS:CD2	2.36	0.60
13:L:57:VAL:O	13:L:57:VAL:HG12	2.02	0.60
1:0:1687:C:O2	28:1:9:GLY:HA2	2.00	0.60
24:W:119:HIS:HD2	24:W:120:PRO:O	1.83	0.60
6:E:24:GLY:HA3	6:E:76:VAL:HB	1.84	0.60
22:U:13:ILE:HG23	40:U:3194:HOH:O	2.00	0.60
40:0:3857:HOH:O	14:M:125:ARG:HD2	2.01	0.60
1:0:1666:C:H2'	1:0:1667:A:H5'	1.84	0.60
1:0:2335:C:H2'	1:0:2336:G:C8	2.37	0.60
1:0:2250:G:H2'	1:0:2251:G:O4'	2.02	0.60
25:X:43:VAL:HG12	25:X:44:ASP:N	2.17	0.60
12:K:13:GLU:O	12:K:16:SER:HB2	2.02	0.60
1:0:2055:A:H4'	19:R:132:ARG:HH21	1.67	0.60
13:L:17:SER:O	13:L:19:LYS:N	2.35	0.60
1:0:2315:C:H5"	40:0:7987:HOH:O	2.02	0.60
9:H:26:ILE:HA	9:H:123:ILE:HG21	1.84	0.60
3:B:274:GLU:HA	3:B:292:GLY:O	2.01	0.60
17:P:115:SER:C	17:P:117:SER:H	2.05	0.59
10:I:85:GLY:O	10:I:86:GLU:HG3	2.02	0.59
21:T:43:ASN:ND2	21:T:108:ARG:CZ	2.61	0.59
7:F:57:GLU:O	7:F:61:MET:HG3	2.02	0.59
10:I:88:GLN:HA	10:I:91:PHE:CE2	2.37	0.59
10:I:91:PHE:HA	10:I:131:GLY:HA3	1.83	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
6:E:20:ILE:HD11	6:E:40:VAL:CG1	2.32	0.59
1:0:1308:A:C4'	4:C:226:GLY:HA3	2.32	0.59
1:0:694:A:H2'	1:0:695:C:H5'	1.83	0.59
8:G:64:ASN:N	8:G:64:ASN:HD22	2.00	0.59
1:0:333:G:O2'	1:0:334:G:H5'	2.02	0.59
11:J:130:VAL:HG12	11:J:131:THR:N	2.16	0.59
1:0:2468:A:N6	30:3:50:GLY:HA2	2.17	0.59
7:F:58:GLU:OE1	14:M:27:ARG:NH2	2.33	0.59
8:G:23:ILE:HD13	8:G:67:LEU:HD23	1.83	0.59
31:9:107:C:H2'	31:9:108:C:C6	2.37	0.59
1:0:2781:U:H2'	1:0:2782:G:H5'	1.84	0.59
1:0:308:U:H5'	1:0:309:C:OP1	2.02	0.59
1:0:1001:U:O2'	1:0:1002:G:H5'	2.02	0.59
1:0:2537:G:H5"	1:0:2538:A:H5"	1.84	0.59
5:D:84:LEU:HA	5:D:87:ALA:HB3	1.85	0.59
28:1:2:GLY:O	28:1:6:PRO:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:81:GLN:H	2:A:92:ASN:ND2	2.01	0.59
17:P:83:LYS:HG3	17:P:84:ALA:H	1.67	0.59
6:E:7:ILE:HD11	6:E:11:VAL:C	2.22	0.59
24:W:88:THR:HB	40:W:6679:HOH:O	2.03	0.59
5:D:50:VAL:O	5:D:71:ALA:HA	2.02	0.59
7:F:30:LYS:HB2	7:F:97:ALA:HB3	1.85	0.59
1:0:2735:U:H2'	1:0:2736:U:C6	2.37	0.59
15:N:34:LEU:HD13	15:N:47:LEU:CD2	2.33	0.59
12:K:62:PRO:HG3	12:K:65:ARG:HH21	1.68	0.59
1:0:2301:A:H5''	1:0:2302:A:H5'	1.85	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
17:P:13:VAL:HG13	17:P:14:LEU:N	2.17	0.59
1:0:645:U:OP2	13:L:4:LYS:HE2	2.02	0.59
24:W:22:GLU:HG2	24:W:27:HIS:CD2	2.37	0.59
1:0:1940:C:H1'	40:0:4154:HOH:O	2.02	0.59
22:U:14:GLU:O	22:U:17:THR:HB	2.03	0.59
5:D:159:PRO:O	5:D:163:VAL:HG23	2.03	0.59
15:N:154:LEU:O	15:N:155:GLU:HB3	2.03	0.59
1:0:1681:G:H5''	1:0:1682:A:H5'	1.84	0.59
13:L:136:ALA:HB3	40:L:6166:HOH:O	2.02	0.59
1:0:2534:C:H1'	40:0:7954:HOH:O	2.02	0.59
5:D:138:GLY:HA2	31:9:29:C:O3'	2.03	0.59
1:0:1766:U:O2	1:0:1778:A:H5'	2.02	0.59
2:A:94:LEU:N	2:A:94:LEU:HD23	2.17	0.59
1:0:2880:A:H2'	1:0:2881:C:H5'	1.84	0.59
14:M:74:LYS:CD	14:M:91:ILE:HD11	2.33	0.59
15:N:77:ASN:OD1	15:N:79:PRO:HD2	2.02	0.59
3:B:97:LEU:O	3:B:98:THR:HG23	2.03	0.59
15:N:73:ALA:HB1	15:N:74:PRO:HD2	1.85	0.59
2:A:17:ARG:HD2	40:A:1373:HOH:O	2.02	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.03	0.58
17:P:13:VAL:HG13	17:P:14:LEU:H	1.66	0.58
30:3:34:LYS:HB2	30:3:34:LYS:NZ	2.18	0.58
40:0:4499:HOH:O	8:G:12:ILE:HG23	2.03	0.58
26:Y:117:LEU:HA	26:Y:174:VAL:HG11	1.85	0.58
14:M:166:ALA:HB2	14:M:169:ARG:HH21	1.67	0.58
4:C:27:ARG:NH1	4:C:30:LEU:HG	2.18	0.58
2:A:167:LYS:HE3	27:Z:50:VAL:HA	1.85	0.58
1:0:195:C:H2'	1:0:196:G:H5'	1.85	0.58
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.51	0.58
10:I:107:LYS:HB3	10:I:110:ASP:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.19	0.58
5:D:134:LEU:HD11	5:D:166:ILE:HD11	1.83	0.58
5:D:58:VAL:HB	5:D:62:ASP:CB	2.33	0.58
2:A:167:LYS:CE	27:Z:50:VAL:HG13	2.34	0.58
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	1.84	0.58
14:M:47:ASP:CG	14:M:48:LYS:H	2.05	0.58
24:W:27:HIS:C	24:W:28:HIS:HD2	2.05	0.58
2:A:125:ASN:HB3	2:A:158:VAL:HG12	1.84	0.58
1:O:2437:A:H2'	1:O:2438:G:C8	2.38	0.58
15:N:115:VAL:HG23	15:N:116:PHE:H	1.68	0.58
1:O:2588:OMG:N1	32:4:75:C:N3	2.39	0.58
2:A:192:VAL:CG1	2:A:208:HIS:H	2.17	0.58
9:H:41:LYS:HD3	9:H:46:TYR:OH	2.03	0.58
2:A:135:VAL:HG11	2:A:147:ARG:NH2	2.18	0.58
1:O:290:C:O2'	1:O:291:C:H5'	2.02	0.58
1:O:1119:G:H5'	11:J:52:GLN:HE21	1.68	0.58
31:9:91:C:H2'	31:9:92:G:O4'	2.03	0.58
1:O:2434:A:O2'	30:3:27:SER:HB3	2.04	0.58
1:O:2781:U:C2'	1:O:2782:G:H5'	2.33	0.58
26:Y:99:ALA:HB2	26:Y:233:TYR:CZ	2.38	0.58
7:F:13:GLU:OE2	7:F:78:GLU:HG2	2.02	0.58
1:O:1066:U:H2'	1:O:1067:A:C8	2.37	0.58
30:3:70:ARG:HD3	30:3:77:ALA:HB2	1.84	0.58
13:L:55:GLN:HA	13:L:58:GLN:NE2	2.08	0.58
3:B:36:PRO:CG	3:B:169:GLY:H	2.16	0.58
17:P:103:THR:O	17:P:107:GLU:HG3	2.04	0.58
1:O:308:U:H2'	21:T:52:ARG:NH2	2.18	0.58
1:O:933:C:H4'	1:O:1297:U:H4'	1.86	0.58
15:N:61:ALA:HB2	15:N:88:ALA:HB2	1.86	0.58
14:M:133:LEU:O	14:M:134:ILE:HD13	2.04	0.58
18:Q:64:GLU:HG3	18:Q:74:ASP:CG	2.23	0.58
5:D:67:ASP:O	5:D:69:ILE:HG13	2.02	0.58
23:V:11:MET:HB3	23:V:15:GLU:HB2	1.85	0.58
25:X:51:ASP:OD2	25:X:52:PRO:HD2	2.04	0.58
13:L:148:GLU:HA	40:L:6153:HOH:O	2.02	0.58
19:R:125:ARG:HG2	40:R:3539:HOH:O	2.04	0.58
1:O:1202:A:H2'	1:O:1203:G:O4'	2.03	0.58
21:T:48:VAL:HG21	21:T:96:VAL:CG1	2.33	0.58
1:O:926:A:C4'	13:L:39:GLU:HG2	2.33	0.58
1:O:644:G:N3	1:O:644:G:H5'	2.19	0.58
16:O:38:ARG:HD3	40:O:7674:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:136:VAL:HG22	4:C:137:PRO:HA	1.85	0.58
4:C:14:GLY:O	4:C:15:GLU:HB3	2.04	0.58
5:D:154:LYS:HD2	5:D:154:LYS:N	2.14	0.58
9:H:41:LYS:HG2	9:H:42:ASP:H	1.69	0.58
6:E:14:GLU:HG2	6:E:15:GLN:H	1.68	0.58
10:I:94:ASP:OD1	10:I:133:THR:HB	2.04	0.58
6:E:100:ASP:HB2	40:E:2789:HOH:O	2.04	0.58
1:O:247:A:H2'	40:O:8472:HOH:O	2.04	0.58
20:S:6:LYS:NZ	20:S:61:GLU:HG2	2.19	0.58
14:M:99:ARG:NH1	14:M:99:ARG:HG2	2.07	0.57
1:O:420:U:H5'	1:O:1920:C:C2	2.39	0.57
9:H:76:LEU:HD21	9:H:149:VAL:HA	1.86	0.57
18:Q:27:GLN:HE21	31:9:8:G:H4'	1.69	0.57
27:Z:62:ALA:HA	27:Z:69:ASP:HA	1.84	0.57
3:B:147:VAL:O	3:B:147:VAL:HG12	2.04	0.57
5:D:86:THR:O	5:D:90:LEU:HG	2.04	0.57
24:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.57
1:O:2766:A:H5'	40:O:4808:HOH:O	2.03	0.57
1:O:2353:A:H4'	1:O:2354:A:O5'	2.04	0.57
1:O:2618:G:O2'	32:4:76:5AA:N1	2.33	0.57
1:O:2321:A:H2	1:O:2378:U:H3	1.50	0.57
1:O:2533:C:C5'	1:O:2533:C:H6	2.14	0.57
17:P:105:LEU:CD2	17:P:137:LEU:HD21	2.33	0.57
1:O:2345:A:H3'	1:O:2346:C:C6	2.38	0.57
1:O:2374:G:H2'	1:O:2375:A:C8	2.39	0.57
1:O:1181:A:H2'	1:O:1182:C:H5'	1.87	0.57
14:M:164:THR:CG2	14:M:165:GLY:N	2.66	0.57
17:P:103:THR:HA	17:P:106:ARG:HH12	1.69	0.57
1:O:2769:C:O2'	1:O:2770:G:H5'	2.04	0.57
26:Y:117:LEU:HD12	26:Y:174:VAL:HG13	1.87	0.57
1:O:2703:A:H2'	1:O:2704:C:H6	1.68	0.57
25:X:72:VAL:HG22	25:X:85:VAL:CG1	2.32	0.57
1:O:1183:C:H42	1:O:1184:C:H41	1.52	0.57
1:O:2676:C:H4'	11:J:70:PHE:CD1	2.40	0.57
1:O:297:U:H2'	1:O:298:C:H6	1.67	0.57
1:O:1654:U:C2'	2:A:47:HIS:HD2	2.17	0.57
3:B:56:ASP:CB	3:B:322:ARG:HE	2.17	0.57
1:O:1451:C:H5'	1:O:1505:U:C5	2.38	0.57
3:B:238:ASN:HD22	3:B:240:GLY:H	1.52	0.57
5:D:49:PRO:HA	5:D:73:VAL:HG22	1.86	0.57
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:92:G:C4'	23:V:44:GLY:HA3	2.31	0.57
23:V:44:GLY:O	23:V:48:GLU:HG2	2.05	0.57
1:0:100:C:H2'	1:0:101:C:H6	1.68	0.57
40:0:6085:HOH:O	30:3:79:LEU:HB2	2.04	0.57
23:V:39:ALA:N	23:V:40:PRO:CD	2.68	0.57
2:A:125:ASN:CB	2:A:158:VAL:HG12	2.35	0.57
5:D:10:PHE:CG	5:D:11:HIS:N	2.73	0.57
24:W:34:LEU:HD12	24:W:107:LEU:HD11	1.86	0.57
16:O:14:LEU:HD23	16:O:102:ILE:HD11	1.87	0.57
14:M:73:ARG:HD2	14:M:73:ARG:N	2.18	0.57
26:Y:235:GLU:CD	26:Y:235:GLU:N	2.54	0.57
31:9:116:C:O2'	31:9:117:G:H5'	2.05	0.57
6:E:8:PRO:HB2	6:E:11:VAL:HG23	1.87	0.57
1:0:1829:A:H2'	1:0:1830:C:H5'	1.86	0.57
1:0:1566:C:H2'	1:0:1567:G:H8	1.70	0.57
1:0:1486:A:C5	29:2:2:LYS:HG3	2.39	0.57
1:0:228:C:H2'	1:0:229:G:H5'	1.85	0.57
24:W:142:ASP:HB3	24:W:145:GLY:H	1.70	0.57
9:H:61:ARG:HG3	9:H:61:ARG:NH1	2.20	0.57
1:0:1882:C:OP1	2:A:192:VAL:HG23	2.05	0.57
3:B:232:TRP:HD1	3:B:235:ARG:HD2	1.68	0.57
3:B:199:TYR:HE2	3:B:268:ARG:HB2	1.70	0.57
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.37	0.57
1:0:1829:A:N6	27:Z:42:TYR:HA	2.19	0.57
15:N:114:LYS:O	15:N:118:ILE:HG13	2.05	0.57
17:P:55:LYS:CG	17:P:56:GLY:N	2.66	0.57
13:L:143:THR:HG22	13:L:144:ASP:N	2.19	0.57
3:B:215:VAL:HA	3:B:220:VAL:HG22	1.85	0.57
1:0:2457:U:H4'	30:3:80:ARG:O	2.04	0.57
1:0:1416:G:H2'	1:0:1417:G:H5'	1.86	0.57
1:0:1522:A:H1'	1:0:1665:G:N2	2.19	0.57
1:0:57:C:H42	1:0:89:G:H1	1.53	0.57
20:S:57:THR:HG22	20:S:58:MET:N	2.20	0.57
38:0:2924:MYL:HBC	38:0:2924:MYL:OAJ	2.04	0.56
1:0:2507:G:H2'	1:0:2510:C:H42	1.69	0.56
1:0:1183:C:H2'	40:0:5603:HOH:O	2.05	0.56
5:D:25:MET:HE3	5:D:37:ALA:CB	2.34	0.56
5:D:172:VAL:HG12	5:D:173:GLU:N	2.19	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
15:N:24:LEU:HD13	18:Q:26:PRO:HB3	1.86	0.56
2:A:81:GLN:HB2	2:A:92:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:135:G:H5''	14:M:39:ARG:NH1	2.20	0.56
15:N:181:ASP:O	15:N:184:ILE:HG22	2.04	0.56
3:B:195:ARG:N	3:B:198:GLU:OE1	2.36	0.56
8:G:71:LEU:O	8:G:73:ASP:N	2.38	0.56
1:0:952:G:OP1	18:Q:42:LYS:HE2	2.05	0.56
1:0:581:G:O2'	1:0:582:U:H5'	2.04	0.56
2:A:191:GLY:HA2	2:A:194:MET:HE3	1.87	0.56
12:K:64:MET:HA	12:K:67:GLN:HE21	1.69	0.56
30:3:88:LEU:HD23	30:3:90:PHE:HE2	1.70	0.56
7:F:81:ASP:HA	7:F:92:GLY:HA3	1.87	0.56
21:T:41:ARG:NH1	21:T:42:VAL:O	2.39	0.56
1:0:164:G:H3'	40:0:8187:HOH:O	2.04	0.56
14:M:111:ASN:HB2	40:M:1852:HOH:O	2.04	0.56
26:Y:112:GLU:HA	26:Y:112:GLU:OE1	2.04	0.56
1:0:699:C:H5'	40:0:8623:HOH:O	2.05	0.56
1:0:807:A:O2'	1:0:808:A:H5'	2.05	0.56
1:0:2488:A:H1'	40:0:3183:HOH:O	2.04	0.56
23:V:42:ASN:HB3	40:V:7247:HOH:O	2.04	0.56
1:0:636:G:H1'	1:0:2058:G:C4	2.40	0.56
1:0:779:U:H3'	40:0:4557:HOH:O	2.05	0.56
1:0:1625:U:H4'	40:0:3427:HOH:O	2.06	0.56
1:0:2105:C:H4'	40:0:5147:HOH:O	2.05	0.56
25:X:72:VAL:CG2	25:X:85:VAL:HG12	2.32	0.56
2:A:30:ARG:HG2	2:A:31:LYS:H	1.70	0.56
3:B:56:ASP:HB2	3:B:322:ARG:HH21	1.70	0.56
4:C:35:VAL:HG21	4:C:227:GLY:HA2	1.88	0.56
1:0:671:A:O2'	1:0:672:G:H2'	2.05	0.56
40:0:5620:HOH:O	18:Q:11:ARG:HD3	2.04	0.56
1:0:1387:G:H1'	17:P:28:GLN:HE22	1.68	0.56
13:L:104:ASP:O	13:L:105:TYR:HB3	2.04	0.56
1:0:2064:U:H5'	1:0:2652:U:H4'	1.87	0.56
1:0:1268:C:O2'	1:0:1269:G:H5'	2.05	0.56
1:0:2460:A:H5''	30:3:59:ASP:OD1	2.06	0.56
1:0:1667:A:H5'	1:0:1667:A:C8	2.32	0.56
7:F:46:GLU:OE1	7:F:100:ASP:HA	2.06	0.56
24:W:99:ALA:HA	24:W:102:SER:OG	2.06	0.56
1:0:1120:U:H6	1:0:1120:U:H5''	1.70	0.56
1:0:2689:A:C2'	1:0:2690:U:H5'	2.35	0.56
1:0:2241:C:H2'	1:0:2242:U:C6	2.41	0.56
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.87	0.56
1:0:210:U:O2'	1:0:211:U:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:15:PRO:HA	14:M:20:LEU:HD23	1.86	0.56
19:R:39:THR:O	19:R:42:GLU:N	2.38	0.56
8:G:68:GLU:HA	8:G:71:LEU:HD12	1.88	0.56
13:L:34:GLY:HA3	13:L:38:HIS:CE1	2.41	0.56
1:0:951:A:O2'	1:0:952:G:H5'	2.06	0.56
3:B:145:HIS:HD2	3:B:146:THR:O	1.88	0.56
16:O:14:LEU:CD2	16:O:102:ILE:HD11	2.35	0.56
1:0:338:C:H4'	4:C:174:ILE:CD1	2.35	0.56
14:M:61:ILE:N	14:M:61:ILE:HD12	2.21	0.56
40:0:6374:HOH:O	28:1:46:ARG:HA	2.04	0.56
28:1:26:SER:HB3	28:1:35:SER:OG	2.06	0.56
14:M:84:LYS:HG2	30:3:46:ILE:O	2.05	0.56
30:3:25:VAL:HG22	30:3:68:LYS:HE3	1.87	0.56
1:0:2252:A:C5	1:0:2253:G:H1'	2.41	0.56
27:Z:54:GLU:HG2	27:Z:57:MET:HE2	1.88	0.56
24:W:90:TYR:HE2	24:W:99:ALA:HB2	1.71	0.56
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.56
17:P:42:GLU:O	17:P:46:GLU:HG3	2.05	0.56
1:0:745:G:O6	16:O:68:GLY:HA3	2.06	0.56
15:N:147:ILE:HD12	40:9:4707:HOH:O	2.05	0.56
1:0:1714:C:O2'	1:0:1715:C:H5'	2.06	0.56
1:0:1184:C:H1'	40:0:7308:HOH:O	2.04	0.56
1:0:736:A:H2'	1:0:737:A:O4'	2.05	0.56
20:S:14:ALA:HA	20:S:25:GLN:NE2	2.21	0.56
1:0:2073:G:OP2	1:0:2490:A:H5'	2.05	0.56
25:X:76:ARG:NH1	25:X:76:ARG:HG3	2.19	0.56
15:N:143:ARG:HG2	15:N:172:PHE:CD2	2.41	0.56
14:M:138:HIS:ND1	14:M:139:PRO:HD2	2.20	0.56
40:0:4782:HOH:O	24:W:119:HIS:HE1	1.87	0.56
17:P:14:LEU:HD13	17:P:51:ALA:HB2	1.87	0.56
28:1:22:CYS:HA	40:1:2086:HOH:O	2.05	0.56
10:I:102:GLN:HA	10:I:105:GLU:OE2	2.06	0.56
15:N:132:ASN:O	15:N:135:VAL:HG12	2.06	0.56
1:0:2281:C:C2'	1:0:2282:U:H5'	2.34	0.56
40:0:4808:HOH:O	3:B:267:LYS:HA	2.06	0.56
17:P:138:GLU:O	17:P:140:TYR:N	2.39	0.56
1:0:2438:G:H5'	40:0:5494:HOH:O	2.05	0.56
1:0:1038:G:O2'	1:0:1039:G:H5'	2.06	0.56
21:T:115:GLU:HG3	21:T:116:ASP:N	2.21	0.56
11:J:25:GLN:HE22	11:J:116:LEU:HB3	1.69	0.56
6:E:77:THR:OG1	6:E:78:GLU:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2006:C:H3'	1:0:2007:A:H2'	1.87	0.56
1:0:1118:A:C3'	1:0:1118:A:C8	2.88	0.56
14:M:69:LYS:O	14:M:73:ARG:NH2	2.36	0.56
29:2:43:ARG:HG2	40:2:6577:HOH:O	2.06	0.56
1:0:2565:C:H4'	40:0:3660:HOH:O	2.06	0.56
5:D:78:GLU:HB3	5:D:82:GLU:OE2	2.06	0.56
17:P:135:ALA:CB	17:P:139:ARG:HH12	2.12	0.55
21:T:28:SER:HA	21:T:97:ARG:HD3	1.88	0.55
1:0:1666:C:C2'	1:0:1667:A:H5''	2.36	0.55
10:I:124:VAL:O	10:I:124:VAL:HG12	2.06	0.55
5:D:23:VAL:HG23	5:D:23:VAL:O	2.06	0.55
26:Y:152:LYS:HB3	26:Y:160:LYS:HG3	1.88	0.55
14:M:31:TRP:HA	14:M:34:GLU:HG3	1.88	0.55
3:B:14:GLY:HA2	3:B:15:PRO:C	2.26	0.55
1:0:2827:A:H2'	1:0:2828:G:O4'	2.05	0.55
9:H:174:LEU:HA	40:H:5702:HOH:O	2.06	0.55
1:0:1118:A:C8	1:0:1119:G:H5''	2.41	0.55
1:0:1701:A:H4'	1:0:1702:U:C5'	2.34	0.55
30:3:25:VAL:HG12	30:3:27:SER:H	1.71	0.55
13:L:143:THR:HG22	13:L:145:LEU:H	1.71	0.55
15:N:139:TRP:HA	15:N:139:TRP:HE3	1.70	0.55
1:0:2345:A:H3'	1:0:2346:C:H6	1.72	0.55
12:K:24:THR:HG22	12:K:105:ARG:HG2	1.88	0.55
14:M:183:THR:OG1	14:M:184:ARG:N	2.39	0.55
1:0:2466:G:H2'	40:0:7450:HOH:O	2.06	0.55
1:0:2755:G:H1'	40:0:3447:HOH:O	2.06	0.55
4:C:127:ARG:HH11	4:C:127:ARG:HG2	1.71	0.55
40:0:4939:HOH:O	14:M:68:ARG:HG3	2.06	0.55
1:0:1586:G:O2'	1:0:1587:U:H5'	2.06	0.55
1:0:2780:C:H2'	1:0:2781:U:H6	1.71	0.55
1:0:1940:C:H4'	40:0:7130:HOH:O	2.06	0.55
1:0:2044:G:OP1	25:X:23:HIS:HE1	1.89	0.55
5:D:12:GLU:O	5:D:15:GLU:HG2	2.06	0.55
1:0:303:C:O2'	1:0:304:G:H5'	2.06	0.55
4:C:153:VAL:O	4:C:157:LEU:HG	2.06	0.55
40:0:3422:HOH:O	30:3:50:GLY:HA3	2.06	0.55
11:J:22:VAL:O	11:J:26:VAL:HG23	2.06	0.55
1:0:1477:C:O2'	1:0:1478:U:H5'	2.06	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.87	0.55
13:L:73:VAL:HG23	13:L:74:THR:H	1.70	0.55
14:M:28:GLN:HA	14:M:31:TRP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:419:A:H1'	1:0:1921:A:C2	2.40	0.55
40:0:7150:HOH:O	2:A:177:HIS:HE1	1.90	0.55
6:E:68:HIS:O	6:E:72:MET:HG3	2.07	0.55
31:9:61:C:H2'	31:9:62:A:H8	1.71	0.55
32:4:176:DA:O4'	32:4:175:C:H2'	2.06	0.55
30:3:2:GLN:O	30:3:3:MET:HB2	2.06	0.55
14:M:77:HIS:HB2	14:M:81:ARG:CZ	2.36	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.87	0.55
1:0:1162:G:H1'	10:I:112:LEU:CD1	2.35	0.55
1:0:2240:U:O2'	1:0:2241:C:H5'	2.05	0.55
1:0:1921:A:O2'	1:0:1922:A:H5'	2.06	0.55
6:E:49:ILE:HD11	6:E:69:ILE:HD12	1.89	0.55
1:0:1278:A:H4'	1:0:1279:U:C4	2.41	0.55
22:U:39:ASN:HD22	22:U:49:LEU:CD1	2.19	0.55
1:0:1557:G:H2'	1:0:1558:C:H6	1.72	0.55
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.55
1:0:216:A:O2'	1:0:217:C:H5'	2.06	0.55
31:9:35:C:H5"	40:9:4078:HOH:O	2.05	0.55
1:0:248:A:H5'	1:0:249:G:OP2	2.07	0.55
3:B:141:ARG:HD2	3:B:163:GLU:OE2	2.07	0.55
1:0:1616:A:H5"	1:0:1617:C:OP1	2.07	0.55
1:0:1304:U:H2'	1:0:1305:C:C6	2.41	0.55
24:W:4:LEU:HD22	24:W:54:PHE:HB3	1.89	0.55
24:W:4:LEU:CD1	24:W:52:VAL:HG21	2.36	0.55
11:J:43:ARG:HG2	40:J:5361:HOH:O	2.06	0.55
4:C:237:GLU:HB2	40:C:5218:HOH:O	2.07	0.55
1:0:2319:C:H3'	30:3:1:MET:H2	1.68	0.55
1:0:2409:C:H4'	30:3:17:HIS:CG	2.42	0.55
4:C:236:THR:HG22	4:C:239:ALA:CB	2.36	0.55
5:D:18:ILE:HG12	5:D:134:LEU:HD23	1.86	0.55
7:F:29:VAL:HA	7:F:99:THR:HG22	1.89	0.55
14:M:47:ASP:CG	14:M:48:LYS:N	2.60	0.55
10:I:123:VAL:C	10:I:125:GLY:H	2.09	0.55
13:L:35:ARG:HB2	13:L:43:HIS:CD2	2.42	0.55
1:0:2090:G:H2'	1:0:2091:G:C8	2.42	0.55
16:O:15:LYS:O	16:O:16:SER:C	2.45	0.55
14:M:164:THR:HG22	14:M:165:GLY:N	2.21	0.55
5:D:58:VAL:HG12	5:D:60:GLU:HG2	1.88	0.55
13:L:67:ARG:O	13:L:71:GLU:HG3	2.07	0.55
5:D:19:GLU:HG3	40:D:6165:HOH:O	2.05	0.55
1:0:214:U:H5'	40:0:5454:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:N2	1:0:1246:A:C2	2.65	0.55
12:K:58:THR:HG22	12:K:59:LYS:HG3	1.87	0.55
19:R:132:ARG:HG2	19:R:133:ALA:N	2.21	0.55
1:0:952:G:N3	1:0:2302:A:H2'	2.21	0.55
1:0:2790:C:HO2'	1:0:2791:U:H6	1.55	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.55
1:0:2851:G:H2'	1:0:2902:A:H61	1.71	0.55
10:I:133:THR:HG22	10:I:134:ILE:H	1.72	0.55
1:0:2135:A:O2'	1:0:2136:G:H5'	2.06	0.55
5:D:36:ASN:HA	40:D:7500:HOH:O	2.06	0.55
1:0:485:A:N3	1:0:487:G:H5''	2.22	0.55
1:0:2404:G:H5''	40:0:4170:HOH:O	2.06	0.55
4:C:129:HIS:HA	4:C:165:ASP:OD1	2.07	0.55
25:X:49:ARG:HD3	25:X:84:ILE:HG12	1.89	0.55
29:2:36:ASN:HD22	29:2:39:ARG:HG2	1.71	0.55
1:0:371:U:H2'	1:0:372:A:C8	2.41	0.55
27:Z:62:ALA:HA	27:Z:68:GLU:O	2.07	0.55
1:0:1922:A:H2'	30:3:33:MET:HG2	1.89	0.55
18:Q:19:ARG:HH21	31:9:11:A:P	2.29	0.55
1:0:2862:G:H4'	3:B:336:GLN:O	2.06	0.55
5:D:163:VAL:HA	40:D:6326:HOH:O	2.07	0.54
14:M:52:GLN:HE22	14:M:118:TYR:HB3	1.71	0.54
2:A:191:GLY:HA2	2:A:194:MET:CE	2.38	0.54
1:0:2363:G:H4'	18:Q:11:ARG:HE	1.71	0.54
1:0:1825:U:O2'	1:0:1826:C:H5'	2.07	0.54
1:0:834:G:H4'	1:0:835:U:OP2	2.06	0.54
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.21	0.54
1:0:1434:A:H2'	1:0:1436:C:C5	2.41	0.54
5:D:95:THR:C	5:D:97:GLN:H	2.10	0.54
11:J:39:VAL:HG22	11:J:107:ASN:HA	1.88	0.54
15:N:78:MET:HB2	15:N:79:PRO:HD3	1.90	0.54
1:0:1829:A:H61	27:Z:42:TYR:HA	1.71	0.54
1:0:2362:A:H2'	1:0:2363:G:C8	2.43	0.54
17:P:16:VAL:HG13	17:P:20:ARG:NH1	2.23	0.54
1:0:113:A:H3'	1:0:114:A:H5''	1.88	0.54
1:0:1072:G:OP2	26:Y:154:ARG:NH2	2.40	0.54
1:0:2442:G:H3'	40:0:6128:HOH:O	2.06	0.54
1:0:383:A:H2'	1:0:384:G:O4'	2.07	0.54
30:3:62:THR:HG22	30:3:63:LYS:N	2.22	0.54
30:3:83:TRP:HA	40:3:4958:HOH:O	2.08	0.54
3:B:36:PRO:HA	3:B:167:GLY:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1446:U:C2'	20:S:55:GLN:NE2	2.70	0.54
24:W:4:LEU:CD2	24:W:54:PHE:HB3	2.37	0.54
10:I:96:SER:HB3	10:I:99:GLN:HE21	1.72	0.54
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.89	0.54
10:I:101:LYS:O	10:I:105:GLU:HG3	2.07	0.54
1:0:110:C:H2'	1:0:111:C:H6	1.72	0.54
25:X:71:ARG:HD3	40:X:2171:HOH:O	2.08	0.54
14:M:122:GLN:OE1	14:M:127:LYS:HE2	2.07	0.54
1:0:31:C:H2'	40:0:7619:HOH:O	2.06	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.54
2:A:167:LYS:HD2	27:Z:53:ILE:HG21	1.90	0.54
3:B:199:TYR:CE2	3:B:268:ARG:HB2	2.42	0.54
22:U:13:ILE:HG12	22:U:32:CYS:HB3	1.90	0.54
1:0:1386:G:O2'	1:0:1387:G:H5'	2.07	0.54
19:R:50:VAL:O	19:R:53:GLY:N	2.40	0.54
1:0:1805:G:H2'	1:0:1806:G:H8	1.70	0.54
1:0:1074:G:H4'	1:0:1260:G:C6	2.42	0.54
31:9:57:A:H2'	31:9:58:G:H5'	1.89	0.54
21:T:48:VAL:HG22	21:T:49:GLU:N	2.23	0.54
1:0:613:C:H2'	1:0:614:U:C6	2.42	0.54
5:D:163:VAL:O	5:D:167:GLU:HB2	2.08	0.54
14:M:134:ILE:CG2	14:M:141:ILE:HD13	2.36	0.54
1:0:722:G:H22	1:0:938:G:P	2.30	0.54
15:N:100:ALA:O	15:N:129:ILE:HG23	2.06	0.54
24:W:29:VAL:O	24:W:30:ASN:HB2	2.07	0.54
40:0:3133:HOH:O	3:B:214:PRO:HD2	2.08	0.54
3:B:279:THR:HG22	3:B:280:VAL:N	2.23	0.54
8:G:20:VAL:O	8:G:24:VAL:HG23	2.07	0.54
27:Z:54:GLU:HG2	27:Z:57:MET:HE1	1.90	0.54
1:0:2032:U:H2'	1:0:2033:G:C5'	2.38	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.89	0.54
4:C:19:PRO:HG2	4:C:22:PHE:CD1	2.43	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
2:A:70:ALA:HB1	27:Z:89:THR:HG21	1.89	0.54
29:2:9:LYS:O	29:2:12:ALA:HB3	2.07	0.54
1:0:2269:C:H2'	1:0:2270:G:O4'	2.08	0.54
1:0:2588:OMG:C6	32:4:76:5AA:H102	2.43	0.54
1:0:2505:G:O2'	1:0:2506:A:H5'	2.08	0.54
1:0:1181:A:C2'	1:0:1182:C:H5'	2.37	0.54
31:9:92:G:H2'	31:9:93:A:H8	1.64	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:22:ALA:O	8:G:25:GLU:HB3	2.07	0.54
19:R:18:LEU:HD12	19:R:143:VAL:HG11	1.90	0.54
4:C:26:VAL:HG21	4:C:123:LEU:HD11	1.88	0.54
1:0:1942:A:H2'	1:0:1943:C:C6	2.42	0.54
1:0:2281:C:H2'	1:0:2282:U:H5'	1.90	0.54
6:E:3:VAL:HG22	6:E:49:ILE:HB	1.90	0.54
1:0:1419:U:H5'	1:0:1420:C:OP2	2.07	0.54
1:0:2459:G:OP1	30:3:64:LYS:HB2	2.08	0.54
2:A:217:ARG:CG	2:A:217:ARG:HH11	2.20	0.54
13:L:134:GLU:HG3	40:L:4812:HOH:O	2.07	0.54
1:0:820:G:O2'	1:0:856:G:H4'	2.07	0.54
31:9:7:G:H5'	40:9:5071:HOH:O	2.06	0.54
1:0:1894:C:N4	1:0:1939:U:H2'	2.23	0.54
2:A:39:ALA:O	2:A:61:GLU:HG3	2.08	0.54
19:R:123:GLN:HA	19:R:137:ASN:OD1	2.07	0.54
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.90	0.54
1:0:2832:C:OP1	19:R:71:LYS:HE3	2.08	0.54
17:P:115:SER:O	17:P:117:SER:N	2.41	0.54
23:V:1:THR:CG2	23:V:2:VAL:H	2.17	0.54
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.90	0.54
12:K:45:PRO:HB2	40:K:7169:HOH:O	2.07	0.54
1:0:1213:C:C2'	1:0:1214:G:H5'	2.38	0.54
1:0:138:U:OP2	1:0:139:C:H5	1.90	0.54
1:0:2812:A:H2	1:0:2814:A:H62	1.56	0.54
24:W:131:PRO:O	24:W:136:GLY:N	2.41	0.54
30:3:2:GLN:HG3	30:3:91:GLN:NE2	2.23	0.54
3:B:36:PRO:HG3	3:B:169:GLY:N	2.20	0.54
31:9:29:C:C2'	31:9:30:C:H5'	2.36	0.54
21:T:23:VAL:HG23	21:T:41:ARG:HG3	1.90	0.54
2:A:171:LYS:HG2	2:A:174:ASN:ND2	2.23	0.54
25:X:20:GLU:CG	25:X:21:PRO:HD2	2.38	0.54
3:B:41:PHE:HB3	3:B:190:MET:CE	2.38	0.54
1:0:2346:C:O2'	5:D:52:THR:HG21	2.06	0.54
1:0:2783:A:H3'	40:0:4201:HOH:O	2.08	0.54
1:0:105:G:O2'	1:0:106:A:H5'	2.07	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
1:0:1244:U:H4'	1:0:1246:A:O4'	2.08	0.53
3:B:162:MET:HE3	3:B:310:ARG:HD3	1.88	0.53
12:K:23:ASN:ND2	12:K:108:GLU:H	2.01	0.53
1:0:1641:A:C2'	1:0:1642:A:H5'	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:101:LYS:HG2	27:Z:104:ARG:HH12	1.72	0.53
17:P:7:LYS:HD3	17:P:23:PHE:CZ	2.43	0.53
21:T:51:LEU:O	21:T:52:ARG:HD3	2.08	0.53
1:0:485:A:O2'	1:0:487:G:H5'	2.08	0.53
1:0:1753:C:O2	3:B:229:ARG:NH2	2.39	0.53
1:0:392:U:O2'	14:M:182:LYS:HE2	2.08	0.53
6:E:21:THR:HG23	6:E:30:THR:OG1	2.08	0.53
1:0:2428:G:H5'	40:0:6155:HOH:O	2.07	0.53
9:H:48:VAL:HA	9:H:170:ARG:O	2.07	0.53
12:K:98:VAL:HG13	12:K:102:GLU:HA	1.85	0.53
15:N:38:LYS:HE2	15:N:107:ASN:HD22	1.70	0.53
1:0:1603:A:H5''	1:0:1605:G:H5'	1.90	0.53
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.53
3:B:51:VAL:HG23	3:B:330:VAL:HG22	1.91	0.53
22:U:14:GLU:OE1	22:U:15:PRO:HD2	2.08	0.53
1:0:1856:C:H5'	1:0:1858:A:O4'	2.08	0.53
1:0:1794:G:P	17:P:133:SER:HB2	2.47	0.53
1:0:2320:U:C2'	30:3:2:GLN:HB2	2.38	0.53
1:0:170:U:H5'	30:3:48:ASN:HB3	1.91	0.53
5:D:63:ILE:HG13	5:D:64:ARG:N	2.23	0.53
3:B:162:MET:HG3	3:B:310:ARG:NH1	2.23	0.53
18:Q:59:GLN:OE1	18:Q:75:ILE:HB	2.08	0.53
1:0:1555:G:H4'	1:0:1630:A:C2	2.43	0.53
31:9:95:C:O2'	31:9:96:C:H5'	2.09	0.53
24:W:13:MET:HE3	24:W:17:ILE:HG22	1.90	0.53
1:0:2825:C:H4'	1:0:2826:G:O5'	2.09	0.53
21:T:49:GLU:HB3	21:T:59:GLU:HG2	1.90	0.53
1:0:420:U:H5'	1:0:1920:C:O2	2.09	0.53
8:G:67:LEU:O	8:G:71:LEU:HG	2.08	0.53
23:V:39:ALA:C	23:V:41:GLU:H	2.11	0.53
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.44	0.53
19:R:47:LEU:O	19:R:51:ILE:HG13	2.09	0.53
2:A:9:ARG:HG2	2:A:16:PHE:CD2	2.43	0.53
15:N:4:PRO:HG3	31:9:69:U:OP1	2.08	0.53
1:0:1664:A:OP1	1:0:1664:A:H8	1.91	0.53
1:0:2893:C:O2'	1:0:2894:C:H5'	2.08	0.53
7:F:26:THR:HG21	7:F:102:GLY:C	2.28	0.53
30:3:11:CYS:HA	40:3:3538:HOH:O	2.07	0.53
30:3:2:GLN:HB3	30:3:91:GLN:HG3	1.90	0.53
11:J:74:ARG:O	11:J:78:ILE:HG12	2.08	0.53
28:1:18:LYS:HA	28:1:25:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:25:LYS:HG2	28:1:25:LYS:O	2.09	0.53
1:0:2768:A:H2'	1:0:2769:C:O4'	2.07	0.53
6:E:172:PRO:HB3	40:E:6931:HOH:O	2.09	0.53
12:K:105:ARG:HD2	40:K:3385:HOH:O	2.08	0.53
1:0:1735:C:OP2	3:B:234:ARG:HG3	2.08	0.53
17:P:40:VAL:O	17:P:44:VAL:HG23	2.08	0.53
9:H:128:ALA:HA	40:H:175:HOH:O	2.09	0.53
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.73	0.53
11:J:64:GLY:HA3	36:J:8821:CL:CL	2.45	0.53
5:D:60:GLU:HG3	5:D:60:GLU:O	2.08	0.53
9:H:50:ILE:HG12	9:H:168:VAL:HG22	1.90	0.53
20:S:18:MET:HG3	20:S:74:ALA:HB1	1.90	0.53
3:B:215:VAL:HB	40:B:5430:HOH:O	2.09	0.53
1:0:2780:C:H2'	1:0:2781:U:C6	2.43	0.53
5:D:47:GLN:NE2	5:D:75:LEU:HD23	2.23	0.53
1:0:703:G:O2'	1:0:704:C:H5'	2.09	0.53
1:0:338:C:H4'	4:C:174:ILE:HD11	1.90	0.53
20:S:49:VAL:HG13	20:S:66:VAL:HG13	1.91	0.53
30:3:64:LYS:HE2	30:3:84:ARG:NH1	2.24	0.53
31:9:1:U:H4'	31:9:3:A:OP1	2.08	0.53
1:0:2421:G:H1'	40:0:8242:HOH:O	2.07	0.53
7:F:46:GLU:HG3	40:F:3461:HOH:O	2.08	0.53
2:A:192:VAL:HG12	2:A:192:VAL:O	2.09	0.53
1:0:1839:A:H5'	1:0:2643:G:H4'	1.90	0.53
1:0:2842:G:H2'	1:0:2843:A:H5'	1.91	0.53
5:D:141:VAL:HG21	31:9:57:A:C8	2.44	0.53
2:A:88:ILE:HD13	2:A:100:PRO:CD	2.35	0.53
1:0:1544:U:O4	1:0:1640:C:H2'	2.09	0.53
3:B:30:PRO:HB2	3:B:39:GLN:HE21	1.72	0.53
13:L:108:VAL:HB	13:L:125:PHE:HD2	1.74	0.53
1:0:363:C:H2'	1:0:364:U:H6	1.72	0.53
7:F:53:ASP:OD1	7:F:80:GLN:N	2.42	0.53
26:Y:117:LEU:N	26:Y:174:VAL:HG21	2.23	0.53
1:0:196:G:H2'	40:L:6170:HOH:O	2.08	0.53
1:0:1521:C:H2'	1:0:1522:A:O4'	2.09	0.53
21:T:55:PHE:CD2	21:T:77:VAL:HG13	2.44	0.53
1:0:2860:G:H1'	40:0:6383:HOH:O	2.09	0.53
1:0:2819:C:O4'	3:B:96:PRO:HB2	2.09	0.53
1:0:2507:G:H2'	1:0:2510:C:N4	2.24	0.53
4:C:236:THR:HG22	4:C:239:ALA:HB2	1.91	0.53
1:0:1166:A:OP1	1:0:1174:A:H4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:166:ALA:HB2	14:M:169:ARG:NH2	2.23	0.53
1:0:421:C:H4'	1:0:1919:A:C6	2.44	0.53
24:W:52:VAL:HG22	24:W:53:ALA:H	1.73	0.53
8:G:24:VAL:O	8:G:28:GLU:HG3	2.09	0.53
11:J:69:TYR:O	11:J:69:TYR:CD2	2.62	0.53
1:0:2614:C:O2'	1:0:2615:U:H5'	2.09	0.53
1:0:1803:C:H2'	1:0:1804:A:C8	2.44	0.53
1:0:2824:C:H5''	1:0:2825:C:H5'	1.91	0.53
20:S:20:PHE:CD2	20:S:20:PHE:N	2.72	0.53
1:0:1857:A:N6	1:0:2247:C:H1'	2.24	0.53
1:0:1508:C:H5'	20:S:21:GLN:NE2	2.24	0.53
1:0:424:C:H2'	1:0:425:U:H6	1.72	0.53
1:0:2372:A:H2'	1:0:2373:U:C6	2.44	0.53
1:0:2659:U:H5''	40:0:8735:HOH:O	2.09	0.53
1:0:449:A:N7	4:C:43:LYS:HG2	2.24	0.53
1:0:708:A:H2'	1:0:709:G:O4'	2.09	0.53
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.09	0.53
31:9:115:C:H2'	31:9:116:C:H6	1.74	0.53
30:3:69:TYR:HB2	30:3:78:HIS:CE1	2.44	0.53
15:N:34:LEU:HD13	15:N:47:LEU:HD21	1.90	0.53
1:0:932:U:O2'	1:0:1296:A:H1'	2.08	0.53
10:I:108:HIS:H	10:I:109:PRO:HD2	1.74	0.53
28:1:42:SER:HB2	40:1:354:HOH:O	2.09	0.53
1:0:2415:A:N3	15:N:26:LEU:HD13	2.24	0.53
30:3:10:TYR:HB2	30:3:17:HIS:HE1	1.74	0.52
15:N:37:ARG:NH1	31:9:6:C:OP1	2.42	0.52
2:A:217:ARG:HG3	2:A:217:ARG:HH11	1.75	0.52
1:0:1496:A:H2'	1:0:1497:G:O4'	2.09	0.52
1:0:2325:U:H2'	1:0:2326:C:C6	2.44	0.52
22:U:20:MET:HG3	22:U:30:HIS:CE1	2.44	0.52
1:0:1262:C:O2'	24:W:120:PRO:HD3	2.08	0.52
1:0:1566:C:H2'	1:0:1567:G:C8	2.44	0.52
1:0:834:G:H3'	1:0:835:U:H4'	1.91	0.52
1:0:2830:U:O2'	1:0:2831:C:H5'	2.09	0.52
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.52
8:G:63:ARG:N	40:G:2569:HOH:O	2.41	0.52
26:Y:145:LYS:O	26:Y:147:ARG:HG2	2.08	0.52
16:O:62:GLY:O	16:O:79:VAL:HG23	2.09	0.52
14:M:159:VAL:HG12	36:M:8818:CL:CL	2.47	0.52
1:0:2612:A:H4'	40:0:8224:HOH:O	2.09	0.52
1:0:2714:U:H4'	3:B:10:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2055:A:H5'	19:R:134:SER:HB2	1.91	0.52
21:T:41:ARG:HG2	21:T:41:ARG:NH1	2.23	0.52
10:I:95:LEU:HD22	10:I:99:GLN:HB3	1.89	0.52
10:I:133:THR:HG22	10:I:134:ILE:N	2.23	0.52
1:O:1008:C:O2'	1:O:1009:U:H5'	2.09	0.52
1:O:1815:A:H2'	1:O:1816:C:O4'	2.10	0.52
1:O:2740:G:H2'	1:O:2741:A:O4'	2.08	0.52
1:O:1114:A:O2'	1:O:1115:U:H5'	2.09	0.52
21:T:71:VAL:CG1	21:T:90:PRO:HB3	2.30	0.52
1:O:93:C:H5'	23:V:1:THR:HB	1.90	0.52
3:B:51:VAL:HG23	3:B:329:TYR:O	2.08	0.52
1:O:2609:G:N2	3:B:238:ASN:HD21	2.07	0.52
1:O:1416:G:C2'	1:O:1417:G:H5'	2.39	0.52
6:E:69:ILE:HA	6:E:72:MET:HE2	1.90	0.52
9:H:73:ASN:HB2	9:H:88:MET:CE	2.39	0.52
25:X:34:ARG:NH1	25:X:48:VAL:O	2.42	0.52
1:O:857:A:H4'	2:A:176:HIS:CD2	2.45	0.52
1:O:2371:G:H5'	40:O:3898:HOH:O	2.08	0.52
1:O:621:C:H2'	1:O:622:G:C8	2.45	0.52
11:J:19:MET:HE2	11:J:79:PHE:HA	1.92	0.52
6:E:101:GLU:CB	6:E:117:THR:HA	2.39	0.52
5:D:18:ILE:HG12	5:D:134:LEU:HD21	1.91	0.52
1:O:1294:A:H2'	1:O:1295:G:O4'	2.10	0.52
1:O:911:G:H5'	1:O:932:U:OP1	2.09	0.52
1:O:635:A:H2'	1:O:636:G:H5'	1.90	0.52
11:J:17:CYS:HA	11:J:119:THR:O	2.10	0.52
1:O:1925:G:OP1	30:3:29:ARG:CZ	2.58	0.52
1:O:1170:U:H2'	1:O:1172:G:OP2	2.10	0.52
1:O:1594:C:OP2	17:P:120:ARG:HD2	2.09	0.52
1:O:2909:G:H2'	1:O:2910:A:H8	1.75	0.52
24:W:48:VAL:HG12	24:W:48:VAL:O	2.09	0.52
31:9:73:A:N6	31:9:108:C:H42	2.05	0.52
1:O:1762:C:O2'	1:O:1763:C:H5'	2.10	0.52
4:C:131:PHE:N	4:C:131:PHE:CD2	2.77	0.52
13:L:112:GLY:H	13:L:132:LYS:NZ	2.07	0.52
27:Z:61:HIS:HB2	27:Z:71:VAL:HB	1.91	0.52
1:O:2320:U:O5'	30:3:1:MET:HA	2.09	0.52
1:O:1185:U:OP1	10:I:121:LYS:HD3	2.10	0.52
14:M:83:SER:CB	30:3:47:GLY:HA2	2.37	0.52
40:O:3741:HOH:O	30:3:25:VAL:HG11	2.09	0.52
1:O:2766:A:O2'	1:O:2767:C:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:7:LYS:HD2	17:P:21:VAL:HG21	1.92	0.52
13:L:73:VAL:HG23	13:L:74:THR:N	2.24	0.52
13:L:17:SER:C	13:L:19:LYS:N	2.60	0.52
6:E:15:GLN:HG2	6:E:16:ASP:N	2.25	0.52
4:C:135:GLU:O	4:C:136:VAL:HB	2.10	0.52
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.92	0.52
21:T:102:ASP:O	21:T:103:LEU:HD23	2.10	0.52
22:U:45:GLU:HB2	22:U:48:ASN:ND2	2.24	0.52
5:D:140:ARG:HG3	5:D:140:ARG:HH11	1.74	0.52
12:K:21:ALA:O	12:K:22:ASP:HB3	2.10	0.52
9:H:4:LYS:HE3	9:H:100:GLU:OE2	2.10	0.52
1:O:70:A:H4'	1:O:71:G:O5'	2.10	0.52
40:O:7968:HOH:O	4:C:80:VAL:HA	2.09	0.52
1:O:154:C:H2'	1:O:155:C:C6	2.45	0.52
1:O:2016:U:H2'	1:O:2017:U:O4'	2.09	0.52
31:9:3:A:H2	31:9:21:G:N3	2.08	0.52
36:O:8812:CL:CL	12:K:14:LYS:NZ	2.78	0.52
5:D:103:ASN:HD22	5:D:133:ASN:HA	1.75	0.52
15:N:49:THR:CG2	15:N:56:ASP:HB2	2.39	0.52
1:O:524:A:C5'	19:R:29:LYS:HE2	2.40	0.52
1:O:157:G:H3'	40:O:8533:HOH:O	2.09	0.52
10:I:127:CYS:HB3	10:I:132:VAL:HB	1.92	0.52
2:A:36:ASP:CB	2:A:85:SER:HB2	2.39	0.52
1:O:1279:U:O2	1:O:1279:U:H2'	2.09	0.52
1:O:918:G:H5''	40:O:3194:HOH:O	2.10	0.52
1:O:463:A:H5'	1:O:465:U:O4'	2.10	0.52
1:O:1315:G:C4	26:Y:212:ARG:HB2	2.45	0.52
1:O:1052:G:H2'	1:O:1052:G:N3	2.24	0.52
11:J:80:LYS:HE2	11:J:98:PHE:CZ	2.45	0.52
13:L:144:ASP:HA	13:L:147:GLU:OE1	2.10	0.52
27:Z:53:ILE:HG23	27:Z:93:TYR:HB3	1.91	0.52
40:O:4499:HOH:O	8:G:12:ILE:HA	2.10	0.52
1:O:2311:A:H5'	9:H:120:PHE:CD1	2.45	0.52
18:Q:41:LEU:HB3	18:Q:52:PHE:CZ	2.44	0.52
1:O:2278:U:H5'	40:O:4522:HOH:O	2.09	0.52
12:K:114:ALA:HB3	12:K:117:VAL:HG23	1.91	0.52
27:Z:38:PHE:HB3	27:Z:42:TYR:CD1	2.45	0.52
1:O:2050:G:H5''	19:R:80:TYR:O	2.10	0.52
1:O:1069:C:H2'	1:O:1070:A:O4'	2.10	0.52
1:O:561:G:H2'	1:O:562:A:H8	1.74	0.52
16:O:47:ARG:NH1	16:O:47:ARG:HG3	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:704:C:H2'	1:0:705:C:H6	1.75	0.52
40:K:7438:HOH:O	22:U:20:MET:HE2	2.09	0.52
1:0:2394:A:H5'	40:0:6767:HOH:O	2.10	0.52
1:0:451:C:O2'	1:0:452:G:H5'	2.09	0.52
1:0:1020:A:H2'	1:0:1021:G:C8	2.45	0.52
1:0:1948:G:H1	1:0:1964:U:H3	1.57	0.52
2:A:72:GLU:HG3	27:Z:90:GLY:HA2	1.92	0.52
1:0:2401:A:H2'	1:0:2402:A:C8	2.45	0.52
1:0:2433:A:O4'	38:0:2924:MYL:HBf	2.10	0.51
38:0:2924:MYL:OAS	38:0:2924:MYL:HAGA	2.11	0.51
1:0:1246:A:O2'	1:0:1247:A:H3'	2.10	0.51
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.91	0.51
19:R:39:THR:CB	19:R:42:GLU:HG3	2.39	0.51
1:0:363:C:H2'	1:0:364:U:C6	2.45	0.51
1:0:1168:C:H5'	10:I:83:GLY:HA3	1.92	0.51
1:0:727:G:H3'	1:0:728:C:C6	2.45	0.51
1:0:517:U:H2'	1:0:518:G:H5'	1.91	0.51
1:0:2375:A:H2'	1:0:2376:C:C6	2.45	0.51
14:M:184:ARG:HG3	14:M:185:PRO:HA	1.91	0.51
1:0:2498:C:O2'	1:0:2499:U:H5'	2.10	0.51
1:0:2344:G:N3	1:0:2344:G:H2'	2.25	0.51
3:B:157:LYS:O	3:B:159:PRO:HD3	2.09	0.51
31:9:75:G:H1	31:9:106:U:H3	1.56	0.51
11:J:45:VAL:HG22	11:J:46:ILE:N	2.24	0.51
26:Y:187:VAL:CG2	26:Y:192:ASP:HB2	2.35	0.51
21:T:43:ASN:HB2	21:T:108:ARG:NH1	2.25	0.51
1:0:1167:G:H2'	1:0:1168:C:C6	2.45	0.51
1:0:2414:A:H2'	1:0:2415:A:C8	2.45	0.51
1:0:453:A:H4'	1:0:455:A:N7	2.25	0.51
26:Y:149:GLN:HB3	40:Y:6589:HOH:O	2.09	0.51
4:C:16:VAL:HG12	4:C:17:ASP:H	1.76	0.51
1:0:2541:U:H5'	40:0:4280:HOH:O	2.09	0.51
11:J:52:GLN:HG3	11:J:53:ILE:N	2.25	0.51
1:0:2319:C:H3'	30:3:1:MET:H1	1.72	0.51
4:C:140:VAL:HB	40:C:6502:HOH:O	2.08	0.51
1:0:259:G:H21	14:M:58:GLN:HE22	1.58	0.51
1:0:746:A:C6	16:O:65:LEU:HD13	2.46	0.51
6:E:126:ILE:HA	6:E:131:LEU:HD23	1.93	0.51
31:9:39:U:H3	31:9:42:C:H5''	1.76	0.51
6:E:69:ILE:HA	6:E:72:MET:CE	2.40	0.51
1:0:1020:A:H2'	1:0:1021:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:107:LYS:HA	13:L:124:ASP:O	2.11	0.51
3:B:102:THR:HG23	3:B:182:VAL:HG12	1.91	0.51
1:0:2316:G:H4'	40:0:5391:HOH:O	2.10	0.51
13:L:92:ASP:HA	13:L:121:ILE:HB	1.92	0.51
19:R:132:ARG:HD3	40:R:248:HOH:O	2.10	0.51
1:0:2436:U:H5''	30:3:70:ARG:HH22	1.75	0.51
1:0:2416:G:H2'	1:0:2417:C:C6	2.44	0.51
4:C:31:ILE:HA	4:C:110:ALA:HB1	1.93	0.51
25:X:70:ILE:O	25:X:70:ILE:HG23	2.11	0.51
9:H:157:TYR:CD1	9:H:157:TYR:C	2.84	0.51
7:F:1:PRO:H3	7:F:4:VAL:HG23	1.75	0.51
25:X:61:ARG:HH12	25:X:67:PRO:HD3	1.76	0.51
24:W:82:GLU:HB2	40:W:2749:HOH:O	2.11	0.51
17:P:115:SER:H	17:P:118:GLN:HE21	1.55	0.51
10:I:87:PRO:HB3	40:I:6825:HOH:O	2.10	0.51
30:3:25:VAL:HG22	30:3:68:LYS:CG	2.38	0.51
1:0:775:G:OP1	28:1:16:HIS:HE1	1.93	0.51
1:0:470:U:O2'	28:1:16:HIS:CD2	2.62	0.51
24:W:13:MET:HE1	24:W:18:GLN:HA	1.91	0.51
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
3:B:233:ARG:HH11	3:B:233:ARG:HG2	1.75	0.51
21:T:81:LYS:HD2	21:T:87:VAL:HG11	1.92	0.51
1:0:2594:C:O2'	1:0:2595:U:H5'	2.10	0.51
1:0:95:A:H5''	1:0:97:G:O4'	2.09	0.51
30:3:6:ARG:HH11	30:3:6:ARG:HG2	1.75	0.51
14:M:84:LYS:HA	30:3:46:ILE:O	2.10	0.51
30:3:65:THR:HG21	30:3:88:LEU:HD22	1.93	0.51
1:0:545:G:C8	1:0:545:G:H5'	2.39	0.51
13:L:134:GLU:HA	13:L:138:GLY:O	2.09	0.51
8:G:71:LEU:C	8:G:73:ASP:N	2.62	0.51
1:0:553:G:H2'	1:0:554:G:H5'	1.93	0.51
18:Q:25:PRO:HB2	40:9:4350:HOH:O	2.09	0.51
3:B:51:VAL:CG2	3:B:327:VAL:HG13	2.40	0.51
14:M:157:ASP:HB3	14:M:160:PHE:HD1	1.76	0.51
1:0:154:C:H2'	1:0:155:C:H6	1.75	0.51
21:T:64:ASN:HB3	21:T:73:HIS:HB2	1.92	0.51
4:C:8:LEU:HD11	4:C:143:ASP:O	2.10	0.51
1:0:2276:U:H2'	1:0:2277:U:C6	2.45	0.51
1:0:790:A:H1'	1:0:1710:A:H2'	1.92	0.51
1:0:1592:G:H2'	1:0:1593:C:H6	1.75	0.51
1:0:1996:U:H6	1:0:2586:U:O2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:853:C:H2'	1:0:854:G:O4'	2.11	0.51
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.45	0.51
18:Q:27:GLN:HE21	31:9:8:G:C5'	2.24	0.51
22:U:13:ILE:HG12	22:U:32:CYS:CB	2.41	0.51
3:B:150:ALA:O	3:B:152:PRO:HD3	2.11	0.51
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.51
1:0:1855:G:H4'	1:0:1856:C:O5'	2.10	0.51
16:O:25:VAL:O	16:O:28:ASP:N	2.44	0.51
1:0:155:C:OP1	14:M:189:SER:HB3	2.11	0.51
21:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.51
1:0:2119:C:O2'	1:0:2120:U:H5'	2.11	0.51
1:0:2515:C:H2'	1:0:2516:G:O4'	2.10	0.51
1:0:963:C:H2'	1:0:964:G:C8	2.45	0.51
1:0:1299:G:O6	13:L:6:ARG:HD3	2.11	0.51
1:0:1437:A:O2'	1:0:1438:G:H5'	2.10	0.51
4:C:165:ASP:O	4:C:168:ARG:HB3	2.10	0.51
1:0:2319:C:H3'	30:3:1:MET:CA	2.40	0.51
40:0:7242:HOH:O	21:T:9:LYS:HD2	2.10	0.51
12:K:113:ILE:HD12	12:K:128:ALA:HB2	1.91	0.51
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.91	0.51
1:0:269:G:O3'	1:0:274:G:H4'	2.11	0.51
4:C:123:LEU:O	4:C:126:ASP:HB2	2.11	0.51
1:0:10:U:C6	1:0:10:U:H3'	2.44	0.51
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.45	0.51
1:0:308:U:C4	1:0:342:C:H1'	2.46	0.51
5:D:81:GLU:O	5:D:84:LEU:N	2.44	0.51
1:0:2134:G:N2	1:0:2242:U:C2	2.78	0.51
9:H:49:GLN:O	9:H:169:GLU:HB2	2.11	0.51
1:0:629:A:H2'	1:0:630:A:O4'	2.11	0.51
1:0:412:C:O2'	1:0:413:G:H5'	2.10	0.51
1:0:1514:C:H2'	1:0:1515:A:C8	2.45	0.51
1:0:1333:U:H2'	1:0:1334:C:H6	1.75	0.51
18:Q:91:LEU:O	18:Q:92:ARG:HD2	2.09	0.51
1:0:1180:U:H4'	10:I:86:GLU:HG2	1.92	0.51
1:0:2363:G:O2'	18:Q:11:ARG:HG3	2.10	0.51
4:C:18:LEU:HD12	4:C:19:PRO:HD2	1.93	0.51
1:0:1634:G:H2'	1:0:1635:U:C6	2.45	0.51
1:0:2508:C:H2'	40:0:6319:HOH:O	2.10	0.51
1:0:329:A:OP2	4:C:206:ASN:HB2	2.09	0.51
1:0:1792:C:H2'	1:0:1793:C:H6	1.75	0.51
30:3:60:LYS:CG	30:3:61:PRO:HD2	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:64:PRO:HB2	27:Z:86:TYR:HE2	1.73	0.51
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.51
1:0:2840:A:OP1	3:B:211:THR:HG23	2.11	0.51
12:K:109:LEU:CD1	12:K:113:ILE:HD11	2.40	0.51
1:0:2821:C:H4'	3:B:116:PRO:HB3	1.93	0.51
4:C:123:LEU:O	4:C:126:ASP:N	2.43	0.51
1:0:2782:G:O6	1:0:2790:C:H5''	2.11	0.51
1:0:2796:U:H1'	6:E:143:GLN:OE1	2.10	0.51
22:U:39:ASN:HD22	22:U:49:LEU:HD11	1.75	0.51
1:0:423:A:H2'	1:0:424:C:H6	1.76	0.51
1:0:1636:G:O2'	1:0:1637:A:H5'	2.11	0.51
9:H:117:ARG:HB3	40:H:7374:HOH:O	2.10	0.51
40:0:5660:HOH:O	26:Y:158:LYS:HD3	2.11	0.51
9:H:81:GLY:C	9:H:83:GLU:H	2.15	0.51
1:0:2510:C:H42	1:0:2564:G:N2	2.09	0.50
11:J:131:THR:HG22	11:J:133:GLY:N	2.25	0.50
8:G:23:ILE:HG22	8:G:27:ILE:HD11	1.93	0.50
13:L:94:ARG:NH1	13:L:143:THR:HG21	2.26	0.50
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.50
16:O:21:SER:HB2	16:O:106:PRO:O	2.10	0.50
1:0:1504:A:H4'	1:0:1506:U:C5	2.46	0.50
1:0:1980:U:O2'	1:0:1981:A:H5'	2.10	0.50
1:0:1829:A:C2'	1:0:1830:C:H5'	2.41	0.50
1:0:1552:G:H2'	1:0:1553:C:C6	2.46	0.50
3:B:55:ASN:HB3	3:B:64:GLY:H	1.75	0.50
19:R:33:ARG:NH1	19:R:33:ARG:HB2	2.26	0.50
15:N:80:SER:HB2	40:N:4257:HOH:O	2.11	0.50
7:F:19:ALA:O	7:F:22:VAL:HG22	2.11	0.50
1:0:1966:U:H2'	1:0:1967:U:C6	2.46	0.50
1:0:1178:G:H2'	1:0:1179:C:C6	2.45	0.50
19:R:95:ALA:HB1	19:R:147:LEU:HD11	1.92	0.50
1:0:1183:C:N3	1:0:1184:C:C5	2.79	0.50
1:0:1206:U:H2'	1:0:1207:A:O4'	2.11	0.50
2:A:109:GLU:HG2	2:A:116:GLY:N	2.20	0.50
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.94	0.50
13:L:129:ALA:O	13:L:133:VAL:HG23	2.11	0.50
24:W:80:ASP:C	24:W:84:VAL:HG23	2.31	0.50
2:A:164:ARG:HA	27:Z:93:TYR:CE1	2.45	0.50
1:0:334:G:H2'	1:0:335:U:O4'	2.11	0.50
1:0:2584:G:H4'	40:0:6824:HOH:O	2.10	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2057:U:O5'	1:0:2057:U:H6	1.93	0.50
1:0:162:C:H2'	1:0:163:U:H5'	1.94	0.50
1:0:2590:U:O2	32:4:74:C:H1'	2.12	0.50
1:0:1594:C:C5	17:P:120:ARG:NH1	2.79	0.50
1:0:398:U:H2'	1:0:399:C:C6	2.45	0.50
25:X:22:ASN:OD1	25:X:25:ARG:HD2	2.11	0.50
1:0:1735:C:O2'	1:0:1736:A:H5'	2.10	0.50
4:C:21:VAL:HG13	40:C:3779:HOH:O	2.12	0.50
1:0:2712:G:OP1	12:K:43:ARG:NH1	2.44	0.50
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.50
14:M:69:LYS:CG	14:M:70:GLY:H	2.18	0.50
1:0:2320:U:P	30:3:2:GLN:HG2	2.52	0.50
23:V:7:GLU:O	23:V:11:MET:HG3	2.11	0.50
1:0:877:G:C5'	1:0:878:G:OP1	2.55	0.50
1:0:711:G:C2	1:0:718:C:C2	2.99	0.50
21:T:19:ARG:HD3	21:T:67:LEU:O	2.11	0.50
24:W:88:THR:HG21	24:W:96:LEU:HD13	1.93	0.50
1:0:2694:A:H5''	6:E:90:HIS:CE1	2.47	0.50
4:C:4:THR:HA	4:C:15:GLU:HB3	1.93	0.50
1:0:2869:G:H5'	40:0:4548:HOH:O	2.11	0.50
4:C:111:VAL:HB	40:C:721:HOH:O	2.10	0.50
9:H:79:GLU:O	9:H:80:LEU:HD23	2.11	0.50
1:0:1057:A:H1'	1:0:2492:U:O2'	2.12	0.50
1:0:445:U:H2'	1:0:446:G:H8	1.75	0.50
1:0:219:G:O2'	30:3:51:LYS:HB3	2.11	0.50
30:3:64:LYS:HA	30:3:83:TRP:O	2.10	0.50
1:0:2510:C:N4	1:0:2564:G:H22	2.07	0.50
1:0:1201:C:H5''	40:0:5584:HOH:O	2.10	0.50
12:K:30:LYS:O	12:K:55:VAL:HG13	2.11	0.50
5:D:99:ASP:HB3	5:D:103:ASN:H	1.77	0.50
1:0:1774:G:O2'	1:0:1775:A:H5'	2.12	0.50
4:C:5:ILE:HG22	4:C:6:TYR:N	2.27	0.50
1:0:836:G:H1'	40:0:7509:HOH:O	2.10	0.50
23:V:4:HIS:HB3	40:V:6622:HOH:O	2.12	0.50
1:0:310:U:H2'	1:0:311:C:C6	2.46	0.50
1:0:1783:A:O2'	1:0:1784:U:H5'	2.11	0.50
1:0:1314:U:H5''	1:0:1316:G:O4'	2.11	0.50
3:B:53:LEU:HD21	3:B:270:ILE:HD12	1.93	0.50
29:2:40:ARG:HA	29:2:45:ASN:ND2	2.27	0.50
1:0:80:A:H3'	21:T:43:ASN:OD1	2.12	0.50
12:K:55:VAL:HG12	12:K:56:SER:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:612:U:H2'	1:0:613:C:C6	2.47	0.50
7:F:100:ASP:O	7:F:101:ALA:O	2.30	0.50
1:0:2769:C:C2'	1:0:2770:G:H5'	2.42	0.50
5:D:75:LEU:HB3	5:D:80:ALA:HA	1.93	0.50
26:Y:182:PHE:CG	26:Y:202:ALA:HB2	2.47	0.50
3:B:238:ASN:ND2	3:B:240:GLY:H	2.09	0.50
10:I:119:ALA:O	10:I:123:VAL:HG23	2.12	0.50
1:0:2028:U:H2'	1:0:2029:C:H6	1.76	0.50
10:I:111:LEU:HD22	10:I:122:GLU:OE1	2.11	0.50
1:0:1003:U:H4'	9:H:91:ARG:O	2.11	0.50
12:K:66:ARG:HH11	12:K:66:ARG:HG2	1.77	0.50
1:0:1119:G:OP2	11:J:49:ARG:HD3	2.12	0.50
1:0:1593:C:H5'	17:P:120:ARG:HG2	1.92	0.50
1:0:1351:G:H1'	40:0:3441:HOH:O	2.10	0.50
8:G:64:ASN:ND2	8:G:64:ASN:N	2.59	0.50
24:W:60:GLU:O	24:W:63:GLU:HB2	2.11	0.50
1:0:2904:U:H4'	25:X:8:ARG:HH12	1.77	0.50
3:B:305:ASP:O	3:B:306:LYS:CB	2.59	0.50
1:0:945:U:O2'	24:W:43:GLY:HA3	2.11	0.50
23:V:27:LEU:HA	23:V:49:LEU:HD13	1.93	0.50
20:S:57:THR:CG2	20:S:58:MET:N	2.75	0.50
1:0:583:C:H2'	1:0:584:U:H6	1.76	0.50
1:0:685:C:O2	1:0:748:C:H4'	2.12	0.50
4:C:133:ARG:HG2	4:C:134:ASP:N	2.27	0.50
3:B:332:ASN:HB3	40:B:2649:HOH:O	2.12	0.50
32:4:74:C:H2'	32:4:75:C:H5'	1.93	0.50
21:T:69:LYS:O	21:T:71:VAL:HG23	2.12	0.50
26:Y:189:ASN:HB2	40:Y:651:HOH:O	2.11	0.50
3:B:212:GLN:HB2	3:B:257:THR:CG2	2.38	0.50
1:0:1157:C:H2'	1:0:1158:G:H8	1.75	0.50
1:0:2335:C:H2'	1:0:2336:G:H8	1.75	0.50
2:A:217:ARG:HG2	2:A:229:ALA:CB	2.37	0.50
1:0:292:G:H1'	1:0:360:A:N6	2.27	0.50
18:Q:27:GLN:HB3	40:9:4350:HOH:O	2.12	0.50
1:0:2439:C:H5'	40:0:4534:HOH:O	2.12	0.50
11:J:25:GLN:NE2	11:J:116:LEU:HB3	2.27	0.50
9:H:49:GLN:HG3	9:H:140:TYR:CE2	2.47	0.50
40:0:6935:HOH:O	28:1:41:LYS:HD3	2.11	0.50
1:0:1674:C:P	20:S:34:LYS:HG3	2.52	0.50
15:N:160:SER:HB2	31:9:51:A:H5'	1.94	0.50
9:H:32:ALA:C	9:H:33:GLN:HG3	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:OP2	16:O:37:ARG:HD2	2.12	0.50
1:0:2407:G:O2'	1:0:2408:A:H5'	2.12	0.50
15:N:35:VAL:HG13	40:N:3863:HOH:O	2.12	0.50
1:0:614:U:H2'	1:0:615:G:H8	1.77	0.50
1:0:2070:G:H4'	40:0:2976:HOH:O	2.12	0.50
14:M:82:ARG:O	14:M:86:GLN:HG3	2.12	0.50
17:P:138:GLU:C	17:P:140:TYR:N	2.65	0.50
3:B:5:ARG:HD2	3:B:8:LYS:CE	2.41	0.50
28:1:37:CYS:SG	28:1:39:PHE:HB2	2.52	0.50
5:D:78:GLU:O	5:D:80:ALA:N	2.44	0.50
15:N:115:VAL:HG23	15:N:116:PHE:N	2.27	0.50
16:O:25:VAL:HG23	16:O:26:TRP:H	1.77	0.50
1:0:79:G:N2	1:0:97:G:H1'	2.27	0.50
1:0:2898:G:H1'	3:B:282:GLY:O	2.12	0.50
1:0:1797:A:H4'	1:0:1798:C:C5	2.47	0.50
17:P:91:LYS:O	17:P:95:GLU:HG3	2.12	0.50
1:0:536:A:H3'	40:0:3958:HOH:O	2.12	0.50
14:M:71:SER:HB2	14:M:92:THR:CG2	2.22	0.49
1:0:1163:G:H2'	1:0:1164:U:C5	2.47	0.49
1:0:1185:U:H2'	1:0:1186:C:C6	2.47	0.49
5:D:41:LEU:HA	5:D:44:ILE:CG2	2.40	0.49
26:Y:96:GLU:O	26:Y:235:GLU:HA	2.12	0.49
8:G:64:ASN:O	8:G:68:GLU:HG3	2.12	0.49
9:H:25:GLY:O	9:H:27:PRO:HD3	2.12	0.49
1:0:2703:A:H2'	1:0:2704:C:C6	2.47	0.49
17:P:98:ILE:HD13	17:P:98:ILE:O	2.12	0.49
3:B:279:THR:OG1	3:B:290:VAL:HB	2.12	0.49
14:M:186:SER:HB3	14:M:189:SER:HB3	1.94	0.49
12:K:76:GLN:HA	12:K:93:ASN:HA	1.94	0.49
1:0:1091:U:H4'	26:Y:123:VAL:HG13	1.94	0.49
1:0:1928:C:H2'	1:0:1929:G:O4'	2.12	0.49
16:O:81:PHE:HB2	16:O:86:GLU:HB2	1.93	0.49
4:C:47:GLY:HA2	4:C:92:PRO:HB2	1.92	0.49
21:T:38:ARG:HH11	21:T:38:ARG:HG3	1.76	0.49
14:M:57:LYS:HZ3	14:M:144:ASP:HB2	1.77	0.49
29:2:41:HIS:HD2	29:2:44:ARG:H	1.60	0.49
1:0:484:A:N1	1:0:506:G:H4'	2.28	0.49
16:O:49:GLU:OE2	16:O:71:GLN:HB2	2.12	0.49
24:W:52:VAL:CG2	24:W:53:ALA:N	2.75	0.49
18:Q:28:ARG:HG2	40:9:4350:HOH:O	2.11	0.49
2:A:36:ASP:HB2	2:A:85:SER:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:139:ASP:HB2	3:B:165:ARG:HE	1.78	0.49
17:P:24:ASN:OD1	17:P:26:GLU:N	2.43	0.49
13:L:40:PHE:C	13:L:40:PHE:CD1	2.84	0.49
1:O:920:C:H4'	1:O:921:G:C2	2.47	0.49
4:C:233:THR:HG22	4:C:234:VAL:H	1.77	0.49
1:O:2635:A:O2'	1:O:2636:C:H5'	2.12	0.49
1:O:151:A:H2'	1:O:152:A:O4'	2.13	0.49
1:O:264:G:H1'	1:O:265:U:H5	1.76	0.49
24:W:146:ILE:HG22	24:W:147:ASP:N	2.26	0.49
26:Y:205:ILE:HD12	26:Y:214:ARG:NH1	2.27	0.49
5:D:25:MET:SD	5:D:40:ILE:HD11	2.52	0.49
4:C:96:LYS:HB3	4:C:98:ARG:NH1	2.22	0.49
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.43	0.49
1:O:2748:G:H2'	40:O:7410:HOH:O	2.10	0.49
1:O:229:G:O2'	1:O:230:C:H5'	2.12	0.49
1:O:1553:C:H2'	1:O:1554:C:H6	1.77	0.49
3:B:297:VAL:HB	40:B:4810:HOH:O	2.12	0.49
1:O:2323:G:H5'	40:O:6692:HOH:O	2.12	0.49
1:O:2597:U:H2'	1:O:2598:U:H5'	1.93	0.49
31:9:37:C:O2	31:9:47:A:H1'	2.13	0.49
16:O:89:ILE:HG21	16:O:95:ALA:HB2	1.94	0.49
9:H:54:VAL:HG13	9:H:162:PRO:HG3	1.94	0.49
1:O:1180:U:H2'	1:O:1181:A:O4'	2.13	0.49
14:M:122:GLN:O	14:M:122:GLN:HG3	2.12	0.49
3:B:205:VAL:HB	3:B:307:ARG:HD3	1.95	0.49
3:B:304:PRO:HD2	3:B:307:ARG:NE	2.27	0.49
1:O:398:U:O3'	14:M:179:GLY:HA3	2.12	0.49
1:O:2694:A:H4'	6:E:91:PHE:CE1	2.43	0.49
24:W:122:ARG:HG3	24:W:122:ARG:NH1	2.27	0.49
7:F:36:THR:HG23	7:F:97:ALA:HB2	1.95	0.49
8:G:12:ILE:N	8:G:13:PRO:HD3	2.28	0.49
1:O:2642:G:H2'	1:O:2643:G:O4'	2.12	0.49
1:O:423:A:H2'	1:O:424:C:C6	2.47	0.49
1:O:79:G:H22	1:O:97:G:H1'	1.78	0.49
1:O:2854:A:H2'	1:O:2855:G:H8	1.77	0.49
1:O:2576:A:H4'	1:O:2799:A:C2	2.47	0.49
1:O:1494:A:H1'	1:O:1495:C:C6	2.47	0.49
1:O:1211:G:O2'	1:O:1212:C:H5'	2.12	0.49
30:3:7:PHE:HE1	30:3:9:THR:HG21	1.77	0.49
15:N:15:GLU:OE1	15:N:17:ARG:HD2	2.13	0.49
10:I:118:ASN:HA	10:I:121:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:GLY:O	3:B:308:LEU:HD12	2.12	0.49
18:Q:21:ARG:HG2	18:Q:22:GLY:N	2.26	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.49
3:B:41:PHE:HA	3:B:79:MET:CE	2.42	0.49
1:0:2783:A:H2'	1:0:2784:A:C8	2.48	0.49
10:I:106:GLN:O	10:I:108:HIS:N	2.46	0.49
3:B:294:TYR:HE2	40:B:7123:HOH:O	1.95	0.49
31:9:26:C:H2'	31:9:27:C:C6	2.48	0.49
11:J:54:VAL:HG11	11:J:138:THR:HG21	1.93	0.49
1:0:1235:G:C1'	11:J:63:ILE:HG23	2.42	0.49
1:0:566:A:H2'	1:0:567:U:O4'	2.12	0.49
38:0:2924:MYL:HACB	38:0:2924:MYL:CAN	2.42	0.49
1:0:1119:G:H5'	11:J:52:GLN:NE2	2.27	0.49
4:C:127:ARG:HG2	4:C:127:ARG:NH1	2.27	0.49
12:K:97:ILE:HG22	12:K:98:VAL:N	2.27	0.49
5:D:170:TYR:O	5:D:171:ASP:HB3	2.12	0.49
15:N:143:ARG:HG2	15:N:172:PHE:CE2	2.48	0.49
14:M:48:LYS:HE3	14:M:52:GLN:HE21	1.76	0.49
3:B:140:LEU:HD13	3:B:175:LEU:HA	1.95	0.49
1:0:1787:C:OP1	17:P:68:LYS:HE2	2.12	0.49
2:A:54:PRO:HG2	2:A:160:ALA:HB3	1.94	0.49
3:B:54:VAL:HB	40:B:5136:HOH:O	2.12	0.49
31:9:59:C:O5'	31:9:59:C:H6	1.95	0.49
1:0:2473:U:O3'	1:0:2474:A:H3'	2.13	0.49
14:M:74:LYS:HG2	14:M:87:GLY:O	2.13	0.49
15:N:90:LEU:O	15:N:93:GLN:HB2	2.12	0.49
3:B:84:LEU:HD23	3:B:178:ALA:HB1	1.94	0.49
1:0:926:A:H1'	13:L:38:HIS:O	2.13	0.49
31:9:73:A:H61	31:9:108:C:N4	2.07	0.49
17:P:137:LEU:O	17:P:140:TYR:HB3	2.13	0.49
8:G:12:ILE:HG22	8:G:17:GLN:NE2	2.28	0.49
1:0:654:A:OP2	16:O:38:ARG:HD2	2.13	0.49
7:F:20:LEU:O	7:F:23:ALA:HB3	2.12	0.49
1:0:2906:A:H5'	1:0:2907:C:O4'	2.13	0.49
2:A:21:HIS:CE1	2:A:22:ARG:HG3	2.48	0.49
14:M:181:GLU:N	14:M:181:GLU:OE1	2.39	0.49
14:M:77:HIS:CG	14:M:81:ARG:HB3	2.48	0.49
31:9:115:C:H2'	31:9:116:C:C6	2.48	0.49
2:A:33:GLU:O	2:A:34:ASP:HB2	2.12	0.49
13:L:120:LEU:HB2	13:L:140:VAL:HG23	1.95	0.49
17:P:83:LYS:O	17:P:86:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:64:MET:HA	12:K:67:GLN:NE2	2.28	0.49
17:P:27:ARG:O	17:P:28:GLN:C	2.50	0.49
9:H:54:VAL:HG13	9:H:162:PRO:CG	2.42	0.49
1:O:1573:A:H2'	1:O:1574:C:O4'	2.13	0.49
5:D:37:ALA:O	5:D:40:ILE:HG12	2.12	0.49
11:J:39:VAL:HG13	11:J:40:ASN:ND2	2.28	0.49
1:O:2807:U:P	3:B:27:ASN:HD21	2.36	0.49
1:O:363:C:O2'	1:O:364:U:H5'	2.13	0.49
3:B:87:TYR:O	3:B:138:GLY:N	2.43	0.49
25:X:43:VAL:CG1	25:X:47:ALA:HB3	2.43	0.49
15:N:69:TYR:CD2	15:N:184:ILE:HD11	2.48	0.49
9:H:88:MET:HA	9:H:139:ALA:HA	1.95	0.49
7:F:1:PRO:H3	7:F:4:VAL:CG2	2.25	0.49
1:O:1634:G:H2'	1:O:1635:U:H6	1.78	0.49
1:O:30:U:OP2	4:C:181:ALA:HB2	2.11	0.49
1:O:892:G:H5''	28:1:54:ALA:HB2	1.93	0.49
21:T:61:GLU:HG3	40:T:3851:HOH:O	2.11	0.49
1:O:263:U:C2	7:F:59:ILE:CD1	2.96	0.49
1:O:295:C:H2'	1:O:296:G:O4'	2.12	0.49
1:O:1310:U:OP2	4:C:168:ARG:NH1	2.46	0.49
30:3:4:PRO:HG2	30:3:7:PHE:CD2	2.48	0.49
1:O:1187:U:H2'	40:0:6517:HOH:O	2.13	0.49
6:E:11:VAL:HG12	6:E:12:ASP:N	2.28	0.49
24:W:110:GLN:HA	24:W:110:GLN:HE21	1.76	0.49
1:O:946:C:H2'	1:O:947:U:H6	1.76	0.49
1:O:699:C:H6	1:O:744:G:O4'	1.96	0.49
12:K:125:ALA:C	12:K:127:ALA:H	2.16	0.49
1:O:2894:C:O2'	1:O:2895:C:H5'	2.12	0.49
4:C:28:SER:HB2	40:C:7195:HOH:O	2.13	0.49
13:L:10:SER:O	13:L:11:ARG:HB3	2.12	0.49
26:Y:156:GLY:O	26:Y:157:ILE:C	2.52	0.49
30:3:54:LYS:HE2	40:3:4294:HOH:O	2.12	0.49
20:S:43:GLU:HB3	40:S:7106:HOH:O	2.13	0.49
1:O:969:G:H1	1:O:999:C:N4	2.11	0.49
11:J:48:GLY:HA3	11:J:53:ILE:HD11	1.94	0.48
1:O:2909:G:H2'	1:O:2910:A:C8	2.47	0.48
1:O:1500:U:OP2	17:P:41:ARG:NH2	2.46	0.48
40:0:7267:HOH:O	2:A:211:LYS:HE3	2.13	0.48
24:W:27:HIS:C	24:W:28:HIS:CD2	2.86	0.48
24:W:11:VAL:O	24:W:12:ASN:HB2	2.13	0.48
1:O:1829:A:C8	1:O:1885:A:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2241:C:O2'	1:0:2242:U:H5'	2.13	0.48
17:P:94:TRP:CZ2	17:P:98:ILE:HG13	2.47	0.48
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.95	0.48
1:0:1299:G:N7	13:L:6:ARG:NH1	2.61	0.48
1:0:777:U:O2'	28:1:11:LYS:HG2	2.13	0.48
28:1:13:THR:HG22	28:1:14:THR:N	2.28	0.48
1:0:1363:G:H2'	1:0:1364:G:C8	2.48	0.48
1:0:2038:A:H5''	3:B:222:LYS:HG3	1.95	0.48
1:0:503:G:H2'	1:0:504:G:H8	1.77	0.48
30:3:24:LYS:HE2	30:3:65:THR:HG23	1.95	0.48
1:0:1166:A:P	1:0:1174:A:H4'	2.52	0.48
4:C:96:LYS:CB	4:C:98:ARG:HH12	2.22	0.48
31:9:39:U:H3'	31:9:40:C:H5''	1.95	0.48
1:0:947:U:H2'	1:0:948:G:H8	1.77	0.48
1:0:694:A:C2'	1:0:695:C:H5'	2.42	0.48
21:T:24:ARG:NH2	21:T:39:ASN:HD22	2.11	0.48
1:0:2028:U:H2'	1:0:2029:C:C6	2.48	0.48
1:0:2899:A:H4'	3:B:289:GLU:OE1	2.14	0.48
1:0:1426:C:H2'	40:0:4918:HOH:O	2.13	0.48
9:H:39:LYS:HD3	40:H:6292:HOH:O	2.12	0.48
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.12	0.48
6:E:101:GLU:HA	6:E:118:ILE:HG13	1.95	0.48
3:B:310:ARG:HD2	40:B:4128:HOH:O	2.13	0.48
1:0:243:A:H61	1:0:269:G:H1'	1.78	0.48
1:0:2032:U:H2'	1:0:2033:G:H5''	1.94	0.48
1:0:499:G:O2'	1:0:500:G:H5'	2.13	0.48
25:X:43:VAL:CG1	25:X:44:ASP:N	2.75	0.48
9:H:27:PRO:HD3	9:H:123:ILE:HG22	1.95	0.48
15:N:184:ILE:HG23	15:N:184:ILE:O	2.13	0.48
24:W:13:MET:CE	24:W:17:ILE:HG22	2.43	0.48
15:N:160:SER:CB	31:9:51:A:H5'	2.42	0.48
1:0:2897:C:H2'	1:0:2898:G:H8	1.77	0.48
14:M:57:LYS:NZ	14:M:144:ASP:HB2	2.28	0.48
1:0:2636:C:H4'	32:4:174:C:H4'	1.95	0.48
26:Y:131:GLN:O	26:Y:132:ASP:HB2	2.13	0.48
1:0:2478:U:O2'	1:0:2479:A:H5'	2.12	0.48
30:3:65:THR:HG21	30:3:88:LEU:CD2	2.44	0.48
1:0:2637:A:O5'	32:4:175:C:OP2	2.30	0.48
14:M:24:GLN:HE22	14:M:27:ARG:HH11	1.59	0.48
25:X:20:GLU:HG3	25:X:21:PRO:CD	2.42	0.48
1:0:2614:C:H5''	3:B:232:TRP:CZ3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:232:TRP:CD1	3:B:235:ARG:HD2	2.47	0.48
1:0:553:G:O4'	1:0:1325:G:H5'	2.12	0.48
7:F:13:GLU:OE1	7:F:77:VAL:HG13	2.13	0.48
1:0:1513:C:O2'	1:0:1514:C:H5'	2.12	0.48
1:0:1514:C:H2'	1:0:1515:A:H8	1.77	0.48
1:0:812:A:H2'	1:0:813:C:O4'	2.13	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.27	0.48
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.48
1:0:107:U:H2'	1:0:108:U:H5'	1.95	0.48
1:0:77:G:O2'	1:0:78:G:H5'	2.13	0.48
1:0:535:G:C5	1:0:2063:U:C4	3.01	0.48
1:0:1303:C:O2	1:0:1353:C:H1'	2.13	0.48
1:0:1353:C:H4'	40:0:5388:HOH:O	2.13	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.12	0.48
14:M:91:ILE:HB	40:M:7419:HOH:O	2.13	0.48
1:0:2321:A:H8	1:0:2322:U:O2'	1.96	0.48
3:B:307:ARG:HG3	3:B:307:ARG:HH11	1.78	0.48
29:2:35:ARG:HB3	40:2:2691:HOH:O	2.12	0.48
27:Z:101:LYS:HA	27:Z:104:ARG:HH11	1.78	0.48
13:L:108:VAL:HB	13:L:125:PHE:CD2	2.49	0.48
23:V:23:LEU:HD22	23:V:49:LEU:HD23	1.95	0.48
19:R:72:VAL:CG1	19:R:73:ASP:N	2.76	0.48
2:A:81:GLN:HB2	2:A:92:ASN:ND2	2.28	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.48
30:3:3:MET:CG	30:3:22:VAL:HG11	2.35	0.48
1:0:1180:U:O2'	10:I:87:PRO:HD2	2.14	0.48
3:B:36:PRO:CA	3:B:168:GLY:HA3	2.35	0.48
5:D:173:GLU:O	5:D:174:VAL:O	2.32	0.48
1:0:1016:U:H1'	40:0:8202:HOH:O	2.12	0.48
13:L:115:ARG:O	13:L:116:HIS:CG	2.67	0.48
1:0:314:G:N2	1:0:317:A:C8	2.82	0.48
17:P:27:ARG:HH21	17:P:30:ASP:CG	2.17	0.48
30:3:5:ARG:HG3	30:3:6:ARG:HG3	1.95	0.48
2:A:123:GLY:HA2	2:A:159:VAL:O	2.14	0.48
6:E:137:ASP:O	6:E:141:VAL:HG23	2.13	0.48
1:0:401:C:O2'	14:M:92:THR:HB	2.13	0.48
19:R:99:ALA:CB	19:R:109:MET:HE3	2.41	0.48
12:K:23:ASN:ND2	12:K:108:GLU:HB2	2.28	0.48
1:0:1938:G:O2'	1:0:1939:U:H5'	2.13	0.48
26:Y:106:THR:CG2	26:Y:107:PRO:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:6:TYR:HB3	31:9:11:A:N6	2.28	0.48
1:0:590:A:H2'	1:0:591:A:O4'	2.13	0.48
9:H:143:VAL:HG11	9:H:173:GLU:HG2	1.95	0.48
1:0:2549:C:H1'	40:B:342:HOH:O	2.13	0.48
1:0:1060:C:H5'	1:0:1060:C:H6	1.78	0.48
1:0:2725:G:N1	1:0:2756:U:OP2	2.37	0.48
1:0:2590:U:H1'	32:4:74:C:C2	2.49	0.48
3:B:160:ASP:CB	3:B:308:LEU:HD22	2.44	0.48
1:0:646:G:H5''	4:C:96:LYS:HD2	1.96	0.48
9:H:29:SER:HA	9:H:62:HIS:HD2	1.78	0.48
13:L:34:GLY:C	13:L:36:ASP:H	2.16	0.48
1:0:2634:G:OP2	2:A:204:GLY:N	2.47	0.48
1:0:1774:G:H2'	1:0:1775:A:O4'	2.13	0.48
1:0:228:C:C2'	1:0:229:G:H5'	2.43	0.48
26:Y:152:LYS:CB	26:Y:160:LYS:HG3	2.43	0.48
1:0:622:G:O2'	1:0:623:U:H5'	2.14	0.48
1:0:120:A:C6	28:1:17:THR:HG21	2.48	0.48
1:0:962:C:H2'	1:0:963:C:H5'	1.95	0.48
1:0:1548:U:O2'	1:0:1549:C:H5'	2.14	0.48
28:1:12:ASN:C	28:1:12:ASN:OD1	2.52	0.48
6:E:34:TRP:HB3	40:E:1053:HOH:O	2.13	0.48
15:N:36:ALA:N	40:N:3863:HOH:O	2.47	0.48
19:R:39:THR:HB	19:R:42:GLU:CD	2.35	0.48
19:R:39:THR:HG22	19:R:42:GLU:H	1.79	0.48
11:J:26:VAL:HG13	11:J:36:VAL:CG1	2.41	0.48
13:L:143:THR:O	13:L:147:GLU:HG3	2.13	0.48
3:B:268:ARG:HH21	3:B:322:ARG:HB2	1.78	0.48
1:0:661:G:C5	1:0:686:A:C2	3.02	0.48
6:E:26:ASN:HB3	6:E:76:VAL:O	2.13	0.48
3:B:147:VAL:HG12	3:B:150:ALA:H	1.79	0.48
1:0:843:A:C2	1:0:846:A:C8	3.01	0.48
15:N:72:GLU:HG2	15:N:72:GLU:O	2.13	0.48
1:0:123:U:O2'	1:0:124:C:H5'	2.14	0.48
1:0:1801:A:H3'	40:0:7513:HOH:O	2.14	0.48
1:0:800:G:H4'	40:0:6743:HOH:O	2.14	0.48
24:W:133:LYS:HG3	40:W:5904:HOH:O	2.13	0.48
1:0:2588:OMG:N2	32:4:76:5AA:C2	2.77	0.48
7:F:50:VAL:CG2	7:F:63:ILE:HG21	2.44	0.48
12:K:113:ILE:HG22	12:K:114:ALA:N	2.28	0.48
1:0:2114:C:OP1	2:A:1:GLY:HA2	2.13	0.48
6:E:81:GLU:HG3	6:E:133:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:GLY:O	2:A:36:ASP:HB2	2.14	0.48
1:0:1625:U:C6	1:0:1625:U:H3'	2.48	0.48
3:B:15:PRO:HG2	3:B:17:LYS:HG2	1.96	0.48
1:0:1617:C:C4	1:0:1643:C:H4'	2.49	0.48
1:0:1617:C:C5	1:0:1643:C:H4'	2.49	0.48
1:0:113:A:H3'	1:0:114:A:C5'	2.43	0.48
1:0:449:A:C8	4:C:43:LYS:HG2	2.48	0.48
9:H:91:ARG:NH1	9:H:138:THR:OG1	2.47	0.48
21:T:38:ARG:NH1	21:T:38:ARG:HG3	2.28	0.48
1:0:2483:A:H4'	1:0:2484:U:OP2	2.12	0.48
14:M:66:SER:HB2	14:M:128:TRP:CD1	2.49	0.48
19:R:31:ILE:O	19:R:32:ALA:C	2.52	0.48
2:A:121:ALA:O	2:A:124:VAL:HG22	2.14	0.48
15:N:171:HIS:CE1	40:N:6988:HOH:O	2.67	0.48
6:E:75:GLY:O	6:E:79:GLY:HA2	2.14	0.48
1:0:53:C:H2'	1:0:54:G:O4'	2.14	0.48
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.48
1:0:2590:U:O2	32:4:74:C:Cl'	2.61	0.47
30:3:10:TYR:CG	30:3:11:CYS:N	2.81	0.47
1:0:1684:A:O2'	1:0:1685:A:H5''	2.14	0.47
4:C:236:THR:H	4:C:239:ALA:HB3	1.78	0.47
21:T:48:VAL:HG22	21:T:96:VAL:HG22	1.96	0.47
21:T:49:GLU:OE2	21:T:97:ARG:NH1	2.46	0.47
11:J:107:ASN:C	11:J:107:ASN:ND2	2.64	0.47
1:0:2840:A:H3'	40:0:7562:HOH:O	2.13	0.47
2:A:207:GLN:O	2:A:208:HIS:HB3	2.14	0.47
1:0:926:A:O2'	13:L:41:HIS:CD2	2.62	0.47
1:0:517:U:C2'	1:0:518:G:H5'	2.44	0.47
17:P:69:ARG:HA	17:P:73:HIS:O	2.13	0.47
1:0:2499:U:H2'	1:0:2500:C:H6	1.79	0.47
1:0:35:U:H5'	4:C:47:GLY:O	2.14	0.47
21:T:38:ARG:NH1	40:T:6217:HOH:O	2.45	0.47
1:0:1739:G:O2'	1:0:1740:U:H5'	2.13	0.47
1:0:2271:G:P	2:A:223:ARG:HH12	2.37	0.47
2:A:231:LYS:O	2:A:232:ARG:HB3	2.14	0.47
1:0:862:U:H2'	1:0:863:G:H8	1.79	0.47
1:0:958:G:O2'	1:0:959:C:H5'	2.14	0.47
4:C:219:ASN:O	4:C:222:ASP:HB2	2.14	0.47
1:0:2088:C:H1'	1:0:2841:A:C2	2.49	0.47
1:0:1366:C:H1'	40:0:3715:HOH:O	2.14	0.47
27:Z:70:ARG:HB3	27:Z:70:ARG:HH11	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5'	1.96	0.47
7:F:50:VAL:HG21	7:F:63:ILE:HG21	1.95	0.47
13:L:90:ARG:CA	13:L:119:THR:HB	2.42	0.47
25:X:52:PRO:O	25:X:55:ASN:N	2.48	0.47
9:H:41:LYS:HD3	9:H:46:TYR:CZ	2.48	0.47
1:0:2704:C:H1'	6:E:110:GLU:OE1	2.14	0.47
20:S:20:PHE:HD2	20:S:20:PHE:N	2.11	0.47
4:C:73:GLN:HE21	4:C:73:GLN:HA	1.79	0.47
1:0:88:G:C8	29:2:28:LYS:HB2	2.49	0.47
24:W:39:ASP:OD1	24:W:42:ARG:NH1	2.46	0.47
1:0:1149:U:C5	1:0:1215:A:C5	3.02	0.47
1:0:17:G:H2'	1:0:18:C:C6	2.49	0.47
40:M:674:HOH:O	30:3:46:ILE:HB	2.14	0.47
1:0:1116:U:HO2'	1:0:1118:A:H2	0.74	0.47
31:9:75:G:H2'	31:9:76:G:O4'	2.14	0.47
24:W:147:ASP:O	24:W:151:GLU:HB2	2.15	0.47
1:0:1701:A:H5'	1:0:1702:U:H3'	1.95	0.47
7:F:101:ALA:HA	40:F:5413:HOH:O	2.14	0.47
1:0:1497:G:H2'	1:0:1498:G:H8	1.78	0.47
2:A:199:HIS:CD2	2:A:201:PHE:HB2	2.49	0.47
1:0:319:A:H2'	1:0:320:G:C8	2.49	0.47
22:U:39:ASN:ND2	22:U:49:LEU:CD1	2.77	0.47
10:I:108:HIS:N	10:I:109:PRO:HD2	2.29	0.47
19:R:33:ARG:HH11	19:R:33:ARG:CB	2.27	0.47
1:0:1358:A:N7	1:0:1360:C:C2	2.82	0.47
22:U:8:TYR:CE1	22:U:40:ALA:HB2	2.48	0.47
5:D:55:LYS:O	5:D:56:ARG:HB2	2.14	0.47
1:0:2637:A:O5'	32:4:175:C:P	2.72	0.47
31:9:20:G:O2'	31:9:21:G:H5'	2.14	0.47
3:B:202:VAL:HG11	3:B:301:VAL:HG13	1.96	0.47
3:B:162:MET:HG3	3:B:310:ARG:HH11	1.79	0.47
5:D:170:TYR:CD1	5:D:170:TYR:N	2.83	0.47
2:A:100:PRO:O	2:A:103:VAL:HG23	2.14	0.47
25:X:76:ARG:O	25:X:77:PHE:HB3	2.14	0.47
1:0:820:G:C6	2:A:171:LYS:HB2	2.48	0.47
31:9:107:C:H2'	31:9:108:C:H6	1.79	0.47
1:0:702:G:O2'	1:0:703:G:H5'	2.15	0.47
1:0:228:C:H2'	1:0:229:G:C5'	2.44	0.47
9:H:87:LYS:HG2	9:H:140:TYR:HB2	1.97	0.47
1:0:709:G:O3'	16:O:25:VAL:HG13	2.15	0.47
1:0:579:G:H2'	1:0:580:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:16:ASN:C	29:2:18:ASN:H	2.18	0.47
29:2:16:ASN:C	29:2:18:ASN:N	2.67	0.47
1:0:2887:G:H2'	1:0:2888:U:C6	2.49	0.47
1:0:2604:A:H5'	40:0:4959:HOH:O	2.13	0.47
4:C:214:THR:HG23	40:C:5535:HOH:O	2.15	0.47
24:W:117:ARG:HB3	24:W:117:ARG:HH11	1.79	0.47
19:R:26:LYS:HD3	19:R:62:HIS:CG	2.49	0.47
23:V:12:THR:CG2	23:V:15:GLU:HG3	2.36	0.47
11:J:77:GLY:O	11:J:78:ILE:C	2.53	0.47
30:3:25:VAL:HG13	30:3:68:LYS:CE	2.41	0.47
3:B:217:ARG:HG3	3:B:257:THR:CG2	2.44	0.47
2:A:164:ARG:HB2	40:Z:292:HOH:O	2.13	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.14	0.47
40:0:3944:HOH:O	27:Z:40:ALA:HB3	2.14	0.47
1:0:1632:A:C2'	1:0:1633:C:H5'	2.43	0.47
1:0:944:G:H21	24:W:44:MET:CE	2.27	0.47
9:H:123:ILE:HD12	9:H:123:ILE:N	2.30	0.47
1:0:194:A:H2'	1:0:195:C:O4'	2.15	0.47
10:I:116:LEU:O	10:I:119:ALA:HB3	2.13	0.47
1:0:111:C:O2'	28:1:20:ARG:HG2	2.14	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
7:F:4:VAL:HA	7:F:76:PHE:CZ	2.49	0.47
1:0:1333:U:H2'	1:0:1334:C:C6	2.48	0.47
1:0:29:C:H5'	1:0:1342:C:OP1	2.13	0.47
21:T:32:ARG:NH1	21:T:38:ARG:HH12	2.12	0.47
1:0:1149:U:H5''	1:0:1151:G:O4'	2.14	0.47
1:0:1219:U:H2'	1:0:1220:U:C6	2.50	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.47
14:M:74:LYS:HE2	40:M:444:HOH:O	2.14	0.47
1:0:1163:G:H2'	1:0:1164:U:H5	1.79	0.47
1:0:1174:A:C6	1:0:1201:C:H4'	2.50	0.47
1:0:100:C:C4'	21:T:16:LEU:HB2	2.44	0.47
8:G:71:LEU:C	8:G:73:ASP:H	2.18	0.47
1:0:721:A:H5''	16:O:51:TYR:CE1	2.50	0.47
2:A:33:GLU:OE1	2:A:33:GLU:N	2.42	0.47
28:1:28:HIS:ND1	28:1:31:LYS:HG3	2.30	0.47
5:D:15:GLU:HA	5:D:16:PRO:HD3	1.75	0.47
40:0:8330:HOH:O	14:M:189:SER:HB2	2.13	0.47
1:0:1574:C:H2'	1:0:1575:C:H6	1.78	0.47
7:F:8:VAL:HG13	7:F:12:LEU:HD13	1.96	0.47
19:R:13:THR:HA	19:R:147:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:8:ALA:CB	19:R:13:THR:HG21	2.21	0.47
1:0:2321:A:C2	1:0:2378:U:N3	2.76	0.47
40:0:4371:HOH:O	17:P:117:SER:HB2	2.13	0.47
1:0:734:U:O2'	1:0:736:A:N7	2.40	0.47
3:B:275:GLY:C	3:B:291:ASP:HA	2.35	0.47
1:0:561:G:O2'	1:0:562:A:H5'	2.15	0.47
15:N:11:ARG:O	15:N:13:ARG:N	2.47	0.47
24:W:88:THR:C	24:W:90:TYR:N	2.66	0.47
10:I:96:SER:O	10:I:99:GLN:HB2	2.15	0.47
14:M:52:GLN:NE2	14:M:118:TYR:HB3	2.30	0.47
3:B:80:ARG:HA	3:B:186:GLY:O	2.15	0.47
30:3:70:ARG:HA	30:3:77:ALA:HB2	1.97	0.47
1:0:110:C:H2'	1:0:111:C:C6	2.48	0.47
1:0:422:G:O2'	1:0:423:A:H5'	2.15	0.47
1:0:1634:G:H3'	40:0:8442:HOH:O	2.15	0.47
19:R:33:ARG:HH11	19:R:33:ARG:HB2	1.80	0.47
1:0:1800:G:H1'	17:P:88:GLN:NE2	2.30	0.47
1:0:17:G:H2'	1:0:18:C:H6	1.78	0.47
5:D:151:ILE:CG2	5:D:155:HIS:HB3	2.45	0.47
2:A:69:LEU:HD23	2:A:107:ASN:HB2	1.96	0.47
16:O:69:VAL:HG12	16:O:70:LEU:N	2.29	0.47
2:A:134:ASN:O	2:A:150:PRO:CD	2.63	0.47
18:Q:34:ASP:O	18:Q:37:GLU:HG3	2.15	0.47
1:0:2065:C:O2'	1:0:2066:C:H5'	2.15	0.47
1:0:477:A:C6	1:0:478:C:C4	3.02	0.47
1:0:2639:G:O2'	1:0:2640:U:H5'	2.14	0.47
3:B:91:PRO:HA	11:J:144:THR:OG1	2.14	0.47
3:B:29:TRP:CH2	3:B:164:THR:HA	2.50	0.47
1:0:2590:U:C2	32:4:74:C:N1	2.83	0.47
27:Z:81:CYS:O	27:Z:85:ASP:HA	2.14	0.47
1:0:2504:A:H4'	9:H:74:ARG:HH11	1.80	0.47
10:I:118:ASN:HA	10:I:121:LYS:CD	2.44	0.47
3:B:26:PHE:HD2	3:B:312:ARG:HH21	1.63	0.47
9:H:30:LYS:H	9:H:62:HIS:CD2	2.33	0.47
12:K:115:ARG:HG3	12:K:116:GLU:N	2.29	0.47
1:0:10:U:C3'	1:0:10:U:C6	2.97	0.47
1:0:1296:A:O2'	1:0:1297:U:H5'	2.15	0.47
20:S:6:LYS:HE3	20:S:29:ASP:HA	1.97	0.47
24:W:107:LEU:O	24:W:112:LEU:HB2	2.15	0.47
9:H:73:ASN:HB2	9:H:88:MET:HE1	1.95	0.47
1:0:812:A:H1'	40:0:8538:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:75:ARG:NH2	14:M:78:LYS:NZ	2.62	0.47
29:2:20:ARG:HG3	29:2:20:ARG:HH11	1.79	0.47
1:0:1850:U:O4'	1:0:1941:A:C2	2.68	0.47
3:B:125:GLU:O	3:B:129:ARG:HG3	2.14	0.47
1:0:125:U:H2'	40:0:8310:HOH:O	2.15	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
11:J:77:GLY:O	11:J:80:LYS:N	2.48	0.47
3:B:195:ARG:O	3:B:196:ALA:C	2.52	0.47
3:B:198:GLU:HA	40:B:7384:HOH:O	2.13	0.47
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.47
3:B:27:ASN:N	3:B:27:ASN:HD22	2.06	0.47
24:W:90:TYR:CE2	24:W:99:ALA:HB2	2.50	0.47
1:0:1972:U:C2'	1:0:1973:A:H5''	2.45	0.47
1:0:307:G:H3'	1:0:342:C:OP2	2.14	0.47
1:0:2735:U:H2'	1:0:2736:U:H6	1.79	0.47
24:W:27:HIS:O	24:W:28:HIS:HD2	1.98	0.47
1:0:2831:C:C2'	1:0:2832:C:H5'	2.45	0.47
1:0:697:G:H4'	1:0:730:G:O3'	2.15	0.47
3:B:109:LEU:HD11	3:B:113:LEU:HD12	1.97	0.47
26:Y:144:ARG:CZ	40:Y:7277:HOH:O	2.62	0.47
7:F:32:GLY:N	40:F:3111:HOH:O	2.47	0.47
1:0:1115:U:O2'	1:0:1116:U:H5'	2.15	0.47
17:P:115:SER:N	17:P:118:GLN:NE2	2.53	0.47
10:I:73:LEU:HD12	10:I:107:LYS:HZ1	1.78	0.47
12:K:14:LYS:HG3	12:K:32:ILE:O	2.14	0.47
1:0:1603:A:H5''	1:0:1604:G:H3'	1.97	0.47
1:0:1972:U:H2'	1:0:1973:A:H5''	1.97	0.47
15:N:23:ARG:NH2	15:N:55:ASP:OD2	2.48	0.47
13:L:143:THR:CG2	13:L:144:ASP:N	2.77	0.47
21:T:40:VAL:HG23	21:T:119:ALA:C	2.35	0.47
1:0:500:G:H21	19:R:98:ASN:ND2	2.12	0.47
5:D:76:ARG:O	5:D:77:ASP:HB2	2.15	0.47
1:0:1006:A:N1	1:0:2311:A:H1'	2.30	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.33	0.47
1:0:522:U:O2'	1:0:1366:C:H5'	2.15	0.47
23:V:33:VAL:HG12	23:V:33:VAL:O	2.15	0.47
21:T:18:GLU:O	21:T:21:LYS:HG2	2.15	0.47
16:O:43:VAL:HG11	16:O:115:ARG:HA	1.97	0.47
1:0:1706:G:H1'	1:0:1712:A:H61	1.80	0.47
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.47
1:0:716:G:H1'	40:0:4890:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2289:G:O2'	1:0:2290:U:H5'	2.15	0.47
1:0:2542:C:C1'	40:4:6378:HOH:O	2.62	0.46
30:3:10:TYR:HB2	30:3:17:HIS:CE1	2.50	0.46
25:X:72:VAL:HG23	25:X:86:GLU:O	2.15	0.46
7:F:29:VAL:CA	7:F:99:THR:HG22	2.45	0.46
3:B:195:ARG:O	3:B:198:GLU:HG3	2.14	0.46
31:9:117:G:H2'	31:9:118:C:C6	2.49	0.46
1:0:1972:U:C2'	1:0:1973:A:C5'	2.93	0.46
2:A:186:TRP:CD1	2:A:187:PRO:HA	2.50	0.46
1:0:86:A:C2	29:2:25:VAL:HG13	2.50	0.46
2:A:32:VAL:HG22	2:A:38:ILE:HG13	1.97	0.46
17:P:16:VAL:HG13	17:P:20:ARG:CZ	2.45	0.46
40:0:6342:HOH:O	15:N:4:PRO:HD2	2.15	0.46
1:0:453:A:H3'	40:0:4941:HOH:O	2.14	0.46
1:0:1564:C:H1'	1:0:2738:G:C2	2.51	0.46
4:C:72:LYS:HG2	4:C:77:ALA:HA	1.97	0.46
23:V:12:THR:HG23	23:V:14:ALA:H	1.80	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.46
14:M:83:SER:C	14:M:85:ARG:H	2.17	0.46
11:J:36:VAL:HG12	11:J:37:ALA:N	2.29	0.46
1:0:1883:U:H5''	1:0:2013:G:OP2	2.15	0.46
3:B:84:LEU:CD2	3:B:178:ALA:HB1	2.45	0.46
30:3:34:LYS:HB2	30:3:34:LYS:HZ3	1.78	0.46
1:0:195:C:H5''	40:M:4431:HOH:O	2.13	0.46
1:0:2346:C:H5'	5:D:54:ALA:HB2	1.96	0.46
14:M:60:VAL:C	14:M:61:ILE:HD12	2.36	0.46
9:H:44:ASP:HA	9:H:170:ARG:HH12	1.79	0.46
1:0:709:G:O2'	16:O:25:VAL:CG1	2.63	0.46
1:0:185:G:O3'	1:0:186:A:H4'	2.15	0.46
3:B:204:GLY:O	3:B:261:GLN:HA	2.15	0.46
1:0:770:C:OP1	14:M:79:ALA:HB1	2.14	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.46
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.46
1:0:220:C:H2'	13:L:48:LYS:HE3	1.97	0.46
1:0:558:C:C2'	1:0:559:U:C5'	2.87	0.46
3:B:194:PHE:HA	3:B:198:GLU:OE1	2.15	0.46
8:G:23:ILE:HG22	8:G:27:ILE:CD1	2.46	0.46
5:D:105:SER:CB	5:D:131:THR:HG23	2.45	0.46
1:0:901:G:OP2	13:L:18:HIS:HE1	1.98	0.46
1:0:2694:A:C6	1:0:2702:A:C8	3.04	0.46
3:B:41:PHE:HB3	3:B:190:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
3:B:16:ARG:NH2	40:B:2268:HOH:O	2.43	0.46
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.45	0.46
21:T:24:ARG:HH21	21:T:39:ASN:ND2	2.13	0.46
3:B:71:VAL:HG11	3:B:296:LEU:HB3	1.97	0.46
1:0:2244:A:H1'	40:M:2788:HOH:O	2.14	0.46
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.50	0.46
15:N:63:SER:O	15:N:66:LEU:HB3	2.15	0.46
7:F:110:ASP:O	7:F:114:LYS:N	2.35	0.46
30:3:83:TRP:HZ2	30:3:88:LEU:HD21	1.81	0.46
1:0:2910:A:H5''	40:0:8739:HOH:O	2.15	0.46
30:3:25:VAL:CG2	30:3:68:LYS:HG3	2.43	0.46
22:U:31:PHE:CD2	22:U:37:GLU:HA	2.49	0.46
1:0:1626:A:H2'	1:0:1627:G:C5'	2.45	0.46
12:K:41:LYS:O	12:K:42:ASN:HB2	2.16	0.46
17:P:83:LYS:HG3	17:P:84:ALA:N	2.31	0.46
1:0:2438:G:H2'	1:0:2439:C:C6	2.51	0.46
4:C:142:ASP:OD1	4:C:237:GLU:HB3	2.15	0.46
1:0:1473:U:C1'	28:1:42:SER:HB3	2.46	0.46
6:E:18:LEU:HD13	6:E:34:TRP:CG	2.50	0.46
1:0:1365:C:H4'	40:0:3354:HOH:O	2.16	0.46
14:M:89:THR:O	14:M:89:THR:HG22	2.15	0.46
19:R:113:HIS:O	19:R:145:LEU:HA	2.16	0.46
6:E:132:THR:HB	40:E:2227:HOH:O	2.15	0.46
24:W:130:HIS:NE2	31:9:88:G:OP1	2.46	0.46
3:B:36:PRO:CD	3:B:169:GLY:H	2.29	0.46
11:J:84:ARG:HB2	11:J:98:PHE:CE1	2.51	0.46
1:0:960:G:N3	1:0:960:G:H3'	2.31	0.46
1:0:604:G:H4'	1:0:605:C:O5'	2.15	0.46
15:N:144:GLY:O	15:N:147:ILE:CG2	2.63	0.46
4:C:16:VAL:HG12	4:C:17:ASP:N	2.31	0.46
1:0:79:G:H4'	21:T:20:HIS:CE1	2.50	0.46
1:0:1574:C:H6	1:0:1574:C:O5'	1.98	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.46
4:C:73:GLN:HA	4:C:73:GLN:NE2	2.31	0.46
1:0:647:U:H2'	1:0:648:G:C8	2.50	0.46
1:0:2045:G:H5''	40:0:6966:HOH:O	2.15	0.46
14:M:172:GLY:HA2	40:M:199:HOH:O	2.15	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.46
1:0:1163:G:H5'	10:I:110:ASP:O	2.15	0.46
21:T:48:VAL:CG2	21:T:49:GLU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:167:GLY:O	14:M:171:ARG:HG3	2.16	0.46
1:0:1702:U:H5'	40:0:7857:HOH:O	2.16	0.46
1:0:1377:C:O2'	1:0:1378:G:H5''	2.16	0.46
1:0:1762:C:H2'	1:0:1763:C:C6	2.44	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
3:B:56:ASP:HB2	3:B:322:ARG:NE	2.30	0.46
2:A:179:MET:HG2	2:A:186:TRP:HB2	1.98	0.46
1:0:86:A:H3'	1:0:86:A:OP2	2.16	0.46
1:0:2135:A:O4'	1:0:2243:C:N4	2.49	0.46
1:0:453:A:H4'	1:0:455:A:C8	2.51	0.46
40:0:3360:HOH:O	16:O:39:THR:HB	2.15	0.46
1:0:941:G:C5	1:0:942:U:C4	3.03	0.46
2:A:14:SER:O	2:A:15:THR:C	2.54	0.46
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.46
1:0:2590:U:C2	32:4:74:C:C6	3.03	0.46
1:0:402:U:H2'	1:0:403:C:C6	2.51	0.46
22:U:56:ARG:HG3	22:U:56:ARG:NH1	2.29	0.46
1:0:1181:A:H2'	1:0:1182:C:C5'	2.45	0.46
1:0:711:G:O2'	1:0:712:C:H5'	2.16	0.46
1:0:2720:C:O2	12:K:87:ARG:NH2	2.48	0.46
19:R:39:THR:O	19:R:40:ALA:C	2.53	0.46
1:0:2011:A:H5'	1:0:2013:G:H1'	1.97	0.46
1:0:1496:A:H5'	1:0:1572:A:H1'	1.97	0.46
3:B:268:ARG:NH2	3:B:322:ARG:HB2	2.31	0.46
1:0:553:G:H5'	40:0:7958:HOH:O	2.15	0.46
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.46
1:0:86:A:O4'	29:2:29:THR:HG22	2.16	0.46
1:0:2438:G:H2'	1:0:2439:C:H6	1.81	0.46
14:M:28:GLN:O	14:M:32:ARG:HG3	2.15	0.46
1:0:212:A:O4'	1:0:214:U:C6	2.69	0.46
4:C:107:ARG:O	4:C:111:VAL:HG23	2.16	0.46
23:V:25:THR:CG2	23:V:29:ASN:ND2	2.79	0.46
4:C:235:PHE:N	4:C:235:PHE:CD1	2.84	0.46
1:0:1393:A:C2	1:0:1726:G:H4'	2.51	0.46
9:H:53:ILE:HG23	9:H:134:GLU:O	2.16	0.46
1:0:772:G:H2'	1:0:773:A:O4'	2.16	0.46
9:H:18:THR:HG22	9:H:95:HIS:O	2.15	0.46
9:H:31:ILE:HG23	40:H:6314:HOH:O	2.15	0.46
1:0:401:C:H2'	1:0:402:U:O4'	2.16	0.46
5:D:159:PRO:O	5:D:162:ALA:HB3	2.15	0.46
1:0:698:A:C5'	13:L:110:GLY:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:32:ALA:HA	20:S:36:GLU:OE1	2.16	0.46
4:C:27:ARG:NH1	4:C:29:ASP:OD1	2.47	0.46
13:L:73:VAL:HG21	13:L:116:HIS:CD2	2.50	0.46
12:K:125:ALA:O	12:K:127:ALA:N	2.40	0.46
1:O:1925:G:O2'	1:O:1926:G:H5'	2.15	0.46
9:H:154:ARG:HA	9:H:157:TYR:CE2	2.51	0.46
3:B:233:ARG:NH1	3:B:233:ARG:HG2	2.31	0.46
1:O:1495:C:H1'	1:O:1573:A:H1'	1.97	0.46
1:O:1850:U:H2'	1:O:1851:G:H8	1.80	0.46
15:N:64:SER:C	15:N:66:LEU:H	2.19	0.46
1:O:1098:A:H2'	1:O:1099:G:O4'	2.16	0.46
11:J:29:GLN:O	11:J:32:ASP:N	2.49	0.46
40:O:3432:HOH:O	3:B:300:SER:HB3	2.15	0.46
1:O:669:G:O2'	1:O:670:G:H5'	2.15	0.46
4:C:84:VAL:HG12	4:C:85:LYS:HG2	1.97	0.46
1:O:1154:A:H2'	1:O:1155:G:C8	2.50	0.46
14:M:5:TYR:O	14:M:7:TYR:N	2.49	0.46
14:M:102:GLU:OE2	14:M:164:THR:HG21	2.16	0.46
1:O:542:A:H2'	1:O:543:G:O4'	2.16	0.46
14:M:97:ILE:CD1	14:M:127:LYS:HD2	2.40	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.41	0.46
1:O:710:G:O2'	1:O:711:G:H5'	2.16	0.46
1:O:1209:C:H2'	1:O:1210:G:C8	2.47	0.46
1:O:272:A:N1	1:O:369:G:H5''	2.31	0.46
1:O:137:U:OP1	1:O:259:G:O2'	2.34	0.46
14:M:139:PRO:HA	14:M:142:GLN:HB2	1.98	0.46
28:1:34:CYS:HB3	28:1:39:PHE:H	1.81	0.46
1:O:705:C:C2'	1:O:705:C:O2	2.64	0.46
10:I:102:GLN:C	10:I:104:ALA:H	2.19	0.46
1:O:2416:G:O2'	15:N:25:ARG:HG2	2.15	0.46
1:O:1332:C:O2'	1:O:1333:U:H5'	2.16	0.46
1:O:1550:A:H2'	1:O:1551:C:O4'	2.15	0.46
14:M:180:SER:N	14:M:181:GLU:OE1	2.49	0.46
7:F:83:LEU:HD11	7:F:96:ALA:HB3	1.96	0.46
16:O:18:ALA:HB2	16:O:27:GLY:N	2.31	0.46
1:O:1545:C:H2'	1:O:1546:G:O4'	2.16	0.46
20:S:50:GLU:HB3	20:S:67:ARG:HH21	1.81	0.46
9:H:98:LEU:HD11	9:H:127:ALA:HB2	1.96	0.46
1:O:1652:C:H4'	27:Z:76:THR:HG21	1.98	0.46
1:O:2624:A:H1'	40:O:5545:HOH:O	2.15	0.46
15:N:157:PRO:HA	40:N:2957:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1330:A:H5''	1:0:1331:G:OP2	2.16	0.46
1:0:2551:C:O2'	1:0:2552:C:H5'	2.16	0.46
1:0:700:A:H5''	1:0:701:U:O5'	2.16	0.46
1:0:1909:A:H1'	1:0:2267:G:H5'	1.97	0.46
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.46	0.46
1:0:2072:G:C6	1:0:2533:C:H1'	2.50	0.46
1:0:1351:G:H3'	40:0:4676:HOH:O	2.16	0.46
15:N:86:LEU:HD12	15:N:125:ALA:CB	2.45	0.46
13:L:66:VAL:HG13	13:L:110:GLY:HA2	1.98	0.46
1:0:136:C:H4'	14:M:138:HIS:CD2	2.51	0.46
1:0:1497:G:H2'	1:0:1498:G:C8	2.51	0.46
9:H:56:GLU:C	9:H:132:ALA:HB2	2.37	0.46
3:B:13:PHE:N	3:B:13:PHE:CD1	2.83	0.46
28:1:28:HIS:O	28:1:32:LYS:N	2.47	0.46
24:W:125:HIS:HE1	40:W:3071:HOH:O	1.99	0.46
15:N:34:LEU:HD13	15:N:47:LEU:HD22	1.98	0.46
1:0:1296:A:H3'	40:0:6001:HOH:O	2.16	0.46
1:0:2461:U:O2	1:0:2466:G:H1'	2.16	0.46
1:0:1992:U:H2'	1:0:1994:A:OP2	2.16	0.46
1:0:923:A:H2'	40:0:4815:HOH:O	2.16	0.46
40:0:6414:HOH:O	4:C:175:LYS:HE3	2.16	0.46
27:Z:52:GLU:O	27:Z:55:SER:HB3	2.16	0.46
1:0:675:U:H2'	1:0:676:C:H5'	1.98	0.46
1:0:955:A:H2'	1:0:956:G:O4'	2.15	0.46
12:K:63:GLU:HB2	40:K:6344:HOH:O	2.16	0.46
1:0:1987:C:O2'	1:0:1988:C:H5'	2.16	0.46
31:9:63:C:O2'	31:9:64:C:H5'	2.16	0.46
1:0:2749:U:H5'	40:0:7896:HOH:O	2.15	0.46
1:0:2514:U:OP1	1:0:2572:G:H1'	2.16	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.97	0.45
3:B:217:ARG:HD3	3:B:218:TRP:NE1	2.31	0.45
13:L:91:VAL:CG1	13:L:120:LEU:HD23	2.46	0.45
6:E:14:GLU:CG	6:E:15:GLN:H	2.29	0.45
20:S:6:LYS:HZ3	20:S:61:GLU:HG2	1.80	0.45
1:0:875:A:C2	2:A:194:MET:SD	3.10	0.45
15:N:144:GLY:O	15:N:147:ILE:HG22	2.16	0.45
1:0:2089:A:C2'	1:0:2090:G:H5'	2.46	0.45
1:0:263:U:C4	7:F:54:VAL:HG13	2.50	0.45
1:0:2002:C:H2'	1:0:2003:U:C5'	2.46	0.45
7:F:48:VAL:CG2	7:F:74:PHE:HB3	2.45	0.45
19:R:114:VAL:HG13	19:R:114:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2793:A:H2'	1:0:2794:G:H5'	1.97	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.50	0.45
30:3:60:LYS:C	30:3:62:THR:H	2.19	0.45
29:2:40:ARG:HG3	29:2:45:ASN:CB	2.45	0.45
1:0:2382:A:H1'	30:3:10:TYR:CE2	2.51	0.45
1:0:1181:A:N1	1:0:1192:A:O2'	2.48	0.45
15:N:143:ARG:HB3	15:N:143:ARG:HE	1.49	0.45
1:0:273:G:H2'	1:0:274:G:C8	2.51	0.45
1:0:1891:G:H1'	1:0:1972:U:C2	2.52	0.45
15:N:48:VAL:HG13	15:N:56:ASP:O	2.16	0.45
4:C:246:ARG:NE	40:C:5065:HOH:O	2.50	0.45
1:0:944:G:H21	24:W:44:MET:HE2	1.82	0.45
1:0:319:A:H4'	1:0:338:C:C5	2.51	0.45
18:Q:86:VAL:HG13	18:Q:91:LEU:HD11	1.98	0.45
1:0:2878:U:H2'	1:0:2879:A:O4'	2.16	0.45
21:T:79:LEU:HG	21:T:89:ARG:HB2	1.98	0.45
14:M:152:ALA:O	14:M:155:GLN:N	2.46	0.45
4:C:161:ASP:HA	40:C:2972:HOH:O	2.16	0.45
1:0:2408:A:HO2'	30:3:10:TYR:HD1	1.59	0.45
1:0:1182:C:H1'	1:0:1192:A:H8	1.81	0.45
12:K:12:LEU:HB2	12:K:47:ALA:O	2.16	0.45
1:0:1306:U:OP1	4:C:184:ARG:NH1	2.48	0.45
1:0:2779:G:N7	1:0:2790:C:C2	2.84	0.45
2:A:199:HIS:HD2	2:A:201:PHE:HB2	1.80	0.45
2:A:135:VAL:CG2	2:A:147:ARG:HB3	2.45	0.45
3:B:175:LEU:O	3:B:175:LEU:HD23	2.17	0.45
3:B:87:TYR:HD1	40:B:3693:HOH:O	1.99	0.45
1:0:653:U:H3	1:0:752:G:H1	1.64	0.45
15:N:183:ASP:O	15:N:184:ILE:C	2.54	0.45
1:0:729:C:C2	1:0:743:G:C2	3.04	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.45
1:0:1805:G:H2'	1:0:1806:G:C8	2.50	0.45
17:P:111:GLU:HG2	17:P:111:GLU:O	2.15	0.45
2:A:26:ASP:O	2:A:28:GLU:HG3	2.15	0.45
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.45
31:9:55:U:H4'	31:9:56:A:C8	2.52	0.45
1:0:1163:G:H1	1:0:1184:C:N4	2.14	0.45
1:0:368:C:H2'	1:0:369:G:H5'	1.99	0.45
27:Z:43:GLY:O	27:Z:47:ARG:NE	2.49	0.45
1:0:2807:U:OP2	3:B:28:SER:HB2	2.17	0.45
15:N:49:THR:HG22	15:N:56:ASP:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:524:A:H5''	19:R:29:LYS:HE2	1.97	0.45
2:A:76:VAL:CG2	27:Z:87:LYS:HB3	2.46	0.45
5:D:23:VAL:HG22	5:D:73:VAL:HB	1.98	0.45
24:W:142:ASP:O	24:W:143:THR:C	2.54	0.45
1:0:2842:G:H5'	19:R:68:HIS:O	2.16	0.45
6:E:94:GLN:HG3	40:E:4917:HOH:O	2.17	0.45
31:9:98:C:H2'	31:9:99:U:H6	1.81	0.45
26:Y:108:ASP:OD1	26:Y:108:ASP:N	2.47	0.45
4:C:7:ASP:C	4:C:9:ASP:H	2.20	0.45
1:0:1813:U:O2'	17:P:81:LYS:HE3	2.16	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.52	0.45
1:0:219:G:O5'	1:0:220:C:H5''	2.16	0.45
31:9:56:A:C3'	31:9:57:A:H5''	2.46	0.45
1:0:2637:A:C6	32:4:176:DA:H2'	2.48	0.45
1:0:2379:G:N3	1:0:2418:G:H2'	2.31	0.45
1:0:2502:C:H4'	9:H:158:ASN:ND2	2.31	0.45
1:0:2503:A:C5'	9:H:155:ARG:HH12	2.13	0.45
12:K:34:VAL:O	12:K:35:HIS:C	2.55	0.45
1:0:614:U:H2'	1:0:615:G:C8	2.51	0.45
1:0:558:C:HO2'	1:0:559:U:H5''	1.80	0.45
20:S:15:MET:O	20:S:18:MET:HB3	2.16	0.45
1:0:1477:C:H4'	1:0:1868:G:OP1	2.16	0.45
14:M:120:VAL:HG11	14:M:130:GLU:HG3	1.98	0.45
1:0:317:A:OP1	21:T:52:ARG:O	2.34	0.45
5:D:23:VAL:O	5:D:72:LYS:HA	2.16	0.45
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.97	0.45
2:A:45:ILE:HD12	27:Z:89:THR:CG2	2.46	0.45
9:H:49:GLN:NE2	9:H:170:ARG:HE	2.15	0.45
2:A:173:GLY:O	2:A:176:HIS:HB3	2.15	0.45
9:H:91:ARG:H	9:H:91:ARG:HG2	1.44	0.45
4:C:138:VAL:O	4:C:234:VAL:HA	2.16	0.45
1:0:633:C:O2'	1:0:634:G:H5'	2.15	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.17	0.45
1:0:2248:C:H2'	1:0:2249:G:H8	1.82	0.45
1:0:2706:A:H2'	1:0:2707:C:O4'	2.17	0.45
26:Y:178:HIS:CG	26:Y:179:PRO:HD2	2.52	0.45
40:M:533:HOH:O	30:3:46:ILE:HD12	2.17	0.45
14:M:74:LYS:O	14:M:88:VAL:HG12	2.16	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.45
1:0:2507:G:H22	1:0:2512:U:H5''	1.80	0.45
24:W:139:GLY:O	24:W:141:HIS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:380:A:H2'	40:0:6974:HOH:O	2.15	0.45
2:A:1:GLY:HA2	2:A:197:VAL:HG23	1.98	0.45
15:N:154:LEU:O	15:N:155:GLU:CB	2.65	0.45
1:0:2828:G:H8	1:0:2828:G:O5'	2.00	0.45
9:H:48:VAL:HB	9:H:141:CYS:O	2.16	0.45
14:M:186:SER:HB3	14:M:189:SER:CB	2.47	0.45
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.45
24:W:117:ARG:CB	24:W:117:ARG:HH11	2.29	0.45
4:C:7:ASP:O	4:C:9:ASP:N	2.49	0.45
16:O:33:LEU:HA	16:O:40:HIS:NE2	2.32	0.45
16:O:112:ARG:HG3	16:O:113:VAL:N	2.32	0.45
1:0:2602:G:H2'	1:0:2603:G:C8	2.52	0.45
16:O:45:LEU:HD11	16:O:88:LYS:HB2	1.99	0.45
1:0:473:A:O2'	1:0:474:C:H5'	2.17	0.45
24:W:73:LEU:O	24:W:74:GLU:HG2	2.17	0.45
38:0:2924:MYL:HBG	40:0:5669:HOH:O	2.17	0.45
31:9:14:G:N2	31:9:68:G:H1'	2.32	0.45
13:L:133:VAL:HG13	40:L:4360:HOH:O	2.16	0.45
15:N:11:ARG:HA	15:N:14:ARG:NE	2.32	0.45
15:N:42:HIS:CG	15:N:62:HIS:HE1	2.34	0.45
1:0:2781:U:H2'	1:0:2782:G:C5'	2.45	0.45
27:Z:53:ILE:HG12	40:Z:5979:HOH:O	2.15	0.45
1:0:747:G:H3'	40:0:4594:HOH:O	2.15	0.45
14:M:118:TYR:CZ	14:M:130:GLU:HB2	2.52	0.45
1:0:292:G:H1'	1:0:360:A:H61	1.82	0.45
1:0:1412:U:O4	1:0:1681:G:H2'	2.16	0.45
25:X:41:PHE:CZ	25:X:74:ALA:HB3	2.51	0.45
26:Y:117:LEU:CD1	26:Y:181:GLY:HA2	2.46	0.45
4:C:142:ASP:OD2	4:C:238:SER:OG	2.35	0.45
1:0:1839:A:H3'	40:0:5104:HOH:O	2.17	0.45
1:0:466:A:H2'	1:0:467:G:O4'	2.17	0.45
13:L:97:VAL:HG12	13:L:98:GLU:O	2.16	0.45
1:0:1088:A:C6	1:0:1291:A:H1'	2.51	0.45
1:0:293:A:O2'	1:0:294:C:H5'	2.16	0.45
1:0:353:G:H2'	1:0:354:A:C8	2.51	0.45
1:0:1890:U:H4'	1:0:2010:A:C6	2.52	0.45
4:C:78:ARG:CG	4:C:78:ARG:NH1	2.73	0.45
5:D:63:ILE:HG13	5:D:64:ARG:H	1.81	0.45
5:D:169:THR:C	5:D:170:TYR:HD1	2.20	0.45
2:A:217:ARG:NH1	2:A:217:ARG:CG	2.79	0.45
3:B:98:THR:HG21	3:B:127:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2524:G:H21	1:0:2526:C:N4	2.15	0.45
1:0:12:U:C2'	1:0:13:G:H5'	2.46	0.45
1:0:2330:U:H4'	1:0:2331:C:OP1	2.17	0.45
1:0:1069:C:H4'	1:0:1081:A:O2'	2.17	0.45
19:R:92:LEU:HD23	19:R:145:LEU:HD21	1.99	0.45
1:0:1456:C:H2'	1:0:1457:U:C6	2.51	0.45
6:E:162:PHE:N	6:E:162:PHE:CD1	2.84	0.45
1:0:2283:G:C5	9:H:116:MET:HB3	2.51	0.45
1:0:2804:C:H2'	1:0:2805:A:O4'	2.17	0.45
1:0:2443:C:H3'	40:0:7933:HOH:O	2.17	0.45
40:0:8798:HOH:O	26:Y:186:ARG:HD2	2.15	0.45
1:0:59:A:H5'	40:0:2959:HOH:O	2.16	0.45
21:T:71:VAL:HG11	21:T:90:PRO:CB	2.34	0.45
1:0:1183:C:C2	1:0:1184:C:C5	3.05	0.45
15:N:37:ARG:CZ	40:N:3863:HOH:O	2.65	0.45
13:L:90:ARG:NH2	13:L:121:ILE:HD11	2.32	0.45
12:K:82:ARG:O	12:K:85:GLY:N	2.43	0.45
27:Z:57:MET:HE3	40:Z:5656:HOH:O	2.17	0.45
1:0:1378:G:C6	1:0:2747:C:H2'	2.52	0.45
13:L:148:GLU:C	13:L:148:GLU:OE1	2.55	0.45
1:0:244:C:O5'	1:0:244:C:H6	1.99	0.45
24:W:142:ASP:O	24:W:145:GLY:N	2.50	0.45
1:0:1387:G:C1'	17:P:28:GLN:HE22	2.30	0.45
1:0:2134:G:C6	1:0:2258:A:C8	3.04	0.45
13:L:43:HIS:O	13:L:44:GLU:C	2.55	0.45
1:0:1516:U:H2'	1:0:1517:C:C6	2.52	0.45
1:0:1287:A:C5	1:0:1288:U:C5	3.05	0.45
4:C:61:PHE:HB3	40:C:6056:HOH:O	2.15	0.45
18:Q:48:PRO:HD2	40:Q:5227:HOH:O	2.16	0.45
1:0:1968:A:H2'	1:0:1969:A:C8	2.51	0.45
1:0:1785:G:OP1	17:P:76:GLY:HA3	2.16	0.45
1:0:624:U:H3'	40:0:8802:HOH:O	2.16	0.45
14:M:50:ARG:N	14:M:54:TYR:HB3	2.31	0.45
1:0:2100:A:H5'	40:C:7192:HOH:O	2.16	0.45
9:H:70:LEU:O	9:H:72:ALA:N	2.50	0.45
1:0:2908:A:H8	1:0:2908:A:O5'	2.00	0.45
7:F:28:ALA:CB	7:F:99:THR:HG23	2.47	0.45
7:F:58:GLU:OE2	14:M:27:ARG:NH2	2.49	0.45
26:Y:219:GLU:CG	26:Y:220:GLU:N	2.77	0.45
1:0:820:G:C5	2:A:171:LYS:HB2	2.51	0.45
1:0:944:G:O2'	1:0:945:U:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:117:LEU:HD11	26:Y:181:GLY:HA2	1.98	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
1:0:1010:C:OP1	15:N:5:ARG:NH1	2.49	0.45
1:0:1815:A:H4'	1:0:2751:C:O4'	2.16	0.45
1:0:1055:G:N2	1:0:1057:A:H3'	2.32	0.45
4:C:7:ASP:OD1	4:C:11:ASN:N	2.49	0.45
6:E:146:ALA:O	6:E:150:GLN:HG2	2.17	0.45
1:0:1025:C:H5'	24:W:23:MET:O	2.17	0.45
1:0:1200:A:H3'	40:0:4912:HOH:O	2.17	0.45
1:0:1743:G:H1'	40:0:3739:HOH:O	2.17	0.45
6:E:22:VAL:O	6:E:28:SER:HA	2.17	0.45
11:J:71:TYR:CD1	11:J:72:PRO:HD2	2.52	0.45
1:0:1523:G:H2'	1:0:1524:U:O4'	2.16	0.45
40:0:4366:HOH:O	2:A:215:ILE:HD12	2.16	0.45
12:K:130:MET:SD	22:U:25:ASP:O	2.75	0.45
1:0:220:C:H5'	40:L:166:HOH:O	2.17	0.44
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.17	0.44
7:F:28:ALA:C	7:F:99:THR:HG23	2.37	0.44
12:K:74:VAL:HG21	12:K:96:VAL:HG23	2.00	0.44
9:H:6:ALA:HA	9:H:61:ARG:NH1	2.32	0.44
1:0:1771:U:O2	27:Z:43:GLY:HA2	2.17	0.44
1:0:1766:U:H2'	1:0:1776:A:N6	2.31	0.44
1:0:309:C:H42	1:0:322:G:H1	1.65	0.44
3:B:279:THR:CG2	3:B:280:VAL:N	2.79	0.44
24:W:117:ARG:CB	24:W:117:ARG:NH1	2.80	0.44
2:A:65:ARG:O	2:A:66:ARG:HG3	2.17	0.44
14:M:176:LYS:HB3	14:M:176:LYS:HE2	1.85	0.44
1:0:2645:U:H6	1:0:2645:U:OP2	2.00	0.44
1:0:2432:C:H2'	40:0:5669:HOH:O	2.16	0.44
1:0:1164:U:OP1	10:I:69:PRO:HA	2.18	0.44
1:0:316:A:H1'	1:0:336:G:N3	2.32	0.44
1:0:1278:A:O2'	1:0:1279:U:H3'	2.17	0.44
1:0:1557:G:H2'	1:0:1558:C:C6	2.51	0.44
1:0:1747:A:H5'	1:0:2585:G:OP1	2.17	0.44
1:0:862:U:H2'	1:0:863:G:C8	2.52	0.44
1:0:1523:G:C5	1:0:1524:U:C4	3.05	0.44
1:0:2719:A:C2	3:B:70:PRO:HG3	2.53	0.44
1:0:1864:C:H2'	1:0:1865:A:O4'	2.17	0.44
1:0:245:C:H2'	1:0:246:G:H5'	1.99	0.44
1:0:2004:U:H2'	40:0:6540:HOH:O	2.16	0.44
1:0:2103:A:O2'	1:0:2104:C:OP1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:2:GLN:HG3	30:3:91:GLN:CD	2.38	0.44
1:0:1190:G:H4'	1:0:1207:A:N1	2.33	0.44
12:K:34:VAL:HB	40:K:7169:HOH:O	2.17	0.44
7:F:60:VAL:O	7:F:61:MET:C	2.56	0.44
5:D:172:VAL:HG12	5:D:173:GLU:H	1.82	0.44
24:W:99:ALA:HA	24:W:102:SER:HG	1.81	0.44
1:0:2765:C:H2'	1:0:2766:A:H8	1.82	0.44
1:0:1350:U:H1'	40:0:5164:HOH:O	2.16	0.44
1:0:111:C:H2'	1:0:112:G:O4'	2.17	0.44
1:0:2576:A:H4'	1:0:2799:A:N1	2.33	0.44
1:0:2887:G:H2'	1:0:2888:U:O4'	2.16	0.44
2:A:132:ASP:OD2	2:A:133:ARG:N	2.45	0.44
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.16	0.44
1:0:2471:G:H4'	40:0:7361:HOH:O	2.16	0.44
30:3:11:CYS:SG	30:3:12:PRO:HD2	2.58	0.44
1:0:2509:A:H2'	1:0:2510:C:O4'	2.18	0.44
17:P:115:SER:C	17:P:117:SER:N	2.69	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.50	0.44
12:K:34:VAL:HG21	12:K:46:LYS:O	2.18	0.44
9:H:30:LYS:H	9:H:62:HIS:HD2	1.66	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
9:H:61:ARG:HG3	40:H:3845:HOH:O	2.17	0.44
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.50	0.44
20:S:22:ASN:OD1	20:S:74:ALA:N	2.43	0.44
28:1:5:THR:N	28:1:6:PRO:CD	2.79	0.44
1:0:816:G:H5'	1:0:1598:A:H4'	1.98	0.44
1:0:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.66	0.44
1:0:933:C:H5''	40:0:7590:HOH:O	2.17	0.44
1:0:776:A:H1'	1:0:779:U:O4	2.18	0.44
10:I:102:GLN:C	10:I:104:ALA:N	2.71	0.44
1:0:113:A:OP2	1:0:114:A:H2'	2.17	0.44
16:O:25:VAL:HG23	16:O:26:TRP:N	2.32	0.44
1:0:684:G:H2'	1:0:685:C:C6	2.52	0.44
1:0:1675:C:H5''	29:2:5:LYS:HD2	1.99	0.44
26:Y:189:ASN:C	26:Y:189:ASN:ND2	2.70	0.44
5:D:167:GLU:C	5:D:169:THR:H	2.20	0.44
7:F:47:LEU:O	7:F:98:VAL:HG23	2.18	0.44
5:D:20:LYS:HG2	5:D:133:ASN:HB3	2.00	0.44
20:S:15:MET:O	20:S:18:MET:N	2.50	0.44
24:W:99:ALA:O	24:W:103:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:88:THR:HG22	24:W:90:TYR:CD1	2.52	0.44
1:O:262:A:O2'	7:F:93:SER:HB2	2.16	0.44
10:I:129:SER:O	10:I:130:LEU:HD23	2.18	0.44
1:O:2133:U:H4'	1:O:2134:G:C5'	2.48	0.44
1:O:2672:C:O2'	1:O:2673:U:H5'	2.17	0.44
6:E:152:THR:HG21	6:E:165:GLY:HA2	1.98	0.44
1:O:102:A:H2'	1:O:103:C:O4'	2.17	0.44
17:P:5:ALA:O	17:P:8:ARG:HB3	2.18	0.44
1:O:869:G:H1'	40:O:7376:HOH:O	2.17	0.44
1:O:146:U:O2'	1:O:147:G:H5'	2.17	0.44
4:C:150:THR:HA	4:C:203:ALA:O	2.18	0.44
14:M:83:SER:C	14:M:85:ARG:N	2.71	0.44
2:A:192:VAL:O	2:A:207:GLN:HG2	2.18	0.44
20:S:18:MET:HA	20:S:23:LYS:O	2.17	0.44
29:2:36:ASN:O	29:2:39:ARG:HG3	2.17	0.44
28:1:15:THR:HB	28:1:28:HIS:NE2	2.33	0.44
3:B:175:LEU:C	3:B:175:LEU:CD2	2.86	0.44
1:O:1683:G:C2	1:O:1693:A:O4'	2.71	0.44
3:B:329:TYR:CE2	22:U:15:PRO:HG2	2.52	0.44
3:B:279:THR:OG1	3:B:290:VAL:O	2.34	0.44
11:J:59:LYS:O	11:J:63:ILE:HG13	2.17	0.44
2:A:215:ILE:HG13	2:A:216:SER:N	2.33	0.44
1:O:327:A:OP1	4:C:149:LYS:NZ	2.41	0.44
1:O:1935:C:H2'	1:O:1936:C:C6	2.53	0.44
1:O:2299:G:O6	18:Q:1:PRO:HA	2.16	0.44
1:O:1205:U:C2'	1:O:1206:U:C5'	2.89	0.44
1:O:506:G:N2	1:O:509:A:H5'	2.25	0.44
1:O:1187:U:C2	1:O:1189:A:OP2	2.70	0.44
1:O:2765:C:H2'	1:O:2766:A:C8	2.53	0.44
24:W:59:GLN:NE2	24:W:97:ALA:HB3	2.33	0.44
4:C:121:ALA:HA	4:C:136:VAL:HG11	2.00	0.44
4:C:5:ILE:CG2	4:C:6:TYR:N	2.81	0.44
7:F:96:ALA:HA	40:F:3111:HOH:O	2.18	0.44
2:A:55:VAL:O	2:A:55:VAL:HG13	2.18	0.44
21:T:82:THR:C	21:T:84:GLY:H	2.20	0.44
38:O:2924:MYL:CBD	38:O:2924:MYL:OAR	2.55	0.44
1:O:1593:C:H1'	40:O:5409:HOH:O	2.17	0.44
1:O:1180:U:H1'	40:I:1549:HOH:O	2.17	0.44
10:I:87:PRO:C	10:I:89:GLU:H	2.21	0.44
12:K:34:VAL:HG21	12:K:47:ALA:HB2	1.98	0.44
3:B:62:ARG:HA	3:B:65:MET:HE3	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:89:ASN:ND2	17:P:89:ASN:C	2.70	0.44
13:L:17:SER:H	13:L:20:ASN:ND2	2.15	0.44
1:0:313:U:H2'	1:0:314:G:O4'	2.17	0.44
1:0:645:U:O2	1:0:761:A:H2	2.01	0.44
20:S:59:ASP:C	20:S:61:GLU:H	2.21	0.44
14:M:66:SER:HB2	14:M:128:TRP:NE1	2.32	0.44
6:E:94:GLN:HB2	6:E:105:GLU:HB2	1.99	0.44
24:W:6:GLN:CB	24:W:26:ILE:HD11	2.48	0.44
2:A:93:THR:HG23	2:A:154:ALA:O	2.18	0.44
1:0:328:U:O4'	4:C:202:THR:HG22	2.17	0.44
18:Q:40:HIS:HD2	18:Q:60:THR:HG23	1.82	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.52	0.44
14:M:71:SER:OG	14:M:72:ALA:N	2.50	0.44
1:0:2717:C:C2'	1:0:2718:C:C5'	2.82	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.44
19:R:96:VAL:HA	19:R:99:ALA:HB3	2.00	0.44
19:R:99:ALA:O	19:R:104:PHE:HB2	2.18	0.44
11:J:40:ASN:N	11:J:106:GLY:O	2.50	0.44
4:C:96:LYS:HD3	4:C:98:ARG:NH1	2.33	0.44
31:9:114:G:H2'	31:9:115:C:C6	2.53	0.44
1:0:289:G:O2'	1:0:290:C:H5'	2.17	0.44
1:0:2734:G:O2'	1:0:2735:U:H5'	2.18	0.44
1:0:1625:U:C6	1:0:1625:U:C3'	3.00	0.44
1:0:302:A:O2'	1:0:303:C:H5'	2.18	0.44
1:0:1279:U:H5''	1:0:1280:A:OP2	2.18	0.44
3:B:141:ARG:HG2	3:B:165:ARG:HA	1.98	0.44
6:E:21:THR:HA	6:E:30:THR:HA	2.00	0.44
24:W:13:MET:HE3	24:W:17:ILE:CG2	2.47	0.44
3:B:102:THR:CG2	3:B:182:VAL:HG12	2.48	0.44
1:0:1551:C:H2'	1:0:1552:G:H8	1.83	0.44
1:0:1994:A:P	12:K:66:ARG:HH22	2.40	0.44
3:B:74:ILE:HG13	40:B:4810:HOH:O	2.18	0.44
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.44
1:0:1541:G:O2'	1:0:1542:G:H5'	2.18	0.44
3:B:48:MET:N	40:B:2534:HOH:O	2.50	0.44
16:O:48:ILE:C	16:O:50:ARG:N	2.72	0.44
1:0:514:G:H2'	1:0:514:G:OP1	2.17	0.44
31:9:18:U:H2'	31:9:19:G:H8	1.81	0.44
1:0:1746:A:H5''	40:O:5395:HOH:O	2.17	0.44
1:0:659:A:H5''	40:O:6799:HOH:O	2.17	0.44
1:0:2324:G:N2	1:0:2377:U:H1'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1594:C:H5	17:P:120:ARG:NH1	2.15	0.43
17:P:114:LEU:HA	17:P:118:GLN:NE2	2.33	0.43
23:V:12:THR:HG22	23:V:15:GLU:OE2	2.18	0.43
6:E:116:THR:CG2	6:E:151:LEU:HD22	2.39	0.43
1:0:1305:C:O2'	1:0:1306:U:H5'	2.18	0.43
13:L:66:VAL:HG23	13:L:67:ARG:N	2.33	0.43
4:C:2:GLN:HB3	40:C:3249:HOH:O	2.18	0.43
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.43
4:C:35:VAL:HG11	4:C:227:GLY:N	2.33	0.43
1:0:2006:C:H2'	1:0:2007:A:C8	2.53	0.43
14:M:159:VAL:HG13	14:M:160:PHE:N	2.33	0.43
7:F:20:LEU:HD13	7:F:49:PHE:CZ	2.53	0.43
6:E:23:GLU:HG2	6:E:28:SER:HB3	2.00	0.43
1:0:2103:A:HO2'	1:0:2104:C:P	2.40	0.43
15:N:44:ARG:HG3	15:N:45:ALA:N	2.32	0.43
19:R:84:ALA:O	19:R:88:PHE:HD1	2.01	0.43
14:M:146:ASP:O	14:M:147:LEU:HD23	2.18	0.43
3:B:123:ALA:O	3:B:126:GLU:HB3	2.17	0.43
1:0:2504:A:H4'	9:H:74:ARG:NH1	2.34	0.43
4:C:46:TYR:H	4:C:98:ARG:HH21	1.65	0.43
1:0:1626:A:H2'	1:0:1627:G:H5'	1.99	0.43
1:0:524:A:H5'	19:R:29:LYS:HE2	2.00	0.43
17:P:89:ASN:HD22	17:P:90:SER:N	2.16	0.43
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.43
10:I:134:ILE:HG22	10:I:135:GLU:N	2.33	0.43
20:S:6:LYS:O	20:S:7:HIS:HB3	2.18	0.43
1:0:57:C:N4	1:0:89:G:H1	2.15	0.43
1:0:808:A:C5	1:0:809:G:H1'	2.54	0.43
13:L:114:VAL:HG21	13:L:132:LYS:HB3	2.00	0.43
21:T:17:HIS:O	21:T:20:HIS:HD2	2.00	0.43
1:0:35:U:O2'	1:0:36:C:H5'	2.18	0.43
1:0:1264:U:P	24:W:117:ARG:HH22	2.40	0.43
21:T:82:THR:C	21:T:84:GLY:N	2.72	0.43
40:0:3998:HOH:O	3:B:216:LYS:HA	2.18	0.43
1:0:2596:A:H3'	40:0:8372:HOH:O	2.18	0.43
16:O:97:SER:C	16:O:99:GLU:H	2.21	0.43
5:D:169:THR:O	5:D:170:TYR:HB2	2.18	0.43
4:C:246:ARG:CB	4:C:246:ARG:HH11	2.27	0.43
1:0:1375:A:O2'	1:0:1376:G:H5'	2.18	0.43
1:0:686:A:O2'	1:0:747:G:H4'	2.18	0.43
1:0:65:C:H2'	1:0:66:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:37:A:C2	1:0:446:G:C2	3.07	0.43
16:O:96:VAL:HG12	16:O:97:SER:N	2.33	0.43
28:1:10:LYS:HG3	40:1:2979:HOH:O	2.18	0.43
6:E:166:VAL:HB	40:E:6341:HOH:O	2.17	0.43
1:0:2026:C:H2'	1:0:2027:U:H6	1.81	0.43
1:0:1750:C:H5''	40:0:8211:HOH:O	2.17	0.43
1:0:2053:G:H4'	19:R:136:TRP:CE2	2.53	0.43
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.43	0.43
1:0:1319:G:H1'	40:0:3460:HOH:O	2.17	0.43
4:C:95:GLU:HG3	40:C:7650:HOH:O	2.18	0.43
27:Z:70:ARG:NH1	27:Z:82:SER:C	2.68	0.43
4:C:72:LYS:HD2	40:C:5079:HOH:O	2.18	0.43
11:J:130:VAL:CG1	11:J:131:THR:N	2.81	0.43
1:0:170:U:H2'	1:0:171:C:H5'	1.99	0.43
4:C:98:ARG:NH1	4:C:98:ARG:HG2	2.31	0.43
13:L:41:HIS:O	13:L:42:ASN:HB2	2.17	0.43
24:W:88:THR:O	24:W:90:TYR:N	2.52	0.43
15:N:27:LEU:CD2	15:N:50:LEU:HD22	2.47	0.43
1:0:2779:G:H21	6:E:143:GLN:NE2	2.16	0.43
1:0:2615:U:C5	1:0:2616:G:C6	3.07	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.05	0.43
14:M:120:VAL:CG1	14:M:130:GLU:HG3	2.48	0.43
1:0:1629:G:N2	1:0:1632:A:OP2	2.52	0.43
20:S:52:VAL:HG22	20:S:66:VAL:HG22	2.01	0.43
27:Z:90:GLY:HA3	27:Z:95:PRO:O	2.18	0.43
14:M:4:ALA:O	14:M:7:TYR:HB2	2.18	0.43
1:0:1899:C:H5''	2:A:216:SER:N	2.33	0.43
9:H:92:LYS:HG3	9:H:130:VAL:HG22	2.00	0.43
1:0:1028:U:H5'	1:0:1031:G:O4'	2.18	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.43
4:C:132:ASP:HB3	40:C:2669:HOH:O	2.18	0.43
15:N:15:GLU:HB3	15:N:17:ARG:HG3	2.00	0.43
1:0:827:A:H2'	1:0:828:G:O4'	2.18	0.43
9:H:122:LYS:O	9:H:124:VAL:HG13	2.18	0.43
2:A:170:VAL:HG21	27:Z:50:VAL:HG21	2.00	0.43
1:0:553:G:C2'	1:0:554:G:H5'	2.49	0.43
40:0:7516:HOH:O	2:A:21:HIS:HB2	2.19	0.43
1:0:1738:C:O2'	1:0:1739:G:H5'	2.18	0.43
12:K:27:ARG:HD2	12:K:60:GLY:HA2	2.01	0.43
1:0:1786:C:OP1	17:P:74:GLN:HG2	2.18	0.43
3:B:266:ASN:OD1	3:B:317:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2541:U:O2'	32:4:76:5AA:H4'	2.18	0.43
1:0:2433:A:O5'	1:0:2433:A:H8	2.01	0.43
30:3:62:THR:CG2	30:3:63:LYS:N	2.81	0.43
11:J:19:MET:HE3	11:J:132:LEU:CD1	2.30	0.43
22:U:9:CYS:HA	22:U:52:THR:CG2	2.47	0.43
3:B:26:PHE:HE1	3:B:310:ARG:HB3	1.82	0.43
14:M:81:ARG:HH11	14:M:81:ARG:HB2	1.80	0.43
13:L:30:ARG:NH1	13:L:30:ARG:HG3	2.30	0.43
24:W:122:ARG:NH1	24:W:152:ALA:O	2.49	0.43
1:0:1695:G:N3	28:1:9:GLY:HA3	2.33	0.43
15:N:159:TYR:HE1	31:9:50:G:H5''	1.84	0.43
1:0:1171:A:H2'	1:0:1172:G:H5'	2.00	0.43
1:0:1051:C:H2'	1:0:1052:G:O4'	2.18	0.43
3:B:71:VAL:HG11	3:B:296:LEU:HD22	2.01	0.43
1:0:550:C:H2'	1:0:551:A:O4'	2.18	0.43
1:0:1286:A:H5''	40:0:7804:HOH:O	2.18	0.43
1:0:391:U:H5''	40:0:5416:HOH:O	2.18	0.43
2:A:140:LEU:HB3	2:A:141:PRO:HD2	2.00	0.43
1:0:2529:G:H3'	40:0:6917:HOH:O	2.19	0.43
1:0:324:G:O2'	1:0:325:U:H5'	2.19	0.43
2:A:213:LYS:HB2	40:A:242:HOH:O	2.18	0.43
24:W:128:VAL:HG12	24:W:138:LEU:HD21	2.01	0.43
21:T:114:SER:OG	21:T:117:ASP:HB2	2.19	0.43
1:0:1808:C:O2'	1:0:1809:G:H5'	2.19	0.43
1:0:1537:C:H1'	40:0:6076:HOH:O	2.18	0.43
11:J:131:THR:HG22	11:J:134:GLU:H	1.84	0.43
1:0:1186:C:H42	1:0:1190:G:H22	1.66	0.43
7:F:28:ALA:HB3	7:F:99:THR:HG23	2.00	0.43
9:H:96:GLN:NE2	9:H:129:ARG:NH2	2.66	0.43
5:D:75:LEU:HB3	5:D:80:ALA:CA	2.49	0.43
1:0:1441:G:H2'	1:0:1442:A:H8	1.83	0.43
6:E:14:GLU:CG	6:E:15:GLN:N	2.80	0.43
6:E:26:ASN:CB	6:E:76:VAL:O	2.67	0.43
20:S:6:LYS:HB2	20:S:27:ALA:O	2.19	0.43
5:D:52:THR:N	5:D:70:GLY:O	2.52	0.43
3:B:139:ASP:CB	3:B:165:ARG:HE	2.31	0.43
9:H:49:GLN:O	9:H:49:GLN:HG2	2.18	0.43
1:0:2415:A:H2'	1:0:2416:G:H5'	1.99	0.43
1:0:1553:C:H6	1:0:1553:C:O5'	2.02	0.43
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.43
9:H:53:ILE:HA	9:H:134:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1730:G:H4'	1:0:1731:C:H6	1.82	0.43
1:0:74:G:H5'	23:V:9:ARG:HH22	1.83	0.43
1:0:251:C:H2'	1:0:252:C:H6	1.83	0.43
11:J:75:PRO:HB3	11:J:132:LEU:HB3	2.01	0.43
30:3:11:CYS:SG	30:3:13:HIS:CD2	3.11	0.43
5:D:137:PRO:O	5:D:139:TYR:N	2.52	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.18	0.43
1:0:1166:A:N3	1:0:1166:A:H2'	2.33	0.43
5:D:25:MET:HE2	5:D:41:LEU:HD11	2.01	0.43
1:0:281:U:O2'	1:0:282:C:H5'	2.19	0.43
8:G:64:ASN:ND2	8:G:64:ASN:H	2.16	0.43
15:N:7:LYS:HB2	40:Q:5853:HOH:O	2.19	0.43
15:N:164:ASP:CG	15:N:167:ASP:HA	2.39	0.43
2:A:135:VAL:HG22	2:A:136:ALA:N	2.33	0.43
17:P:80:ARG:HG2	17:P:87:ARG:NH2	2.33	0.43
1:0:945:U:H2'	1:0:946:C:C6	2.54	0.43
1:0:1262:C:O2	24:W:120:PRO:HG2	2.19	0.43
5:D:23:VAL:CG2	5:D:23:VAL:O	2.66	0.43
1:0:304:G:H1'	1:0:347:A:N6	2.33	0.43
1:0:1515:A:H2'	1:0:1516:U:C6	2.53	0.43
1:0:1220:U:O2'	1:0:1221:G:H5'	2.18	0.43
1:0:125:U:C2	1:0:128:A:C2	3.07	0.43
1:0:255:A:H2'	1:0:256:C:C6	2.54	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:593:A:H2'	1:0:594:C:H5'	2.01	0.43
1:0:2834:G:OP1	25:X:39:LYS:HE2	2.18	0.43
1:0:82:C:H4'	1:0:99:A:O2'	2.19	0.43
1:0:2647:C:H1'	40:0:5844:HOH:O	2.18	0.43
26:Y:109:LEU:HA	40:Y:4541:HOH:O	2.18	0.43
14:M:74:LYS:O	14:M:88:VAL:HA	2.18	0.43
27:Z:81:CYS:HB3	27:Z:86:TYR:H	1.83	0.43
1:0:2502:C:H2'	1:0:2503:A:C5'	2.35	0.43
11:J:42:GLU:O	11:J:131:THR:HG23	2.19	0.43
14:M:101:ALA:O	14:M:102:GLU:C	2.56	0.43
28:1:25:LYS:HD2	29:2:48:ASP:HA	2.01	0.43
1:0:1741:U:C4	1:0:2033:G:C8	3.07	0.43
4:C:79:ARG:O	4:C:87:ARG:N	2.51	0.43
1:0:85:C:H3'	1:0:86:A:H2'	2.00	0.43
1:0:1095:U:O2	24:W:120:PRO:HG2	2.18	0.43
24:W:142:ASP:C	24:W:144:GLU:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
26:Y:160:LYS:HD3	26:Y:160:LYS:HA	1.79	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.19	0.43
13:L:32:ASP:O	13:L:35:ARG:HB3	2.19	0.43
28:1:20:ARG:N	40:1:513:HOH:O	2.52	0.43
1:0:1804:A:H2'	1:0:1805:G:C8	2.53	0.43
4:C:22:PHE:HA	4:C:116:ALA:HA	2.01	0.43
3:B:278:PRO:HD3	3:B:294:TYR:CZ	2.53	0.43
1:0:1800:G:H2'	1:0:1801:A:H8	1.83	0.43
1:0:17:G:O2'	1:0:18:C:H5'	2.18	0.43
1:0:1850:U:H2'	1:0:1851:G:C8	2.53	0.43
1:0:696:C:H2'	1:0:697:G:O4'	2.18	0.43
1:0:1935:C:H2'	1:0:1936:C:H6	1.84	0.43
21:T:53:GLY:HA3	40:T:6384:HOH:O	2.18	0.43
15:N:180:LEU:N	15:N:180:LEU:HD12	2.34	0.43
1:0:1409:G:C2	1:0:1410:G:C8	3.07	0.43
1:0:2631:U:H5''	40:0:5654:HOH:O	2.19	0.43
1:0:1430:G:H5''	40:0:3794:HOH:O	2.18	0.43
1:0:2387:U:H2'	1:0:2388:C:C6	2.53	0.43
1:0:220:C:H2'	40:L:166:HOH:O	2.18	0.43
11:J:131:THR:HG22	11:J:133:GLY:H	1.83	0.43
11:J:74:ARG:CB	11:J:74:ARG:HH11	2.25	0.43
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.67	0.43
18:Q:16:ASN:ND2	18:Q:45:PRO:HD2	2.29	0.43
19:R:4:TYR:CZ	19:R:15:LYS:HB3	2.54	0.43
1:0:603:A:H1'	1:0:605:C:C2	2.53	0.43
1:0:195:C:C2'	1:0:196:G:H5'	2.46	0.43
26:Y:146:PRO:O	26:Y:154:ARG:HG3	2.19	0.43
17:P:67:LYS:O	17:P:68:LYS:C	2.57	0.43
1:0:1055:G:OP2	9:H:99:ARG:NH1	2.52	0.43
1:0:920:C:OP1	13:L:37:LYS:NZ	2.52	0.43
1:0:2271:G:N3	1:0:2271:G:H2'	2.34	0.43
1:0:675:U:O2'	4:C:42:ARG:NH1	2.52	0.43
1:0:2758:G:H2'	1:0:2759:C:C6	2.54	0.43
27:Z:99:GLY:O	27:Z:103:VAL:HG23	2.19	0.43
13:L:130:ARG:O	13:L:131:GLU:C	2.57	0.43
1:0:1102:C:H1'	1:0:1109:U:C4	2.54	0.43
1:0:667:C:H2'	1:0:668:C:H6	1.84	0.43
23:V:5:VAL:HG23	40:V:2271:HOH:O	2.19	0.43
40:0:8286:HOH:O	16:O:42:GLU:HB2	2.18	0.43
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:844:A:C6	1:0:882:A:C6	3.06	0.43
1:0:2911:C:H2'	1:0:2912:C:C6	2.54	0.43
1:0:1116:U:O2'	1:0:1118:A:C2	2.47	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.49	0.42
21:T:49:GLU:HG2	21:T:99:THR:CG2	2.49	0.42
19:R:39:THR:HB	19:R:42:GLU:OE1	2.19	0.42
14:M:23:LEU:HD13	14:M:27:ARG:NH2	2.34	0.42
40:C:2822:HOH:O	21:T:2:LYS:HE2	2.18	0.42
1:0:1477:C:C5'	1:0:1868:G:C5'	2.97	0.42
1:0:2526:C:H5'	1:0:2526:C:C6	2.54	0.42
1:0:1838:U:O2'	1:0:2644:C:H5'	2.19	0.42
3:B:181:ILE:HG22	3:B:186:GLY:HA2	2.01	0.42
30:3:34:LYS:HG3	30:3:35:TRP:H	1.84	0.42
10:I:97:VAL:HG12	10:I:101:LYS:HE3	2.00	0.42
24:W:131:PRO:O	24:W:136:GLY:CA	2.67	0.42
4:C:80:VAL:HA	4:C:81:PRO:HD3	1.88	0.42
1:0:107:U:C2'	1:0:108:U:H5'	2.49	0.42
1:0:2103:A:O2'	1:0:2104:C:P	2.77	0.42
4:C:149:LYS:O	4:C:150:THR:C	2.57	0.42
1:0:1908:G:N1	1:0:1930:A:OP2	2.51	0.42
1:0:2493:C:O2	1:0:2493:C:H2'	2.19	0.42
18:Q:23:THR:HG22	18:Q:24:SER:N	2.34	0.42
1:0:121:U:OP2	29:2:10:ARG:NH2	2.47	0.42
1:0:1388:U:H2'	1:0:1389:G:O4'	2.19	0.42
7:F:107:ASP:O	7:F:108:VAL:C	2.57	0.42
1:0:2317:C:P	30:3:61:PRO:HG2	2.58	0.42
31:9:54:A:C2'	31:9:55:U:H5'	2.48	0.42
3:B:160:ASP:HB3	3:B:308:LEU:HD22	2.01	0.42
16:O:71:GLN:HA	16:O:92:VAL:HG11	2.01	0.42
13:L:110:GLY:HA3	13:L:129:ALA:HA	2.01	0.42
25:X:52:PRO:O	25:X:53:SER:C	2.58	0.42
24:W:80:ASP:O	24:W:81:ASP:C	2.57	0.42
3:B:52:VAL:N	3:B:329:TYR:O	2.43	0.42
24:W:56:GLU:O	24:W:143:THR:HG23	2.19	0.42
1:0:699:C:C2'	1:0:744:G:N3	2.82	0.42
19:R:68:HIS:CG	19:R:76:ASP:HB2	2.54	0.42
1:0:2474:A:N7	1:0:2621:PSU:H4'	2.34	0.42
6:E:18:LEU:HD13	6:E:34:TRP:CD1	2.53	0.42
7:F:48:VAL:HG23	7:F:74:PHE:CB	2.49	0.42
24:W:23:MET:C	24:W:25:ASN:H	2.23	0.42
1:0:48:A:H2'	1:0:49:A:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:49:GLU:HA	28:1:49:GLU:OE2	2.19	0.42
1:0:2332:A:H3'	1:0:2333:G:H8	1.84	0.42
1:0:2617:G:H4'	40:0:3214:HOH:O	2.18	0.42
1:0:2545:U:OP2	3:B:2:GLN:NE2	2.46	0.42
18:Q:77:ASP:O	18:Q:79:GLY:N	2.51	0.42
1:0:2637:A:N6	32:4:176:DA:C2'	2.62	0.42
1:0:1185:U:H5'	40:0:7308:HOH:O	2.17	0.42
1:0:2070:G:H2'	1:0:2072:G:OP1	2.19	0.42
3:B:258:GLY:N	3:B:260:HIS:CE1	2.78	0.42
19:R:39:THR:O	19:R:41:GLY:N	2.52	0.42
8:G:73:ASP:N	8:G:73:ASP:OD1	2.52	0.42
15:N:20:TYR:HA	15:N:23:ARG:HB3	2.01	0.42
4:C:131:PHE:N	4:C:131:PHE:HD2	2.09	0.42
26:Y:125:LYS:HB2	26:Y:126:PRO:HD2	2.01	0.42
3:B:147:VAL:CG1	3:B:150:ALA:HB2	2.49	0.42
5:D:10:PHE:N	40:D:7345:HOH:O	2.53	0.42
1:0:1397:C:H1'	17:P:28:GLN:OE1	2.19	0.42
1:0:212:A:O3'	1:0:213:G:H4'	2.19	0.42
17:P:68:LYS:O	17:P:73:HIS:HB2	2.20	0.42
30:3:6:ARG:HG2	30:3:6:ARG:NH1	2.34	0.42
26:Y:132:ASP:OD1	26:Y:135:LYS:HD2	2.18	0.42
23:V:25:THR:HG23	23:V:29:ASN:ND2	2.34	0.42
14:M:98:GLN:NE2	14:M:117:SER:OG	2.49	0.42
1:0:215:A:OP1	13:L:52:LYS:NZ	2.45	0.42
1:0:2546:U:O2'	3:B:237:GLY:N	2.52	0.42
40:0:8389:HOH:O	9:H:14:LYS:HD3	2.19	0.42
40:0:6068:HOH:O	31:9:83:G:H4'	2.18	0.42
30:3:59:ASP:CG	30:3:63:LYS:HZ1	2.22	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.27	0.42
14:M:164:THR:HG22	14:M:167:GLY:H	1.85	0.42
5:D:166:ILE:HB	40:D:6326:HOH:O	2.20	0.42
14:M:76:ARG:NH1	14:M:77:HIS:CE1	2.88	0.42
17:P:55:LYS:HA	40:P:4732:HOH:O	2.19	0.42
1:0:272:A:C2	1:0:369:G:H5''	2.55	0.42
24:W:68:THR:HG23	24:W:69:ARG:HG2	2.01	0.42
13:L:61:ALA:HB2	13:L:105:TYR:CZ	2.54	0.42
31:9:61:C:H2'	31:9:62:A:C8	2.53	0.42
2:A:134:ASN:O	2:A:150:PRO:HD3	2.20	0.42
1:0:1427:A:O2'	1:0:1428:C:H5'	2.19	0.42
1:0:665:A:H2'	1:0:666:A:C8	2.54	0.42
1:0:2036:C:H1'	12:K:44:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1135:G:C6	1:0:1136:U:C4	3.07	0.42
1:0:472:A:O4'	1:0:774:C:H4'	2.18	0.42
2:A:181:ALA:O	2:A:182:ARG:HG2	2.19	0.42
18:Q:81:GLU:HG3	40:Q:3458:HOH:O	2.20	0.42
31:9:78:G:H22	31:9:103:A:P	2.42	0.42
32:4:74:C:C2'	32:4:75:C:H5'	2.49	0.42
40:0:5147:HOH:O	32:4:176:DA:H2	2.02	0.42
1:0:2382:A:H1'	30:3:10:TYR:HE2	1.84	0.42
4:C:236:THR:O	4:C:239:ALA:HB3	2.18	0.42
1:0:2533:C:O2'	1:0:2534:C:H5'	2.20	0.42
1:0:737:A:H2'	1:0:738:G:C8	2.54	0.42
1:0:2838:A:H2'	1:0:2839:C:O4'	2.20	0.42
1:0:710:G:P	16:O:24:ALA:HB3	2.59	0.42
21:T:23:VAL:C	21:T:93:THR:HG21	2.40	0.42
10:I:95:LEU:CD2	10:I:99:GLN:HB3	2.49	0.42
1:0:2748:G:H1'	40:0:7865:HOH:O	2.18	0.42
14:M:112:LEU:HB3	14:M:133:LEU:HB3	2.02	0.42
26:Y:107:PRO:HB3	26:Y:182:PHE:CE2	2.53	0.42
6:E:126:ILE:HB	6:E:131:LEU:CD2	2.49	0.42
1:0:1167:G:H4'	10:I:130:LEU:HD22	2.00	0.42
15:N:151:ASP:O	15:N:154:LEU:HB2	2.19	0.42
13:L:73:VAL:HG21	13:L:116:HIS:CE1	2.54	0.42
22:U:14:GLU:HA	22:U:15:PRO:HD2	1.91	0.42
1:0:213:G:HO2'	1:0:214:U:P	2.42	0.42
1:0:2811:A:C4'	1:0:2812:A:H5''	2.49	0.42
7:F:1:PRO:N	7:F:4:VAL:HG23	2.33	0.42
24:W:82:GLU:O	24:W:86:GLU:HG3	2.20	0.42
1:0:163:U:O3'	1:0:896:C:H4'	2.20	0.42
1:0:2898:G:O2'	1:0:2899:A:H5'	2.19	0.42
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.52	0.42
1:0:2663:U:C4	1:0:2664:A:C6	3.08	0.42
4:C:200:PRO:HA	40:C:3887:HOH:O	2.19	0.42
13:L:21:ARG:HA	13:L:26:HIS:HD2	1.85	0.42
14:M:94:ARG:HG2	14:M:94:ARG:HH11	1.84	0.42
19:R:95:ALA:HB1	19:R:147:LEU:CD1	2.50	0.42
14:M:99:ARG:NH1	14:M:99:ARG:CG	2.67	0.42
26:Y:187:VAL:CG1	26:Y:205:ILE:HA	2.49	0.42
1:0:541:C:O2'	1:0:542:A:H5''	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.08	0.42
24:W:108:ARG:NH2	24:W:114:PRO:HG2	2.27	0.42
9:H:46:TYR:HA	9:H:47:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:706:G:N2	1:0:707:C:N4	2.66	0.42
1:0:1380:U:O4	1:0:2043:U:H4'	2.19	0.42
15:N:26:LEU:HA	15:N:26:LEU:HD12	1.82	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.55	0.42
3:B:270:ILE:HD13	3:B:270:ILE:HA	1.87	0.42
1:0:921:G:H4'	1:0:924:G:N1	2.34	0.42
1:0:1898:G:H2'	1:0:1899:C:C6	2.55	0.42
40:0:8598:HOH:O	21:T:82:THR:HA	2.20	0.42
1:0:549:A:O2'	1:0:550:C:H5'	2.20	0.42
16:O:35:LYS:HB3	16:O:36:PRO:HD2	2.00	0.42
10:I:114:TYR:CD1	10:I:114:TYR:N	2.87	0.42
4:C:97:ASP:C	4:C:97:ASP:OD2	2.58	0.42
7:F:6:PHE:O	7:F:6:PHE:CD1	2.72	0.42
16:O:59:VAL:HG23	16:O:111:VAL:HG21	2.01	0.42
16:O:100:GLN:O	16:O:103:GLU:N	2.52	0.42
1:0:652:G:H5''	40:0:6351:HOH:O	2.18	0.42
9:H:94:PRO:HB2	9:H:126:THR:HB	2.00	0.42
13:L:142:LEU:HD21	13:L:146:GLY:O	2.19	0.42
14:M:14:ASN:C	14:M:16:GLY:H	2.22	0.42
24:W:129:LYS:HD3	31:9:87:U:H2'	2.00	0.42
30:3:3:MET:HE3	30:3:4:PRO:HD2	2.02	0.42
11:J:39:VAL:O	11:J:40:ASN:HB2	2.19	0.42
11:J:39:VAL:HG13	11:J:40:ASN:HD22	1.84	0.42
1:0:1589:G:H4'	40:0:6458:HOH:O	2.19	0.42
1:0:183:A:H1'	14:M:161:ARG:HH11	1.82	0.42
24:W:90:TYR:HD1	24:W:90:TYR:N	2.17	0.42
13:L:144:ASP:HA	13:L:147:GLU:CD	2.40	0.42
4:C:53:GLY:O	4:C:79:ARG:HA	2.20	0.42
22:U:39:ASN:ND2	22:U:51:TRP:HZ2	2.18	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
9:H:51:SER:HA	9:H:138:THR:HA	2.01	0.42
21:T:4:PRO:O	21:T:8:ARG:HG3	2.20	0.42
1:0:1965:C:H6	1:0:1965:C:O5'	2.01	0.42
38:0:2924:MYL:CAV	38:0:2924:MYL:HABB	2.50	0.42
2:A:109:GLU:HG2	2:A:114:ASP:OD1	2.19	0.42
3:B:320:GLN:NE2	3:B:321:PRO:CD	2.80	0.42
15:N:1:ALA:HB2	31:9:14:G:O2'	2.20	0.42
15:N:108:SER:C	15:N:110:THR:H	2.23	0.42
8:G:23:ILE:C	8:G:25:GLU:N	2.72	0.42
8:G:19:GLU:O	8:G:23:ILE:HG13	2.20	0.42
1:0:1882:C:H2'	1:0:1883:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:9:TYR:O	9:H:59:GLN:HB2	2.20	0.42
1:0:164:G:H4'	13:L:30:ARG:HD2	2.01	0.42
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.52	0.42
1:0:1441:G:H2'	1:0:1442:A:C8	2.54	0.42
1:0:661:G:C6	1:0:686:A:C2	3.07	0.42
1:0:1067:A:O2'	24:W:12:ASN:HA	2.20	0.42
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.42
1:0:1855:G:N7	2:A:142:SER:OG	2.43	0.42
12:K:18:ILE:HG22	12:K:93:ASN:HB2	2.00	0.42
1:0:2757:A:C4	1:0:2896:A:C2	3.08	0.42
1:0:1941:A:H5''	40:0:7014:HOH:O	2.20	0.42
7:F:70:LYS:O	7:F:72:VAL:N	2.44	0.42
15:N:58:LEU:HD12	15:N:58:LEU:N	2.35	0.42
1:0:585:C:H5''	40:0:3708:HOH:O	2.20	0.42
1:0:2607:U:OP2	3:B:243:ASN:HB2	2.19	0.42
9:H:165:ARG:NH1	40:H:6571:HOH:O	2.53	0.42
1:0:2319:C:H3'	30:3:1:MET:HA	2.02	0.42
1:0:2378:U:OP1	30:3:8:ASN:HB3	2.20	0.42
1:0:2324:G:H4'	1:0:2418:G:O2'	2.19	0.42
30:3:8:ASN:ND2	30:3:17:HIS:HD2	2.18	0.42
30:3:3:MET:CE	30:3:4:PRO:HD2	2.49	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.42
1:0:2349:G:H5'	5:D:133:ASN:HD22	1.85	0.42
1:0:544:G:H2'	1:0:545:G:H5'	2.01	0.42
8:G:24:VAL:HA	8:G:27:ILE:HD12	2.02	0.42
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.42
25:X:21:PRO:CG	25:X:24:LYS:HD3	2.49	0.42
1:0:1942:A:O2'	1:0:1943:C:H5'	2.20	0.42
17:P:87:ARG:HG2	17:P:87:ARG:HH11	1.85	0.42
25:X:41:PHE:O	25:X:43:VAL:HG23	2.20	0.42
1:0:1486:A:C4	29:2:2:LYS:HG3	2.55	0.42
3:B:280:VAL:HG13	3:B:333:GLU:O	2.20	0.42
1:0:453:A:C4	1:0:479:G:C8	3.08	0.42
1:0:88:G:N7	29:2:28:LYS:HD2	2.35	0.42
3:B:120:ASP:CG	3:B:123:ALA:HB2	2.40	0.42
1:0:1311:G:C5	1:0:1344:G:C6	3.08	0.42
4:C:178:GLN:C	4:C:180:SER:N	2.69	0.42
13:L:117:GLU:CG	13:L:117:GLU:O	2.68	0.42
25:X:16:ASP:C	25:X:18:ARG:H	2.23	0.42
1:0:1047:U:H2'	1:0:1048:G:C8	2.54	0.42
3:B:154:VAL:HA	3:B:155:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:63:ASN:OD1	19:R:63:ASN:N	2.53	0.42
1:0:2542:C:O2'	32:4:75:C:H1'	2.19	0.42
31:9:55:U:H4'	31:9:56:A:H8	1.84	0.42
11:J:107:ASN:HD22	11:J:108:PRO:N	2.16	0.42
5:D:169:THR:HG22	5:D:169:THR:O	2.20	0.42
24:W:52:VAL:CG2	24:W:53:ALA:H	2.32	0.42
1:0:1384:C:H5'	25:X:30:MET:HG2	2.02	0.42
1:0:1150:A:C2	8:G:20:VAL:HG21	2.54	0.42
1:0:2815:G:H4'	1:0:2816:A:OP2	2.20	0.42
1:0:332:G:H4'	21:T:2:LYS:O	2.20	0.42
4:C:243:VAL:HG22	4:C:243:VAL:O	2.20	0.42
1:0:1013:A:H5''	1:0:2302:A:N6	2.35	0.42
1:0:1630:A:H2'	1:0:1631:A:O4'	2.20	0.42
1:0:65:C:H2'	1:0:66:G:H8	1.85	0.42
2:A:95:PRO:HG2	2:A:98:GLU:CG	2.50	0.42
1:0:645:U:O2	4:C:93:LYS:NZ	2.52	0.42
5:D:22:VAL:HA	5:D:73:VAL:O	2.20	0.42
15:N:69:TYR:CE2	15:N:184:ILE:HD11	2.55	0.42
1:0:1552:G:C6	1:0:1634:G:C6	3.08	0.42
11:J:54:VAL:O	11:J:58:GLU:HB2	2.19	0.42
1:0:2001:G:O2'	1:0:2002:C:H5'	2.20	0.42
7:F:12:LEU:HD22	7:F:75:ILE:HD11	2.02	0.42
1:0:2248:C:H3'	40:0:4476:HOH:O	2.20	0.42
1:0:1457:U:O2'	1:0:1458:A:H5'	2.20	0.42
9:H:14:LYS:HG2	40:H:714:HOH:O	2.19	0.42
26:Y:110:SER:O	26:Y:111:ASP:C	2.58	0.42
30:3:30:GLN:HB3	40:3:5866:HOH:O	2.19	0.42
40:0:3586:HOH:O	2:A:11:ARG:HD3	2.19	0.42
12:K:8:VAL:HG12	12:K:9:THR:N	2.35	0.42
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.42
2:A:188:ASN:HA	40:A:3459:HOH:O	2.19	0.42
1:0:261:A:OP1	14:M:42:ARG:NH2	2.53	0.42
30:3:11:CYS:SG	30:3:13:HIS:HD2	2.42	0.41
15:N:37:ARG:NE	40:N:3863:HOH:O	2.53	0.41
16:O:73:ASP:CG	16:O:73:ASP:O	2.58	0.41
1:0:560:U:H2'	1:0:561:G:H8	1.84	0.41
25:X:76:ARG:NH1	25:X:76:ARG:CG	2.83	0.41
1:0:1329:G:N2	40:0:3448:HOH:O	2.50	0.41
2:A:192:VAL:HG12	2:A:207:GLN:HG2	2.03	0.41
13:L:34:GLY:HA2	40:L:4728:HOH:O	2.20	0.41
13:L:34:GLY:C	13:L:36:ASP:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:213:ALA:CB	4:C:218:VAL:HG23	2.50	0.41
3:B:5:ARG:HD2	3:B:8:LYS:NZ	2.35	0.41
1:0:873:G:H2'	1:0:875:A:N7	2.35	0.41
1:0:1260:G:H3'	1:0:1261:A:C8	2.56	0.41
1:0:2499:U:H2'	1:0:2500:C:C6	2.55	0.41
1:0:2756:U:N3	1:0:2896:A:C2	2.87	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.54	0.41
1:0:1564:C:H1'	1:0:2738:G:N2	2.34	0.41
1:0:408:A:O2'	1:0:409:U:H5'	2.19	0.41
1:0:473:A:O2'	1:0:890:C:H5'	2.19	0.41
2:A:18:ALA:O	2:A:20:SER:N	2.46	0.41
40:0:7242:HOH:O	21:T:9:LYS:HB2	2.20	0.41
2:A:207:GLN:HA	40:A:2643:HOH:O	2.20	0.41
6:E:154:ILE:HG13	6:E:156:ASP:OD1	2.20	0.41
1:0:1571:G:C2'	1:0:1626:A:H61	2.33	0.41
3:B:215:VAL:CA	3:B:220:VAL:HG22	2.48	0.41
23:V:64:GLY:O	23:V:65:ASP:CB	2.64	0.41
1:0:1654:U:H5''	40:0:7237:HOH:O	2.19	0.41
1:0:653:U:H2'	1:0:654:A:C8	2.55	0.41
1:0:2346:C:O3'	5:D:52:THR:CG2	2.69	0.41
27:Z:59:GLU:HB2	27:Z:61:HIS:CE1	2.55	0.41
18:Q:41:LEU:N	18:Q:41:LEU:HD12	2.34	0.41
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.41
1:0:411:A:H4'	1:0:412:C:OP2	2.20	0.41
1:0:1553:C:O2'	1:0:1554:C:H5'	2.19	0.41
1:0:1090:A:C6	1:0:1091:U:C4	3.08	0.41
14:M:5:TYR:C	14:M:7:TYR:H	2.23	0.41
1:0:40:C:H4'	40:0:6666:HOH:O	2.19	0.41
5:D:100:ASP:N	5:D:100:ASP:OD1	2.53	0.41
2:A:62:ASP:N	2:A:62:ASP:OD1	2.52	0.41
11:J:47:THR:HA	11:J:129:PHE:HA	2.01	0.41
25:X:26:ALA:HB3	25:X:63:ARG:HG3	2.02	0.41
1:0:1656:A:H2'	1:0:1657:A:O4'	2.20	0.41
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.41
1:0:1351:G:OP1	4:C:96:LYS:NZ	2.40	0.41
14:M:81:ARG:CZ	14:M:81:ARG:HB2	2.50	0.41
15:N:108:SER:HA	15:N:109:PRO:HD3	1.75	0.41
9:H:30:LYS:N	9:H:62:HIS:HD2	2.18	0.41
13:L:65:ASP:O	13:L:66:VAL:C	2.59	0.41
19:R:18:LEU:HB2	19:R:143:VAL:HG12	1.99	0.41
1:0:1688:G:C6	1:0:1692:C:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	11:J:70:PHE:HD1	1.85	0.41
3:B:215:VAL:N	3:B:220:VAL:HG22	2.35	0.41
1:0:1765:G:O2'	1:0:1766:U:H5'	2.20	0.41
2:A:135:VAL:HG11	2:A:147:ARG:HH21	1.86	0.41
25:X:47:ALA:HB1	25:X:82:GLU:HB3	2.02	0.41
25:X:43:VAL:HG12	25:X:47:ALA:HB3	2.01	0.41
1:0:308:U:C2'	21:T:52:ARG:NH2	2.83	0.41
16:O:14:LEU:HG	16:O:102:ILE:HD11	2.02	0.41
1:0:1343:C:C2'	26:Y:208:LYS:HZ1	2.33	0.41
1:0:1784:U:O2'	1:0:1812:G:H2'	2.20	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.89	0.41
1:0:1994:A:OP1	12:K:66:ARG:NH2	2.54	0.41
1:0:2112:A:H2'	1:0:2113:G:H8	1.85	0.41
19:R:92:LEU:HD23	19:R:145:LEU:CD2	2.51	0.41
7:F:70:LYS:C	7:F:72:VAL:H	2.22	0.41
3:B:66:GLU:OE1	3:B:328:ARG:HD2	2.20	0.41
1:0:287:C:H2'	1:0:288:A:H8	1.84	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.35	0.41
1:0:1355:A:H2'	1:0:1355:A:N3	2.36	0.41
1:0:1405:U:H2'	40:0:6435:HOH:O	2.20	0.41
6:E:107:PHE:C	6:E:109:GLY:N	2.74	0.41
14:M:43:PRO:HG3	14:M:62:VAL:HG21	2.02	0.41
2:A:114:ASP:OD1	2:A:115:GLY:N	2.53	0.41
1:0:1833:U:O2'	1:0:1834:C:H5'	2.20	0.41
3:B:62:ARG:HG2	3:B:62:ARG:HH11	1.85	0.41
2:A:88:ILE:CD1	2:A:100:PRO:HD3	2.43	0.41
15:N:110:THR:HA	15:N:111:PRO:HD3	1.87	0.41
1:0:1544:U:H1'	1:0:1642:A:C2	2.55	0.41
11:J:69:TYR:O	11:J:70:PHE:C	2.58	0.41
1:0:2715:G:O2'	3:B:262:ARG:HD2	2.20	0.41
2:A:76:VAL:HG23	27:Z:87:LYS:HB3	2.01	0.41
1:0:2796:U:H2'	1:0:2797:C:O5'	2.21	0.41
3:B:16:ARG:NH1	40:B:5367:HOH:O	2.52	0.41
13:L:3:LYS:O	13:L:4:LYS:C	2.59	0.41
1:0:2362:A:H8	1:0:2362:A:O5'	2.02	0.41
1:0:2818:A:O2'	3:B:96:PRO:HD2	2.20	0.41
3:B:277:GLU:N	3:B:278:PRO:HD2	2.35	0.41
26:Y:132:ASP:C	26:Y:134:HIS:N	2.72	0.41
1:0:1060:C:H2'	1:0:1061:C:H6	1.86	0.41
1:0:407:A:C2	1:0:408:A:C4	3.08	0.41
14:M:55:LYS:HZ2	14:M:146:ASP:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1930:A:H2'	1:0:1931:A:C8	2.56	0.41
25:X:73:ARG:NH1	25:X:88:GLU:HB2	2.35	0.41
9:H:114:ASP:HA	40:H:3102:HOH:O	2.19	0.41
2:A:165:THR:O	2:A:165:THR:HG22	2.19	0.41
12:K:121:PHE:CD1	12:K:121:PHE:N	2.88	0.41
1:0:1669:G:H2'	1:0:1670:A:C8	2.56	0.41
15:N:32:PRO:HD2	15:N:99:GLU:O	2.21	0.41
1:0:2379:G:H4'	1:0:2380:A:C5'	2.50	0.41
12:K:74:VAL:HG12	12:K:75:ARG:HG3	2.02	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.41
27:Z:54:GLU:HB3	27:Z:58:ASN:ND2	2.36	0.41
5:D:78:GLU:O	5:D:79:MET:C	2.59	0.41
1:0:2092:G:O3'	3:B:239:LEU:HD12	2.20	0.41
1:0:661:G:C6	1:0:662:U:C4	3.08	0.41
1:0:2372:A:H2'	1:0:2373:U:H6	1.84	0.41
1:0:154:C:C2	1:0:155:C:C5	3.08	0.41
9:H:157:TYR:C	9:H:157:TYR:HD1	2.23	0.41
21:T:89:ARG:HG3	21:T:89:ARG:O	2.20	0.41
1:0:40:C:H6	1:0:40:C:O5'	2.04	0.41
1:0:1461:U:H2'	1:0:1462:C:C6	2.56	0.41
15:N:91:ARG:O	15:N:94:GLU:HB2	2.20	0.41
13:L:22:ARG:HG3	40:L:2203:HOH:O	2.20	0.41
20:S:45:TYR:HE2	20:S:81:ILE:HG12	1.84	0.41
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.88	0.41
6:E:121:ASP:O	6:E:122:THR:C	2.59	0.41
1:0:2383:G:C6	1:0:2384:U:C4	3.08	0.41
9:H:66:GLU:O	9:H:70:LEU:HB2	2.21	0.41
1:0:2514:U:H5'	1:0:2572:G:O4'	2.21	0.41
1:0:1186:C:H42	1:0:1190:G:N2	2.19	0.41
1:0:613:C:C2	1:0:614:U:C5	3.09	0.41
1:0:1175:G:H1'	1:0:1193:A:C2'	2.47	0.41
13:L:91:VAL:HG12	13:L:120:LEU:HD23	2.02	0.41
17:P:89:ASN:HD22	17:P:89:ASN:C	2.23	0.41
1:0:960:G:N3	1:0:960:G:C2'	2.82	0.41
1:0:314:G:N2	1:0:316:A:H3'	2.36	0.41
11:J:116:LEU:HB2	11:J:119:THR:HG21	2.03	0.41
1:0:2042:U:H2'	1:0:2043:U:C6	2.56	0.41
1:0:1747:A:O3'	1:0:2584:G:H5'	2.21	0.41
3:B:277:GLU:N	3:B:278:PRO:CD	2.83	0.41
1:0:696:C:O2'	1:0:697:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:8:ARG:HG3	40:P:5725:HOH:O	2.21	0.41
1:0:814:G:C2	1:0:815:U:C2	3.08	0.41
1:0:1757:U:H6	1:0:1757:U:O5'	2.03	0.41
3:B:76:THR:N	3:B:77:PRO:HD3	2.35	0.41
6:E:86:VAL:O	6:E:86:VAL:HG13	2.21	0.41
24:W:91:ASP:HB2	40:W:5425:HOH:O	2.21	0.41
1:0:2312:G:H2'	1:0:2313:C:H5'	2.02	0.41
1:0:905:C:H3'	40:0:4139:HOH:O	2.19	0.41
1:0:2588:OMG:O6	32:4:76:5AA:H102	2.21	0.41
11:J:130:VAL:HG12	11:J:131:THR:H	1.86	0.41
1:0:2468:A:H62	30:3:50:GLY:HA2	1.86	0.41
20:S:53:ASN:N	20:S:53:ASN:ND2	2.68	0.41
24:W:4:LEU:HD22	24:W:4:LEU:HA	1.88	0.41
14:M:27:ARG:O	14:M:30:GLU:N	2.54	0.41
1:0:1662:C:H2'	1:0:1663:G:O4'	2.20	0.41
1:0:1883:U:O2'	1:0:1884:G:H5'	2.20	0.41
31:9:107:C:O2'	31:9:108:C:H5'	2.21	0.41
29:2:35:ARG:HA	29:2:39:ARG:HH22	1.84	0.41
1:0:706:G:N2	1:0:707:C:H41	2.18	0.41
19:R:15:LYS:HE3	40:R:6682:HOH:O	2.21	0.41
13:L:56:LYS:NZ	40:L:6170:HOH:O	2.53	0.41
1:0:2064:U:H4'	1:0:2652:U:O3'	2.21	0.41
1:0:2240:U:H2'	1:0:2241:C:O4'	2.21	0.41
15:N:67:ALA:HA	15:N:71:TRP:H	1.85	0.41
5:D:95:THR:C	5:D:97:GLN:N	2.74	0.41
29:2:9:LYS:HE2	29:2:9:LYS:HB3	1.86	0.41
1:0:1170:U:H1'	1:0:1172:G:N7	2.35	0.41
1:0:1551:C:H2'	1:0:1552:G:C8	2.56	0.41
3:B:294:TYR:CD1	3:B:294:TYR:C	2.93	0.41
1:0:1363:G:H1'	40:0:4299:HOH:O	2.20	0.41
1:0:941:G:O2'	1:0:942:U:H5'	2.20	0.41
16:O:97:SER:C	16:O:99:GLU:N	2.73	0.41
25:X:26:ALA:O	25:X:29:ALA:HB3	2.20	0.41
11:J:127:ILE:HG22	36:J:8801:CL:CL	2.57	0.41
12:K:99:ASP:C	12:K:99:ASP:OD1	2.59	0.41
25:X:10:VAL:HG12	25:X:11:THR:N	2.36	0.41
15:N:112:GLY:HA2	15:N:137:ALA:HB2	2.02	0.41
1:0:1871:U:O4'	1:0:1873:G:C8	2.74	0.41
12:K:2:GLU:O	12:K:3:ALA:C	2.59	0.41
1:0:569:A:H5''	1:0:587:A:N1	2.35	0.41
1:0:437:A:H3'	40:0:4828:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:142:ASP:O	17:P:143:ALA:HB3	2.21	0.41
7:F:106:ALA:O	7:F:109:GLU:HB3	2.21	0.41
1:0:2653:A:H2'	1:0:2654:C:C6	2.56	0.41
26:Y:102:LEU:O	26:Y:227:ARG:HG3	2.20	0.41
6:E:85:GLU:HG2	6:E:130:GLU:HG2	2.02	0.41
27:Z:80:GLN:HG2	27:Z:81:CYS:N	2.35	0.41
27:Z:70:ARG:NH1	27:Z:83:TYR:N	2.68	0.41
12:K:97:ILE:HG22	12:K:98:VAL:H	1.86	0.41
1:0:2421:G:H2'	40:0:8689:HOH:O	2.19	0.41
1:0:332:G:O2'	21:T:7:GLN:HG3	2.21	0.41
1:0:2032:U:C2'	1:0:2033:G:H5''	2.51	0.41
3:B:80:ARG:O	3:B:82:VAL:N	2.53	0.41
1:0:314:G:C2	1:0:317:A:C8	3.08	0.41
3:B:51:VAL:CG2	3:B:330:VAL:HG22	2.50	0.41
14:M:61:ILE:N	14:M:61:ILE:CD1	2.84	0.41
1:0:621:C:H2'	1:0:622:G:H8	1.84	0.41
9:H:119:ALA:O	9:H:120:PHE:C	2.57	0.41
1:0:445:U:H2'	1:0:446:G:C8	2.55	0.41
1:0:800:G:H2'	1:0:801:U:C6	2.56	0.41
1:0:1370:G:O5'	19:R:62:HIS:HB3	2.20	0.41
14:M:5:TYR:C	14:M:7:TYR:N	2.74	0.41
1:0:765:G:H4'	4:C:69:HIS:HB2	2.03	0.41
1:0:2238:A:O2'	1:0:2239:C:H5'	2.21	0.41
1:0:593:A:C2'	1:0:594:C:H5'	2.49	0.41
1:0:2681:A:H4'	1:0:2682:C:OP1	2.20	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.41
26:Y:105:LYS:HE2	26:Y:198:GLY:O	2.20	0.41
1:0:27:U:H2'	1:0:28:G:C8	2.56	0.41
1:0:1119:G:C5	1:0:1243:C:C4	3.08	0.41
1:0:2377:U:O2'	1:0:2378:U:H5'	2.20	0.41
1:0:1592:G:O2'	1:0:1593:C:O5'	2.39	0.41
1:0:1195:G:N2	1:0:1205:U:C2	2.89	0.41
10:I:85:GLY:C	10:I:86:GLU:HG3	2.41	0.41
15:N:37:ARG:HH21	15:N:105:GLY:CA	2.33	0.41
14:M:164:THR:CG2	14:M:166:ALA:H	2.27	0.41
7:F:63:ILE:HB	7:F:64:PRO:CD	2.43	0.41
5:D:170:TYR:O	5:D:171:ASP:CB	2.68	0.41
5:D:173:GLU:HG3	5:D:174:VAL:HG23	2.02	0.41
16:O:49:GLU:O	16:O:49:GLU:HG3	2.20	0.41
11:J:80:LYS:HE3	11:J:101:VAL:O	2.21	0.41
19:R:39:THR:HG23	19:R:107:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1853:C:O2'	2:A:217:ARG:NH2	2.54	0.41
1:0:369:G:O2'	1:0:370:G:H5'	2.21	0.41
1:0:2252:A:H2'	1:0:2253:G:H5'	2.02	0.41
15:N:10:MET:O	15:N:11:ARG:C	2.59	0.41
13:L:144:ASP:O	13:L:147:GLU:HB2	2.21	0.41
1:0:1497:G:H4'	1:0:1627:G:O2'	2.20	0.41
1:0:1896:G:C6	1:0:1897:U:C4	3.09	0.41
16:O:4:ASN:HA	16:O:5:PRO:HD3	1.95	0.41
1:0:524:A:OP1	19:R:29:LYS:NZ	2.52	0.41
1:0:2781:U:O2'	1:0:2782:G:H5'	2.20	0.41
1:0:660:A:N6	1:0:746:A:O4'	2.54	0.41
1:0:1308:A:H4'	4:C:226:GLY:HA3	2.02	0.41
15:N:154:LEU:HG	15:N:155:GLU:N	2.32	0.41
29:2:29:THR:O	29:2:30:ASP:C	2.59	0.41
6:E:24:GLY:CA	6:E:76:VAL:HB	2.49	0.41
6:E:73:PHE:O	6:E:76:VAL:HG22	2.21	0.41
1:0:2043:U:O2'	1:0:2044:G:H5'	2.21	0.41
10:I:123:VAL:C	10:I:125:GLY:N	2.74	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
9:H:141:CYS:HB2	40:H:2934:HOH:O	2.21	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.51	0.41
21:T:55:PHE:O	21:T:56:ALA:C	2.58	0.41
5:D:140:ARG:HG3	5:D:140:ARG:NH1	2.36	0.41
30:3:6:ARG:HB3	30:3:19:GLU:CD	2.41	0.41
18:Q:86:VAL:HG22	18:Q:87:THR:N	2.35	0.41
1:0:1342:C:C4	1:0:1343:C:C5	3.09	0.41
16:O:87:THR:C	16:O:89:ILE:H	2.25	0.41
24:W:117:ARG:HB2	24:W:117:ARG:NH1	2.35	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.03	0.41
1:0:2645:U:C6	1:0:2645:U:OP2	2.74	0.41
3:B:120:ASP:OD2	3:B:123:ALA:HB2	2.21	0.41
6:E:166:VAL:HG12	6:E:167:TYR:N	2.36	0.41
1:0:1809:G:H2'	1:0:1811:A:OP2	2.21	0.41
1:0:73:U:H2'	1:0:74:G:C8	2.55	0.41
1:0:175:G:O6	14:M:94:ARG:NH2	2.52	0.41
1:0:1790:C:H2'	1:0:1791:U:H6	1.85	0.41
1:0:1103:C:O2	11:J:86:MET:HG2	2.20	0.41
1:0:385:C:O5'	1:0:385:C:H6	2.03	0.41
1:0:2245:C:O5'	1:0:2245:C:H6	2.03	0.41
4:C:51:TYR:HE1	28:1:55:GLY:O	2.04	0.41
1:0:1153:C:N3	1:0:2786:G:O6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:101:THR:HG22	5:D:101:THR:O	2.20	0.41
26:Y:100:ARG:HD2	26:Y:232:THR:HB	2.02	0.41
25:X:31:ILE:O	25:X:35:GLU:HG3	2.21	0.41
30:3:25:VAL:HG22	30:3:68:LYS:CE	2.50	0.41
1:0:711:G:H1'	40:0:6793:HOH:O	2.19	0.41
1:0:2720:C:H3'	40:0:5838:HOH:O	2.21	0.41
18:Q:75:ILE:HG12	18:Q:84:ILE:CD1	2.49	0.41
30:3:69:TYR:N	30:3:69:TYR:CD1	2.89	0.41
1:0:2092:G:H5''	1:0:2613:G:OP1	2.21	0.41
14:M:48:LYS:HG3	14:M:52:GLN:HE21	1.86	0.41
1:0:168:C:O2'	1:0:169:A:H5'	2.21	0.41
22:U:30:HIS:HB3	40:U:6215:HOH:O	2.20	0.41
26:Y:127:GLN:O	26:Y:128:PHE:HB2	2.20	0.41
24:W:27:HIS:O	24:W:28:HIS:CD2	2.74	0.41
1:0:581:G:H5'	40:0:7612:HOH:O	2.21	0.41
1:0:210:U:H2'	1:0:211:U:O4'	2.20	0.41
1:0:1804:A:H2'	1:0:1805:G:H8	1.85	0.41
15:N:129:ILE:HA	15:N:130:PRO:HD3	1.98	0.41
24:W:13:MET:HE2	24:W:18:GLN:N	2.36	0.41
9:H:80:LEU:HD12	9:H:86:TYR:CD2	2.56	0.41
1:0:1316:G:H1'	1:0:1340:G:N2	2.36	0.41
11:J:62:ASP:O	11:J:63:ILE:C	2.59	0.41
1:0:2474:A:H4'	1:0:2475:C:O5'	2.21	0.41
1:0:941:G:C6	1:0:942:U:C4	3.09	0.41
3:B:69:VAL:HA	3:B:70:PRO:HD3	1.75	0.41
15:N:176:ARG:HG3	15:N:176:ARG:HH11	1.86	0.41
16:O:105:ASN:HD21	16:O:109:SER:N	2.19	0.41
1:0:625:U:H5''	1:0:1044:C:N4	2.36	0.41
1:0:1795:G:H2'	1:0:1796:A:O4'	2.21	0.41
1:0:1511:U:O2'	1:0:1512:G:H5'	2.20	0.41
1:0:2718:C:H6	1:0:2718:C:H5'	1.87	0.40
2:A:75:GLY:HA3	27:Z:86:TYR:CZ	2.56	0.40
1:0:2263:G:H4'	14:M:70:GLY:HA3	2.00	0.40
1:0:2320:U:H4'	1:0:2321:A:O4'	2.21	0.40
17:P:120:ARG:NH2	17:P:123:TYR:CD2	2.89	0.40
12:K:53:ILE:HG13	12:K:55:VAL:HG23	2.02	0.40
1:0:615:G:H2'	1:0:616:U:C6	2.57	0.40
40:0:4400:HOH:O	27:Z:37:ARG:HD2	2.21	0.40
22:U:9:CYS:CA	22:U:52:THR:HG23	2.46	0.40
3:B:202:VAL:HA	3:B:310:ARG:O	2.22	0.40
1:0:2839:C:H2'	1:0:2840:A:H5''	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:845:U:OP1	28:1:5:THR:OG1	2.37	0.40
19:R:69:LYS:HB2	19:R:72:VAL:HG23	2.04	0.40
1:0:1342:C:H2'	1:0:1343:C:H5'	2.02	0.40
1:0:2896:A:H5'	40:0:5399:HOH:O	2.21	0.40
1:0:2088:C:H1'	1:0:2841:A:N1	2.36	0.40
19:R:63:ASN:O	19:R:64:SER:C	2.59	0.40
25:X:73:ARG:HH12	25:X:88:GLU:HB2	1.86	0.40
30:3:86:GLY:HA2	40:3:3274:HOH:O	2.21	0.40
6:E:97:VAL:HG12	40:E:4191:HOH:O	2.21	0.40
15:N:82:TYR:CD2	15:N:82:TYR:C	2.94	0.40
27:Z:56:GLU:CD	27:Z:94:LYS:HZ2	2.25	0.40
40:0:3623:HOH:O	7:F:31:LYS:HD2	2.20	0.40
25:X:36:HIS:CE1	25:X:40:HIS:CD2	3.09	0.40
1:0:1263:C:H5'	24:W:118:LEU:O	2.21	0.40
40:0:3518:HOH:O	15:N:21:HIS:HD2	2.02	0.40
1:0:401:C:H1'	14:M:92:THR:OG1	2.21	0.40
1:0:2408:A:H4'	30:3:15:ASN:C	2.42	0.40
1:0:170:U:H4'	30:3:48:ASN:O	2.22	0.40
19:R:39:THR:CG2	19:R:42:GLU:HG3	2.51	0.40
13:L:110:GLY:N	13:L:129:ALA:HB2	2.36	0.40
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.40
40:0:6597:HOH:O	18:Q:16:ASN:HB2	2.21	0.40
1:0:1598:A:N6	36:0:8815:CL:CL	2.91	0.40
28:1:28:HIS:ND1	28:1:31:LYS:HE2	2.36	0.40
10:I:127:CYS:N	40:I:5371:HOH:O	2.53	0.40
1:0:1508:C:H5'	20:S:21:GLN:HE22	1.85	0.40
16:O:26:TRP:CE3	16:O:26:TRP:HA	2.56	0.40
2:A:172:ALA:O	2:A:173:GLY:C	2.58	0.40
40:0:7968:HOH:O	4:C:81:PRO:HD3	2.20	0.40
1:0:29:C:O2'	1:0:30:U:H5'	2.21	0.40
1:0:2636:C:H1'	40:0:3790:HOH:O	2.20	0.40
15:N:72:GLU:HG2	15:N:163:PHE:HD1	1.87	0.40
31:9:86:G:C2	31:9:88:G:C8	3.10	0.40
13:L:106:VAL:O	13:L:123:ASP:HB2	2.21	0.40
1:0:2039:A:H2'	1:0:2040:C:C6	2.56	0.40
1:0:2761:A:C4	1:0:2763:G:C8	3.09	0.40
1:0:731:U:O2'	1:0:732:C:H5'	2.21	0.40
1:0:1644:C:H2'	1:0:1645:U:H6	1.86	0.40
11:J:115:VAL:HG12	11:J:115:VAL:O	2.21	0.40
1:0:2608:C:H2'	40:0:8118:HOH:O	2.21	0.40
1:0:1139:U:H2'	1:0:1140:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:61:THR:O	24:W:62:LEU:C	2.59	0.40
11:J:92:GLN:O	11:J:93:ARG:C	2.59	0.40
38:0:2924:MYL:CAL	30:3:51:LYS:O	2.70	0.40
1:0:2459:G:H2'	38:0:2924:MYL:HAA	2.04	0.40
38:0:2924:MYL:HAC	38:0:2924:MYL:HADA	1.86	0.40
15:N:15:GLU:O	15:N:16:ALA:HB3	2.22	0.40
1:0:2504:A:H2'	1:0:2505:G:O4'	2.21	0.40
1:0:2512:U:H4'	1:0:2514:U:O4	2.21	0.40
1:0:189:A:OP1	14:M:171:ARG:NH2	2.54	0.40
7:F:50:VAL:CG1	7:F:60:VAL:HG11	2.50	0.40
3:B:309:VAL:O	3:B:310:ARG:HG2	2.20	0.40
5:D:173:GLU:CG	5:D:174:VAL:H	2.29	0.40
1:0:1758:U:H2'	1:0:1759:A:O4'	2.21	0.40
12:K:82:ARG:HH21	12:K:115:ARG:HG2	1.84	0.40
15:N:18:THR:HG21	40:9:5071:HOH:O	2.21	0.40
18:Q:75:ILE:HD12	18:Q:75:ILE:C	2.42	0.40
1:0:2353:A:O2'	15:N:7:LYS:HB3	2.21	0.40
3:B:254:GLN:NE2	40:B:4243:HOH:O	2.54	0.40
7:F:38:LYS:NZ	14:M:3:SER:HA	2.36	0.40
1:0:1398:G:H2'	1:0:1399:A:H8	1.83	0.40
1:0:154:C:O2'	1:0:155:C:H5'	2.21	0.40
1:0:2050:G:H4'	19:R:82:GLU:HG2	2.03	0.40
26:Y:132:ASP:C	26:Y:134:HIS:H	2.24	0.40
5:D:56:ARG:N	40:D:6752:HOH:O	2.54	0.40
1:0:2103:A:O2'	1:0:2104:C:H5'	2.21	0.40
25:X:26:ALA:HB2	25:X:63:ARG:HA	2.02	0.40
1:0:1847:A:OP1	2:A:175:LYS:HG3	2.21	0.40
1:0:2059:U:H2'	1:0:2060:A:C8	2.56	0.40
1:0:965:A:C2	1:0:1004:C:C2	3.09	0.40
1:0:1888:C:H2'	1:0:1889:C:O4'	2.20	0.40
26:Y:130:ARG:HD2	40:Y:3314:HOH:O	2.21	0.40
1:0:1711:A:H3'	40:0:5721:HOH:O	2.21	0.40
1:0:2618:G:O6	1:0:2619:UR3:H3U2	2.22	0.40
31:9:57:A:H2'	31:9:58:G:C5'	2.52	0.40
14:M:125:ARG:O	14:M:126:GLN:HB3	2.22	0.40
1:0:2408:A:O3'	30:3:16:GLU:HA	2.21	0.40
25:X:84:ILE:C	25:X:85:VAL:CG2	2.89	0.40
15:N:12:ARG:NH2	31:9:6:C:C5	2.90	0.40
1:0:421:C:H4'	1:0:1919:A:N6	2.36	0.40
1:0:1187:U:HO2'	1:0:1189:A:H2	1.70	0.40
3:B:8:LYS:HG3	3:B:220:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2582:G:O3'	12:K:41:LYS:HA	2.21	0.40
10:I:127:CYS:C	10:I:129:SER:N	2.74	0.40
26:Y:117:LEU:HD12	26:Y:174:VAL:CG1	2.50	0.40
1:0:319:A:H2'	1:0:320:G:H8	1.86	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
1:0:47:G:N3	1:0:114:A:C2	2.90	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.40
1:0:2829:G:O2'	1:0:2830:U:H5'	2.22	0.40
15:N:159:TYR:CE1	31:9:50:G:H5''	2.56	0.40
1:0:1314:U:H2'	40:0:5081:HOH:O	2.21	0.40
1:0:812:A:H2'	1:0:813:C:C6	2.56	0.40
1:0:801:U:O4'	17:P:128:GLY:HA3	2.22	0.40
1:0:238:C:H4'	1:0:287:C:OP1	2.21	0.40
6:E:86:VAL:CG1	6:E:129:GLU:HA	2.51	0.40
1:0:234:A:H4'	1:0:437:A:O4'	2.21	0.40
1:0:1103:C:C2	1:0:1241:G:N2	2.90	0.40
1:0:1482:A:O2'	1:0:1483:C:H5'	2.21	0.40
3:B:83:ALA:HA	3:B:100:VAL:O	2.21	0.40
6:E:61:THR:O	6:E:62:ILE:C	2.59	0.40
6:E:119:HIS:O	6:E:140:ALA:HB1	2.20	0.40
1:0:529:G:C5	1:0:530:C:C5	3.09	0.40
1:0:1276:U:H3'	16:O:19:ARG:NH1	2.36	0.40
40:M:1445:HOH:O	30:3:46:ILE:HG12	2.21	0.40
1:0:2408:A:H1'	30:3:10:TYR:CD1	2.57	0.40
21:T:71:VAL:HG12	21:T:72:ILE:N	2.37	0.40
23:V:1:THR:CG2	23:V:2:VAL:N	2.77	0.40
3:B:26:PHE:HD2	3:B:312:ARG:NH2	2.19	0.40
10:I:92:VAL:N	10:I:131:GLY:O	2.55	0.40
1:0:100:C:H2'	1:0:101:C:C6	2.52	0.40
5:D:99:ASP:N	5:D:103:ASN:O	2.49	0.40
1:0:1544:U:H1'	1:0:1642:A:N1	2.37	0.40
1:0:1121:G:H21	1:0:1248:A:C4'	2.35	0.40
1:0:1228:C:H2'	1:0:1229:C:O4'	2.22	0.40
4:C:116:ALA:C	4:C:118:THR:N	2.75	0.40
1:0:2750:G:H2'	1:0:2751:C:C6	2.56	0.40
1:0:1926:G:C2	1:0:1927:A:C4	3.10	0.40
16:O:81:PHE:CD1	16:O:81:PHE:N	2.90	0.40
1:0:2478:U:H2'	1:0:2479:A:C8	2.56	0.40
1:0:1523:G:C6	1:0:1524:U:C4	3.09	0.40
1:0:2102:G:N2	1:0:2104:C:C2	2.90	0.40
1:0:1483:C:O2'	1:0:1484:G:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1196:C:H2'	1:0:1197:G:H5'	2.03	0.40
1:0:60:A:C2	1:0:61:G:C8	3.09	0.40
1:0:497:A:H5''	40:0:8141:HOH:O	2.21	0.40
1:0:318:U:H5'	1:0:339:A:C2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	1.73	0.47

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	235/240 (98%)	193 (82%)	32 (14%)	10 (4%)	3	19
3	B	335/338 (99%)	285 (85%)	38 (11%)	12 (4%)	4	24
4	C	244/246 (99%)	204 (84%)	35 (14%)	5 (2%)	9	39
5	D	134/177 (76%)	91 (68%)	33 (25%)	10 (8%)	1	7
6	E	170/178 (96%)	149 (88%)	20 (12%)	1 (1%)	30	70
7	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	2	11
8	G	25/348 (7%)	18 (72%)	6 (24%)	1 (4%)	4	21
9	H	156/174 (90%)	134 (86%)	15 (10%)	7 (4%)	3	18
10	I	68/162 (42%)	43 (63%)	20 (29%)	5 (7%)	1	7
11	J	140/145 (97%)	120 (86%)	15 (11%)	5 (4%)	4	24
12	K	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	13	47
13	L	141/165 (86%)	105 (74%)	31 (22%)	5 (4%)	4	25
14	M	192/194 (99%)	153 (80%)	29 (15%)	10 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	184/187 (98%)	147 (80%)	27 (15%)	10 (5%)	2	14
16	O	113/116 (97%)	89 (79%)	23 (20%)	1 (1%)	21	62
17	P	141/149 (95%)	118 (84%)	20 (14%)	3 (2%)	9	38
18	Q	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	2	14
19	R	148/155 (96%)	130 (88%)	16 (11%)	2 (1%)	14	49
20	S	79/85 (93%)	66 (84%)	12 (15%)	1 (1%)	15	51
21	T	117/120 (98%)	99 (85%)	15 (13%)	3 (3%)	7	32
22	U	51/66 (77%)	43 (84%)	6 (12%)	2 (4%)	4	22
23	V	63/71 (89%)	52 (82%)	11 (18%)	0	100	100
24	W	152/154 (99%)	121 (80%)	27 (18%)	4 (3%)	7	32
25	X	80/92 (87%)	65 (81%)	13 (16%)	2 (2%)	7	33
26	Y	140/241 (58%)	126 (90%)	13 (9%)	1 (1%)	26	67
27	Z	71/116 (61%)	58 (82%)	10 (14%)	3 (4%)	3	20
28	1	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
29	2	42/50 (84%)	34 (81%)	7 (17%)	1 (2%)	7	34
30	3	90/92 (98%)	64 (71%)	23 (26%)	3 (3%)	5	26
All	All	3705/4466 (83%)	3039 (82%)	545 (15%)	121 (3%)	5	26

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	36	ASP
2	A	37	VAL
3	B	184	ASP
3	B	206	THR
4	C	8	LEU
5	D	16	PRO
5	D	137	PRO
7	F	101	ALA
9	H	70	LEU
10	I	107	LYS
14	M	82	ARG
15	N	154	LEU
15	N	184	ILE
17	P	116	SER
24	W	36	PRO

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Mol	Chain	Res	Type
27	Z	105	ARG
30	3	74	CYS
2	A	74	VAL
3	B	169	GLY
4	C	15	GLU
5	D	79	MET
6	E	151	LEU
7	F	59	ILE
7	F	92	GLY
8	G	72	ASP
9	H	41	LYS
13	L	21	ARG
14	M	35	GLY
14	M	79	ALA
17	P	139	ARG
18	Q	48	PRO
18	Q	78	GLY
20	S	57	THR
21	T	46	ASP
21	T	53	GLY
22	U	11	THR
24	W	49	ASN
25	X	70	ILE
25	X	87	ALA
26	Y	157	ILE
27	Z	64	PRO
30	3	25	VAL
2	A	15	THR
2	A	34	ASP
3	B	107	SER
4	C	142	ASP
5	D	96	SER
5	D	138	GLY
5	D	171	ASP
7	F	61	MET
7	F	100	ASP
9	H	71	SER
10	I	75	LYS
10	I	106	GLN
11	J	7	ASP
11	J	78	ILE
12	K	127	ALA

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Mol	Chain	Res	Type
13	L	18	HIS
13	L	35	ARG
13	L	105	TYR
14	M	6	SER
14	M	76	ARG
15	N	12	ARG
15	N	27	LEU
15	N	61	ALA
15	N	164	ASP
19	R	40	ALA
24	W	72	PRO
24	W	89	ASP
29	2	37	HIS
2	A	119	ALA
3	B	245	SER
5	D	164	ALA
5	D	173	GLU
9	H	143	VAL
12	K	126	SER
13	L	101	ASP
14	M	88	VAL
15	N	139	TRP
15	N	167	ASP
22	U	46	ALA
2	A	14	SER
2	A	208	HIS
3	B	2	GLN
3	B	34	GLY
3	B	81	ALA
3	B	121	PRO
5	D	168	SER
5	D	170	TYR
7	F	44	SER
7	F	71	GLY
9	H	82	GLU
11	J	18	ILE
11	J	76	ASP
11	J	89	HIS
14	M	15	PRO
14	M	49	ALA
14	M	110	PRO
15	N	65	ASP

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Mol	Chain	Res	Type
16	O	17	ALA
18	Q	23	THR
2	A	232	ARG
3	B	182	VAL
3	B	291	ASP
4	C	13	ASP
10	I	124	VAL
10	I	133	THR
14	M	78	LYS
17	P	19	ASN
30	3	3	MET
3	B	181	ILE
4	C	136	VAL
15	N	109	PRO
19	R	106	GLY
2	A	150	PRO
9	H	58	VAL
9	H	171	GLY
18	Q	18	PRO
21	T	40	VAL
18	Q	22	GLY
27	Z	39	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	179/182 (98%)	170 (95%)	9 (5%)	30	68
3	B	282/283 (100%)	264 (94%)	18 (6%)	22	57
4	C	193/193 (100%)	174 (90%)	19 (10%)	10	35
5	D	117/148 (79%)	111 (95%)	6 (5%)	29	66
6	E	152/156 (97%)	145 (95%)	7 (5%)	33	70
7	F	93/94 (99%)	92 (99%)	1 (1%)	80	93
8	G	27/282 (10%)	26 (96%)	1 (4%)	41	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	134/143 (94%)	128 (96%)	6 (4%)	34	71
10	I	58/130 (45%)	56 (97%)	2 (3%)	44	79
11	J	118/121 (98%)	114 (97%)	4 (3%)	44	79
12	K	106/106 (100%)	101 (95%)	5 (5%)	32	70
13	L	113/127 (89%)	103 (91%)	10 (9%)	12	43
14	M	158/158 (100%)	153 (97%)	5 (3%)	46	80
15	N	149/150 (99%)	139 (93%)	10 (7%)	20	56
16	O	93/94 (99%)	90 (97%)	3 (3%)	46	80
17	P	113/117 (97%)	106 (94%)	7 (6%)	23	59
18	Q	79/80 (99%)	78 (99%)	1 (1%)	76	91
19	R	117/122 (96%)	112 (96%)	5 (4%)	35	73
20	S	71/74 (96%)	68 (96%)	3 (4%)	36	73
21	T	105/106 (99%)	98 (93%)	7 (7%)	20	56
22	U	44/52 (85%)	44 (100%)	0	100	100
23	V	51/57 (90%)	51 (100%)	0	100	100
24	W	130/130 (100%)	123 (95%)	7 (5%)	27	64
25	X	66/74 (89%)	60 (91%)	6 (9%)	12	40
26	Y	120/196 (61%)	116 (97%)	4 (3%)	45	79
27	Z	60/94 (64%)	59 (98%)	1 (2%)	68	89
28	1	46/47 (98%)	45 (98%)	1 (2%)	60	86
29	2	42/46 (91%)	40 (95%)	2 (5%)	31	69
30	3	79/79 (100%)	76 (96%)	3 (4%)	40	76
All	All	3095/3641 (85%)	2942 (95%)	153 (5%)	31	69

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	33	GLU
2	A	62	ASP
2	A	78	ASP
2	A	94	LEU
2	A	131	HIS
2	A	153	ARG

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Mol	Chain	Res	Type
2	A	179	MET
2	A	217	ARG
3	B	7	ARG
3	B	11	LEU
3	B	27	ASN
3	B	28	SER
3	B	49	THR
3	B	97	LEU
3	B	103	ASP
3	B	132	HIS
3	B	162	MET
3	B	175	LEU
3	B	190	MET
3	B	234	ARG
3	B	251	VAL
3	B	254	GLN
3	B	277	GLU
3	B	304	PRO
3	B	312	ARG
3	B	324	ASP
4	C	2	GLN
4	C	27	ARG
4	C	46	TYR
4	C	87	ARG
4	C	91	PRO
4	C	101	ASP
4	C	131	PHE
4	C	135	GLU
4	C	143	ASP
4	C	151	GLN
4	C	184	ARG
4	C	187	ARG
4	C	198	ASP
4	C	223	LEU
4	C	233	THR
4	C	234	VAL
4	C	235	PHE
4	C	236	THR
4	C	240	LEU
5	D	24	HIS
5	D	50	VAL
5	D	100	ASP

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Mol	Chain	Res	Type
5	D	131	THR
5	D	137	PRO
5	D	170	TYR
6	E	7	ILE
6	E	15	GLN
6	E	16	ASP
6	E	116	THR
6	E	126	ILE
6	E	155	ASN
6	E	164	ASP
7	F	68	ASP
8	G	73	ASP
9	H	13	ASP
9	H	42	ASP
9	H	62	HIS
9	H	87	LYS
9	H	91	ARG
9	H	157	TYR
10	I	76	ASP
10	I	94	ASP
11	J	39	VAL
11	J	52	GLN
11	J	74	ARG
11	J	107	ASN
12	K	4	LEU
12	K	7	ASP
12	K	10	GLN
12	K	16	SER
12	K	83	PRO
13	L	18	HIS
13	L	26	HIS
13	L	35	ARG
13	L	40	PHE
13	L	70	ASP
13	L	80	ASP
13	L	99	GLU
13	L	127	GLU
13	L	140	VAL
13	L	148	GLU
14	M	46	LEU
14	M	68	ARG
14	M	88	VAL

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Mol	Chain	Res	Type
14	M	99	ARG
14	M	120	VAL
15	N	12	ARG
15	N	17	ARG
15	N	23	ARG
15	N	26	LEU
15	N	47	LEU
15	N	93	GLN
15	N	124	ASP
15	N	127	LEU
15	N	135	VAL
15	N	173	ASP
16	O	3	THR
16	O	67	SER
16	O	81	PHE
17	P	52	LYS
17	P	73	HIS
17	P	89	ASN
17	P	91	LYS
17	P	94	TRP
17	P	98	ILE
17	P	110	ASP
18	Q	35	ASP
19	R	39	THR
19	R	82	GLU
19	R	119	VAL
19	R	142	ASP
19	R	143	VAL
20	S	30	ASP
20	S	53	ASN
20	S	55	GLN
21	T	5	ASP
21	T	39	ASN
21	T	73	HIS
21	T	86	GLU
21	T	89	ARG
21	T	96	VAL
21	T	117	ASP
24	W	4	LEU
24	W	38	THR
24	W	88	THR
24	W	90	TYR

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Mol	Chain	Res	Type
24	W	120	PRO
24	W	125	HIS
24	W	146	ILE
25	X	15	ARG
25	X	27	ASP
25	X	46	ASP
25	X	56	GLU
25	X	79	GLU
25	X	88	GLU
26	Y	169	ARG
26	Y	189	ASN
26	Y	203	VAL
26	Y	235	GLU
27	Z	70	ARG
28	1	5	THR
29	2	16	ASN
29	2	18	ASN
30	3	17	HIS
30	3	34	LYS
30	3	51	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	29	HIS
2	A	47	HIS
2	A	92	ASN
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	39	GLN
3	B	106	HIS
3	B	145	HIS
3	B	221	GLN
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
4	C	2	GLN
4	C	11	ASN
4	C	73	GLN
4	C	129	HIS
4	C	151	GLN

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Mol	Chain	Res	Type
5	D	29	HIS
5	D	47	GLN
5	D	133	ASN
6	E	55	ASN
6	E	74	HIS
6	E	90	HIS
6	E	106	ASN
6	E	143	GLN
7	F	80	GLN
8	G	17	GLN
8	G	64	ASN
9	H	34	HIS
9	H	49	GLN
9	H	59	GLN
9	H	62	HIS
10	I	88	GLN
10	I	106	GLN
11	J	25	GLN
11	J	40	ASN
11	J	52	GLN
11	J	107	ASN
11	J	126	ASN
12	K	10	GLN
12	K	44	HIS
12	K	67	GLN
13	L	18	HIS
13	L	20	ASN
13	L	41	HIS
13	L	42	ASN
13	L	43	HIS
13	L	58	GLN
14	M	24	GLN
14	M	52	GLN
14	M	58	GLN
14	M	77	HIS
14	M	86	GLN
14	M	98	GLN
14	M	170	ASN
15	N	93	GLN
15	N	107	ASN
16	O	91	GLN
17	P	28	GLN

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Mol	Chain	Res	Type
17	P	50	GLN
17	P	66	GLN
17	P	88	GLN
17	P	89	ASN
17	P	118	GLN
18	Q	16	ASN
18	Q	27	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	123	GLN
20	S	25	GLN
20	S	44	GLN
20	S	53	ASN
20	S	55	GLN
21	T	39	ASN
21	T	43	ASN
22	U	39	ASN
22	U	48	ASN
23	V	4	HIS
23	V	29	ASN
23	V	34	GLN
23	V	60	GLN
24	W	27	HIS
24	W	28	HIS
24	W	59	GLN
24	W	110	GLN
24	W	119	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	149	GLN
26	Y	189	ASN
27	Z	61	HIS
28	1	8	GLN
28	1	16	HIS
29	2	16	ASN
29	2	18	ASN
29	2	36	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	8	ASN

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Mol	Chain	Res	Type
30	3	13	HIS
30	3	15	ASN
30	3	30	GLN
30	3	43	ASN
30	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	248 (9%)	18 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/8 (12%)	0	0
All	All	2867/3053 (93%)	266 (9%)	19 (0%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	204	A
1	0	219	G
1	0	237	G

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Mol	Chain	Res	Type
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	368	C
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U

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Mol	Chain	Res	Type
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A

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Mol	Chain	Res	Type
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1474	C
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C

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Mol	Chain	Res	Type
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2104	C
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A

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Mol	Chain	Res	Type
1	0	2317	C
1	0	2321	A
1	0	2322	U
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2570	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2607	U
1	0	2608	C
1	0	2609	G
1	0	2613	G
1	0	2637	A
1	0	2638	G
1	0	2644	C
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G

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Mol	Chain	Res	Type
1	0	2762	C
1	0	2768	A
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2912	C
1	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	603	A
1	0	604	G
1	0	644	G
1	0	699	C

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Mol	Chain	Res	Type
1	0	834	G
1	0	857	A
1	0	871	G
1	0	1352	A
1	0	2011	A
1	0	2103	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2718	C
1	0	2726	U
1	0	2791	U
31	9	65	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	0	2587	1,35	12,22,23	1.05	1 (8%)	19,31,34	3.17	2 (10%)
1	OMG	0	2588	1,32	17,26,27	0.95	1 (5%)	21,38,41	2.52	3 (14%)
1	UR3	0	2619	1	12,22,23	0.77	0	16,32,35	0.75	0
1	PSU	0	2621	1	13,21,22	1.67	2 (15%)	18,30,33	6.10	3 (16%)
1	1MA	0	628	1	14,25,26	1.04	1 (7%)	15,37,40	1.16	1 (6%)
32	5AA	4	76	1,32	16,26,27	0.65	0	15,38,41	1.22	2 (13%)

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
1	OMU	0	2587	1,35	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,32	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
32	5AA	4	76	1,32	-	0/7/29/30	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.00	1.47	1.52
1	0	2587	OMU	C4-N3	2.59	1.37	1.33
1	0	2621	PSU	C4-N3	2.71	1.38	1.33
1	0	2588	OMG	C6-N1	2.83	1.38	1.33
1	0	628	1MA	C6-N6	2.85	1.34	1.29

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.39	114.69	128.33
1	0	2588	OMG	C5-C6-N1	-8.63	111.78	123.59
1	0	628	1MA	C2-N3-C4	-3.60	110.82	116.40
1	0	2587	OMU	C5-C4-N3	-3.34	114.54	123.12
1	0	2588	OMG	N3-C2-N1	-2.26	124.00	127.44
32	4	76	5AA	C9-N6-C6	2.13	126.20	119.48
1	0	2621	PSU	C6-N1-C2	2.68	119.79	115.47
32	4	76	5AA	C2-N1-C6	3.58	119.04	111.43
1	0	2588	OMG	C6-N1-C2	6.63	125.14	115.94
1	0	2587	OMU	C4-N3-C2	13.21	127.22	114.14
1	0	2621	PSU	C4-N3-C2	13.72	127.10	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	5	0
1	0	2619	UR3	1	0
1	0	2621	PSU	1	0
32	4	76	5AA	10	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
38	MYL	0	2924	-	35,37,37	1.19	2 (5%)	38,56,56	1.74	11 (28%)

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
38	MYL	0	2924	-	-	2/21/77/77	1/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	MYL	CAA-CAV	2.66	1.39	1.32
38	0	2924	MYL	CBC-NAP	5.25	1.49	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	CAN-CBH-CBB	-3.13	109.52	113.40
38	0	2924	MYL	OAR-CBC-CBG	-2.91	104.64	109.64
38	0	2924	MYL	CAO-CBA-CBE	-2.89	109.64	114.79
38	0	2924	MYL	CAB-OAQ-CBH	-2.22	110.45	116.36
38	0	2924	MYL	OAS-CBF-CBG	-2.13	106.40	110.23
38	0	2924	MYL	CAD-CAZ-CAY	-2.07	109.90	112.87
38	0	2924	MYL	CAC-CAY-CAZ	-2.04	110.94	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	CBC-NAP-CAW	2.87	126.58	122.67
38	0	2924	MYL	OAR-CBC-NAP	2.98	110.89	107.29
38	0	2924	MYL	CAN-CAV-CAZ	3.44	116.96	112.12
38	0	2924	MYL	OAT-CAY-CAC	4.02	110.94	105.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	OAG-CAW-NAP-CBC
38	0	2924	MYL	CBB-CAW-NAP-CBC

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	CAM-CBC-CBF-CBG-OAR-OAS

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	MYL	22	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	0	2749/2923 (94%)	-0.34	5 (0%) 95 91	31, 61, 109, 181	0
2	A	237/240 (98%)	0.00	5 (2%) 67 45	37, 75, 110, 131	0
3	B	337/338 (99%)	-0.39	0 100 100	37, 65, 93, 103	0
4	C	246/246 (100%)	-0.29	0 100 100	34, 60, 84, 96	0
5	D	140/177 (79%)	1.01	26 (18%) 2 1	80, 118, 140, 148	0
6	E	172/178 (96%)	-0.23	0 100 100	54, 81, 102, 112	0
7	F	119/120 (99%)	0.17	2 (1%) 73 53	65, 93, 121, 135	0
8	G	29/348 (8%)	0.39	1 (3%) 49 25	86, 102, 109, 114	0
9	H	160/174 (91%)	0.13	5 (3%) 52 28	58, 79, 111, 121	0
10	I	70/162 (43%)	1.98	33 (47%) 0 0	137, 154, 180, 181	0
11	J	142/145 (97%)	-0.43	0 100 100	48, 63, 82, 98	0
12	K	132/132 (100%)	-0.28	0 100 100	46, 63, 88, 95	0
13	L	145/165 (87%)	0.21	6 (4%) 41 19	38, 86, 124, 133	0
14	M	194/194 (100%)	0.24	19 (9%) 10 3	38, 60, 136, 151	0
15	N	186/187 (99%)	0.24	6 (3%) 51 27	65, 89, 138, 146	0
16	O	115/116 (99%)	-0.33	0 100 100	51, 70, 84, 91	0
17	P	143/149 (95%)	-0.12	1 (0%) 89 79	52, 69, 87, 93	0
18	Q	95/96 (98%)	-0.15	0 100 100	51, 62, 77, 85	0
19	R	150/155 (96%)	-0.39	0 100 100	42, 56, 77, 89	0
20	S	81/85 (95%)	-0.09	1 (1%) 81 65	57, 76, 99, 111	0
21	T	119/120 (99%)	-0.00	2 (1%) 73 53	55, 73, 106, 125	0
22	U	53/66 (80%)	1.65	19 (35%) 0 0	95, 117, 133, 135	0
23	V	65/71 (91%)	0.84	10 (15%) 3 1	65, 90, 140, 144	0
24	W	154/154 (100%)	-0.23	2 (1%) 79 63	46, 62, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/92 (89%)	-0.01	3 (3%) 45 22	52, 70, 88, 105	0
26	Y	142/241 (58%)	-0.41	1 (0%) 89 79	39, 58, 80, 99	0
27	Z	73/116 (62%)	5.07	46 (63%) 0 0	107, 143, 170, 176	0
28	1	56/57 (98%)	-0.21	0 100 100	34, 47, 58, 62	0
29	2	46/50 (92%)	0.17	3 (6%) 22 8	47, 80, 113, 121	0
30	3	92/92 (100%)	7.73	90 (97%) 0 0	164, 175, 184, 189	0
31	9	122/122 (100%)	-0.56	1 (0%) 87 75	52, 86, 113, 166	0
32	4	5/8 (62%)	1.36	0 100 100	41, 43, 47, 47	0
All	All	6651/7519 (88%)	0.02	287 (4%) 39 18	31, 67, 132, 189	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	24.8
30	3	82	GLY	24.3
27	Z	35	SER	23.2
27	Z	58	ASN	21.8
27	Z	46	SER	20.9
30	3	30	GLN	19.9
30	3	62	THR	19.1
30	3	33	MET	16.1
30	3	38	ARG	15.6
30	3	31	THR	14.6
30	3	32	GLY	14.6
27	Z	36	GLY	14.3
30	3	44	SER	13.6
30	3	35	TRP	13.4
27	Z	49	ARG	13.2
30	3	58	GLY	13.2
30	3	14	CYS	13.1
30	3	39	GLN	12.5
27	Z	50	VAL	12.2
30	3	40	ARG	12.2
30	3	78	HIS	11.3
27	Z	48	ARG	11.2
27	Z	45	VAL	11.0
27	Z	39	GLY	10.8
30	3	72	GLY	10.5
30	3	41	GLU	10.1

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Mol	Chain	Res	Type	RSRZ
30	3	56	PRO	10.0
30	3	52	PHE	10.0
27	Z	44	ARG	9.9
27	Z	51	ALA	9.9
30	3	77	ALA	9.9
30	3	86	GLY	9.8
30	3	57	GLY	9.7
30	3	15	ASN	9.5
30	3	11	CYS	9.5
27	Z	54	GLU	9.5
30	3	13	HIS	9.4
14	M	77	HIS	9.4
30	3	42	ARG	9.3
27	Z	55	SER	9.2
30	3	25	VAL	9.1
30	3	36	ILE	9.1
30	3	71	CYS	9.1
30	3	48	ASN	8.8
30	3	66	ASP	8.8
27	Z	42	TYR	8.8
30	3	34	LYS	8.7
30	3	45	GLY	8.7
30	3	68	LYS	8.4
14	M	70	GLY	8.2
30	3	37	ASP	8.2
30	3	3	MET	8.1
27	Z	38	PHE	8.1
27	Z	57	MET	8.1
30	3	83	TRP	8.1
30	3	23	GLU	8.0
30	3	20	HIS	7.9
27	Z	53	ILE	7.9
30	3	22	VAL	7.8
30	3	64	LYS	7.8
14	M	71	SER	7.7
27	Z	56	GLU	7.6
27	Z	47	ARG	7.4
30	3	43	ASN	7.3
30	3	27	SER	7.3
30	3	1	MET	7.3
30	3	70	ARG	7.2
30	3	74	CYS	7.1

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Mol	Chain	Res	Type	RSRZ
30	3	67	LEU	7.0
27	Z	43	GLY	6.8
27	Z	70	ARG	6.8
30	3	9	THR	6.8
30	3	53	SER	6.8
30	3	69	TYR	6.8
30	3	59	ASP	6.7
30	3	76	LYS	6.7
30	3	84	ARG	6.6
30	3	47	GLY	6.6
30	3	81	GLU	6.4
27	Z	52	GLU	6.4
30	3	8	ASN	6.3
30	3	63	LYS	6.3
30	3	65	THR	6.2
30	3	29	ARG	6.1
27	Z	63	CYS	6.1
14	M	89	THR	6.0
22	U	55	ALA	6.0
27	Z	80	GLN	6.0
30	3	91	GLN	5.8
30	3	73	GLU	5.8
30	3	21	GLU	5.7
20	S	81	ILE	5.7
27	Z	68	GLU	5.7
30	3	46	ILE	5.7
30	3	19	GLU	5.7
5	D	26	GLY	5.7
27	Z	59	GLU	5.7
23	V	1	THR	5.6
14	M	90	ARG	5.5
10	I	73	LEU	5.4
30	3	16	GLU	5.4
10	I	71	ALA	5.3
14	M	80	GLY	5.3
30	3	51	LYS	5.3
27	Z	81	CYS	5.2
22	U	52	THR	5.2
30	3	80	ARG	5.2
5	D	40	ILE	5.2
30	3	17	HIS	5.2
14	M	78	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
10	I	70	THR	5.1
30	3	12	PRO	5.1
30	3	10	TYR	5.1
14	M	87	GLY	5.1
30	3	18	GLN	5.0
30	3	2	GLN	5.0
10	I	72	GLU	5.0
23	V	43	PRO	5.0
31	9	1	U	4.9
27	Z	60	ASP	4.9
27	Z	69	ASP	4.8
5	D	57	THR	4.7
10	I	74	ILE	4.7
30	3	61	PRO	4.7
14	M	86	GLN	4.7
30	3	85	ALA	4.7
14	M	81	ARG	4.7
30	3	50	GLY	4.7
30	3	49	ASP	4.6
23	V	41	GLU	4.5
14	M	76	ARG	4.4
30	3	92	GLU	4.3
10	I	66	GLY	4.3
22	U	48	ASN	4.3
5	D	18	ILE	4.2
22	U	9	CYS	4.1
10	I	76	ASP	4.1
30	3	60	LYS	4.1
27	Z	62	ALA	4.1
27	Z	37	ARG	4.1
23	V	39	ALA	4.1
27	Z	67	GLY	4.1
30	3	26	ARG	4.0
22	U	10	GLY	4.0
30	3	6	ARG	3.9
27	Z	77	GLY	3.9
30	3	55	VAL	3.9
15	N	95	ALA	3.9
27	Z	74	GLN	3.8
10	I	68	PRO	3.8
2	A	237	GLY	3.7
10	I	97	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
10	I	128	THR	3.7
14	M	88	VAL	3.6
10	I	109	PRO	3.5
30	3	24	LYS	3.5
30	3	4	PRO	3.5
5	D	44	ILE	3.5
30	3	87	ARG	3.5
30	3	75	GLY	3.5
30	3	54	LYS	3.5
21	T	116	ASP	3.5
5	D	86	THR	3.4
30	3	5	ARG	3.4
10	I	98	ASP	3.4
9	H	86	TYR	3.4
13	L	80	ASP	3.3
5	D	63	ILE	3.3
30	3	28	GLY	3.3
1	0	1198	U	3.3
10	I	102	GLN	3.3
22	U	36	CYS	3.2
27	Z	93	TYR	3.2
22	U	53	ASP	3.2
14	M	79	ALA	3.2
23	V	36	ALA	3.1
1	0	735	C	3.1
8	G	23	ILE	3.1
23	V	40	PRO	3.1
22	U	47	ARG	3.1
5	D	83	PHE	3.0
10	I	110	ASP	3.0
5	D	92	GLU	3.0
27	Z	78	ILE	3.0
13	L	48	LYS	3.0
27	Z	65	ASN	3.0
27	Z	40	ALA	3.0
27	Z	82	SER	3.0
5	D	61	PHE	3.0
25	X	80	GLU	3.0
2	A	56	ALA	3.0
10	I	99	GLN	2.9
10	I	113	SER	2.9
7	F	49	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
5	D	134	LEU	2.9
5	D	87	ALA	2.9
5	D	69	ILE	2.9
13	L	60	GLU	2.9
10	I	106	GLN	2.8
22	U	54	THR	2.8
10	I	69	PRO	2.8
5	D	88	LEU	2.8
21	T	118	SER	2.8
27	Z	41	ARG	2.8
27	Z	64	PRO	2.7
10	I	82	THR	2.7
1	0	2645	U	2.7
17	P	128	GLY	2.7
10	I	78	ALA	2.7
22	U	46	ALA	2.7
5	D	85	GLN	2.6
2	A	85	SER	2.6
23	V	46	ILE	2.6
5	D	84	LEU	2.6
25	X	88	GLU	2.6
22	U	39	ASN	2.6
5	D	19	GLU	2.6
14	M	73	ARG	2.6
10	I	79	GLY	2.6
25	X	71	ARG	2.6
15	N	179	LEU	2.6
30	3	90	PHE	2.6
10	I	111	LEU	2.5
9	H	174	LEU	2.5
10	I	112	LEU	2.5
15	N	50	LEU	2.5
5	D	70	GLY	2.5
22	U	32	CYS	2.5
5	D	142	ALA	2.5
14	M	85	ARG	2.5
23	V	37	GLY	2.5
10	I	108	HIS	2.5
29	2	35	ARG	2.5
22	U	30	HIS	2.4
5	D	23	VAL	2.4
15	N	166	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
24	W	100	LEU	2.4
10	I	91	PHE	2.4
10	I	104	ALA	2.4
10	I	75	LYS	2.4
29	2	39	ARG	2.4
30	3	79	LEU	2.4
14	M	82	ARG	2.4
27	Z	61	HIS	2.4
13	L	123	ASP	2.3
14	M	75	ARG	2.3
5	D	41	LEU	2.3
5	D	89	PRO	2.3
10	I	118	ASN	2.3
22	U	51	TRP	2.3
5	D	25	MET	2.3
22	U	31	PHE	2.3
5	D	73	VAL	2.3
27	Z	88	PHE	2.3
14	M	14	ASN	2.3
13	L	79	ASP	2.3
22	U	25	ASP	2.3
13	L	75	LEU	2.3
7	F	75	ILE	2.3
26	Y	235	GLU	2.3
29	2	20	ARG	2.3
15	N	160	SER	2.2
10	I	100	VAL	2.2
14	M	16	GLY	2.2
2	A	88	ILE	2.2
10	I	132	VAL	2.2
9	H	82	GLU	2.2
24	W	3	ALA	2.2
27	Z	79	TRP	2.2
5	D	75	LEU	2.2
22	U	12	ASP	2.2
9	H	35	LYS	2.2
27	Z	66	CYS	2.1
10	I	83	GLY	2.1
22	U	45	GLU	2.1
22	U	8	TYR	2.1
2	A	37	VAL	2.1
10	I	103	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
30	3	88	LEU	2.1
1	0	970	U	2.0
10	I	88	GLN	2.0
23	V	38	GLY	2.0
5	D	47	GLN	2.0
23	V	8	ILE	2.0
9	H	76	LEU	2.0
1	0	1197	G	2.0
15	N	57	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	UR3	0	2619	21/22	0.95	0.17	-	41,44,49,50	0
1	OMG	0	2588	24/25	0.96	0.16	-	37,42,44,45	0
1	PSU	0	2621	20/21	0.93	0.19	-	37,39,44,44	0
1	1MA	0	628	23/24	0.96	0.17	-	38,41,42,43	0
1	OMU	0	2587	21/22	0.95	0.14	-	43,46,50,50	0
32	5AA	4	76	24/25	0.77	0.29	-	38,44,48,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8565	1/1	0.89	1.65	69.82	80,80,80,80	0
35	NA	0	8530	1/1	0.79	0.68	42.97	68,68,68,68	0
37	SR	L	8969	1/1	0.55	1.29	40.95	200,200,200,200	0
35	NA	0	8563	1/1	0.72	1.00	34.13	85,85,85,85	0
33	MG	0	8047	1/1	0.85	0.55	24.45	68,68,68,68	0
35	NA	0	8513	1/1	0.76	0.66	21.46	62,62,62,62	0
35	NA	0	8568	1/1	0.39	0.62	21.21	35,35,35,35	0
35	NA	0	8517	1/1	0.81	0.35	20.38	62,62,62,62	0
37	SR	B	8987	1/1	0.79	1.00	20.37	200,200,200,200	0
35	NA	0	8528	1/1	0.57	0.68	19.53	91,91,91,91	0
35	NA	0	8547	1/1	0.94	0.61	19.40	82,82,82,82	0
35	NA	0	8555	1/1	0.89	0.76	17.81	61,61,61,61	0
37	SR	0	8949	1/1	0.44	0.43	15.50	157,157,157,157	0
37	SR	0	8962	1/1	0.07	0.42	14.12	200,200,200,200	0
35	NA	0	8521	1/1	0.60	0.47	12.77	59,59,59,59	0
35	NA	0	8512	1/1	0.89	0.44	12.00	54,54,54,54	0
35	NA	0	8556	1/1	0.72	0.46	10.89	49,49,49,49	0
34	K	0	8401	1/1	0.83	0.36	10.00	132,132,132,132	0
35	NA	0	8519	1/1	0.92	0.36	9.30	69,69,69,69	0
35	NA	0	8527	1/1	0.97	0.34	8.05	75,75,75,75	0
35	NA	0	8553	1/1	0.90	0.36	7.05	98,98,98,98	0
35	NA	0	8559	1/1	0.69	0.32	6.84	99,99,99,99	0
35	NA	0	8542	1/1	0.94	0.34	6.58	51,51,51,51	0
35	NA	0	8569	1/1	0.81	0.37	6.03	63,63,63,63	0
37	SR	0	8992	1/1	0.73	0.29	5.80	164,164,164,164	0
35	NA	0	8562	1/1	0.92	0.21	5.76	49,49,49,49	0
33	MG	0	8080	1/1	0.91	2.92	4.99	126,126,126,126	0
33	MG	0	8043	1/1	0.92	0.21	4.87	48,48,48,48	0
36	CL	0	8805	1/1	0.88	0.24	4.78	101,101,101,101	0
35	NA	0	8522	1/1	0.57	0.27	4.44	71,71,71,71	0
37	SR	0	8904	1/1	0.99	0.23	3.74	65,65,65,65	0
35	NA	0	8564	1/1	0.84	0.21	3.42	94,94,94,94	0
35	NA	0	8557	1/1	0.57	0.16	3.32	72,72,72,72	0
35	NA	0	8545	1/1	0.91	0.26	2.83	25,25,25,25	0
35	NA	M	8539	1/1	0.84	0.26	2.65	51,51,51,51	0
33	MG	Y	8086	1/1	0.87	0.25	2.45	53,53,53,53	0
35	NA	Q	8540	1/1	0.74	0.30	2.29	84,84,84,84	0
33	MG	0	8076	1/1	0.81	0.25	2.25	52,52,52,52	0
35	NA	0	8534	1/1	0.81	0.40	1.97	53,53,53,53	0
34	K	0	8402	1/1	0.71	0.48	1.76	88,88,88,88	0
35	NA	0	8523	1/1	0.83	0.21	1.59	52,52,52,52	0
35	NA	R	8533	1/1	0.83	0.20	1.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	B	8819	1/1	0.87	0.23	1.29	80,80,80,80	0
37	SR	0	8970	1/1	0.94	0.13	1.23	148,148,148,148	0
33	MG	0	8015	1/1	0.97	0.17	1.19	26,26,26,26	0
33	MG	0	8034	1/1	0.93	0.19	1.16	57,57,57,57	0
37	SR	0	8902	1/1	0.99	0.20	1.01	44,44,44,44	0
33	MG	0	8014	1/1	0.94	0.20	0.97	24,24,24,24	0
33	MG	0	8041	1/1	0.94	0.21	0.37	29,29,29,29	0
37	SR	0	8985	1/1	0.89	0.12	0.32	150,150,150,150	0
36	CL	M	8818	1/1	0.94	0.18	0.27	62,62,62,62	0
33	MG	0	8003	1/1	0.93	0.17	0.19	32,32,32,32	0
35	NA	R	8575	1/1	0.97	0.19	0.17	92,92,92,92	0
37	SR	0	8923	1/1	0.91	0.17	0.16	108,108,108,108	0
36	CL	J	8821	1/1	0.93	0.19	0.15	90,90,90,90	0
33	MG	0	8062	1/1	0.98	0.20	0.05	53,53,53,53	0
37	SR	0	8943	1/1	0.82	0.14	0.01	105,105,105,105	0
33	MG	A	8051	1/1	0.99	0.20	-0.05	81,81,81,81	0
33	MG	0	8006	1/1	0.98	0.16	-0.05	44,44,44,44	0
39	CD	U	8701	1/1	0.81	0.40	-0.28	200,200,200,200	0
39	CD	Z	8703	1/1	0.49	0.39	-0.34	200,200,200,200	0
33	MG	A	8050	1/1	0.91	0.18	-0.52	68,68,68,68	0
35	NA	0	8507	1/1	0.81	0.17	-0.53	27,27,27,27	0
33	MG	0	8044	1/1	0.59	0.16	-0.61	51,51,51,51	0
33	MG	0	8058	1/1	0.92	0.12	-0.65	22,22,22,22	0
33	MG	0	8088	1/1	0.53	0.18	-0.77	37,37,37,37	0
38	MYL	0	2924	35/35	0.84	0.26	-0.78	80,83,86,87	0
37	SR	A	8930	1/1	0.49	0.15	-0.82	168,168,168,168	0
37	SR	0	8903	1/1	0.96	0.15	-0.86	62,62,62,62	0
33	MG	0	8084	1/1	0.97	0.11	-0.91	31,31,31,31	0
35	NA	C	8503	1/1	0.88	0.17	-0.96	32,32,32,32	0
33	MG	0	8004	1/1	0.82	0.18	-1.01	25,25,25,25	0
33	MG	0	8016	1/1	0.96	0.19	-1.02	34,34,34,34	0
35	NA	J	8538	1/1	0.69	0.15	-1.10	56,56,56,56	0
35	NA	0	8515	1/1	0.92	0.18	-1.16	39,39,39,39	0
36	CL	L	8810	1/1	0.80	0.17	-1.16	76,76,76,76	0
33	MG	0	8001	1/1	0.98	0.17	-1.34	24,24,24,24	0
37	SR	0	8948	1/1	0.93	0.12	-1.35	113,113,113,113	0
36	CL	0	8812	1/1	0.95	0.11	-1.44	66,66,66,66	0
33	MG	0	8002	1/1	0.97	0.17	-1.48	40,40,40,40	0
35	NA	R	8532	1/1	0.93	0.08	-1.52	52,52,52,52	0
33	MG	0	8028	1/1	0.92	0.15	-1.54	13,13,13,13	0
33	MG	0	8065	1/1	0.73	0.12	-1.57	33,33,33,33	0
37	SR	0	8936	1/1	0.96	0.13	-1.61	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8537	1/1	0.84	0.09	-1.71	40,40,40,40	0
33	MG	0	8012	1/1	0.96	0.17	-1.75	23,23,23,23	0
37	SR	H	8972	1/1	0.96	0.11	-1.77	139,139,139,139	0
39	CD	1	8702	1/1	0.94	0.11	-1.89	78,78,78,78	0
37	SR	A	8929	1/1	0.82	0.07	-1.89	124,124,124,124	0
33	MG	0	8045	1/1	0.87	0.10	-1.93	64,64,64,64	0
37	SR	0	8910	1/1	0.89	0.13	-1.95	107,107,107,107	0
33	MG	0	8011	1/1	0.90	0.16	-2.05	14,14,14,14	0
33	MG	0	8025	1/1	0.91	0.14	-2.10	30,30,30,30	0
39	CD	3	8704	1/1	0.56	0.62	-2.29	200,200,200,200	0
37	SR	0	8935	1/1	0.93	0.09	-2.38	91,91,91,91	0
33	MG	T	8057	1/1	0.80	0.07	-2.65	68,68,68,68	0
33	MG	0	8009	1/1	0.98	0.13	-2.69	22,22,22,22	0
33	MG	0	8021	1/1	0.96	0.10	-2.89	53,53,53,53	0
33	MG	0	8052	1/1	0.91	0.13	-2.91	60,60,60,60	0
37	SR	0	8975	1/1	0.75	0.08	-3.21	158,158,158,158	0
33	MG	0	8010	1/1	0.57	0.14	-3.77	25,25,25,25	0
35	NA	9	8572	1/1	0.94	0.04	-3.91	78,78,78,78	0
35	NA	0	8504	1/1	0.99	0.13	-4.60	32,32,32,32	0
33	MG	0	8013	1/1	0.90	0.08	-13.05	24,24,24,24	0
35	NA	0	8574	1/1	0.56	0.62	-	72,72,72,72	0
37	SR	0	8991	1/1	0.68	0.14	-	197,197,197,197	0
33	MG	0	8083	1/1	0.83	0.18	-	50,50,50,50	0
33	MG	0	8039	1/1	0.83	0.18	-	55,55,55,55	0
35	NA	0	8520	1/1	0.87	0.18	-	63,63,63,63	0
33	MG	0	8078	1/1	0.95	0.85	-	91,91,91,91	0
37	SR	0	8907	1/1	0.96	0.14	-	59,59,59,59	0
37	SR	0	8951	1/1	0.85	0.06	-	144,144,144,144	0
35	NA	0	8573	1/1	0.92	0.15	-	78,78,78,78	0
37	SR	0	8941	1/1	0.38	0.30	-	152,152,152,152	0
33	MG	0	8048	1/1	0.91	0.29	-	41,41,41,41	0
37	SR	0	8920	1/1	0.95	0.14	-	130,130,130,130	0
33	MG	0	8017	1/1	0.82	0.17	-	26,26,26,26	0
36	CL	0	8811	1/1	0.92	0.21	-	87,87,87,87	0
36	CL	0	8815	1/1	0.94	0.21	-	83,83,83,83	0
36	CL	0	8822	1/1	0.89	0.90	-	123,123,123,123	0
35	NA	9	8543	1/1	0.74	0.18	-	68,68,68,68	0
33	MG	0	8082	1/1	0.88	0.23	-	61,61,61,61	0
33	MG	0	8007	1/1	0.96	0.12	-	27,27,27,27	0
37	SR	0	8934	1/1	0.89	0.31	-	168,168,168,168	0
33	MG	0	8069	1/1	0.64	0.43	-	63,63,63,63	0
37	SR	0	8945	1/1	0.77	0.13	-	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	8908	1/1	0.57	0.21	-	116,116,116,116	0
35	NA	0	8561	1/1	0.71	0.26	-	66,66,66,66	0
37	SR	0	8989	1/1	0.68	0.16	-	129,129,129,129	0
35	NA	0	8529	1/1	0.83	0.09	-	45,45,45,45	0
37	SR	0	8973	1/1	0.85	0.12	-	162,162,162,162	0
35	NA	0	8546	1/1	0.84	0.63	-	65,65,65,65	0
37	SR	0	8971	1/1	-0.29	0.34	-	200,200,200,200	0
37	SR	0	8938	1/1	0.57	0.32	-	200,200,200,200	0
37	SR	0	8905	1/1	0.96	0.27	-	78,78,78,78	0
37	SR	0	8947	1/1	0.84	0.78	-	200,200,200,200	0
37	SR	0	8979	1/1	0.74	0.24	-	111,111,111,111	0
37	SR	0	8944	1/1	0.66	0.17	-	169,169,169,169	0
33	MG	0	8019	1/1	0.87	0.16	-	11,11,11,11	0
33	MG	0	8029	1/1	0.78	0.19	-	79,79,79,79	0
37	SR	0	8946	1/1	0.92	0.14	-	127,127,127,127	0
37	SR	0	8982	1/1	0.87	1.36	-	200,200,200,200	0
33	MG	3	8090	1/1	0.04	2.20	-	86,86,86,86	0
36	CL	0	8816	1/1	0.94	0.81	-	89,89,89,89	0
37	SR	0	8966	1/1	0.76	0.13	-	117,117,117,117	0
33	MG	0	8072	1/1	0.95	0.40	-	60,60,60,60	0
33	MG	2	8060	1/1	0.73	0.11	-	62,62,62,62	0
33	MG	0	8038	1/1	0.68	0.20	-	92,92,92,92	0
37	SR	0	8960	1/1	0.76	0.09	-	175,175,175,175	0
37	SR	0	8958	1/1	0.96	0.16	-	120,120,120,120	0
33	MG	9	8074	1/1	0.83	0.11	-	87,87,87,87	0
33	MG	0	8049	1/1	0.94	0.35	-	82,82,82,82	0
36	CL	J	8802	1/1	0.89	0.24	-	84,84,84,84	0
33	MG	0	8059	1/1	0.90	0.15	-	56,56,56,56	0
36	CL	0	8813	1/1	0.82	0.10	-	77,77,77,77	0
37	SR	0	8917	1/1	0.83	0.23	-	157,157,157,157	0
33	MG	0	8070	1/1	0.88	0.09	-	58,58,58,58	0
36	CL	0	8803	1/1	0.63	0.12	-	68,68,68,68	0
36	CL	Y	8820	1/1	0.87	0.21	-	58,58,58,58	0
36	CL	O	8808	1/1	0.67	0.14	-	109,109,109,109	0
39	CD	O	8705	1/1	0.95	0.07	-	117,117,117,117	0
35	NA	0	8511	1/1	0.91	0.26	-	54,54,54,54	0
37	SR	0	8965	1/1	0.16	0.19	-	158,158,158,158	0
37	SR	0	8977	1/1	0.20	0.12	-	200,200,200,200	0
37	SR	0	8983	1/1	0.16	0.28	-	199,199,199,199	0
35	NA	0	8524	1/1	0.96	0.12	-	67,67,67,67	0
33	MG	9	8040	1/1	0.93	0.23	-	89,89,89,89	0
33	MG	0	8033	1/1	0.96	0.20	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	9	8980	1/1	0.39	0.37	-	192,192,192,192	0
35	NA	0	8554	1/1	0.71	0.44	-	106,106,106,106	0
33	MG	0	8018	1/1	0.88	0.14	-	32,32,32,32	0
35	NA	0	8544	1/1	0.05	0.45	-	75,75,75,75	0
37	SR	0	8974	1/1	0.27	0.20	-	163,163,163,163	0
37	SR	0	8911	1/1	0.75	0.10	-	99,99,99,99	0
33	MG	0	8077	1/1	0.89	0.64	-	60,60,60,60	0
35	NA	0	8516	1/1	0.89	0.20	-	39,39,39,39	0
37	SR	0	8955	1/1	0.89	0.13	-	200,200,200,200	0
33	MG	0	8053	1/1	0.76	0.10	-	61,61,61,61	0
33	MG	0	8089	1/1	0.88	0.21	-	42,42,42,42	0
35	NA	0	8536	1/1	0.55	0.19	-	72,72,72,72	0
37	SR	0	8993	1/1	0.36	0.23	-	186,186,186,186	0
36	CL	J	8801	1/1	0.90	0.34	-	88,88,88,88	0
36	CL	A	8809	1/1	0.81	0.79	-	128,128,128,128	0
35	NA	0	8548	1/1	0.39	0.33	-	67,67,67,67	0
33	MG	0	8061	1/1	0.93	0.41	-	48,48,48,48	0
33	MG	0	8030	1/1	0.95	0.39	-	88,88,88,88	0
37	SR	0	8924	1/1	0.82	0.20	-	140,140,140,140	0
35	NA	0	8549	1/1	0.76	0.34	-	124,124,124,124	0
33	MG	0	8008	1/1	0.93	0.15	-	23,23,23,23	0
37	SR	B	8950	1/1	0.90	0.15	-	125,125,125,125	0
37	SR	0	8953	1/1	0.76	1.12	-	200,200,200,200	0
35	NA	0	8535	1/1	0.92	0.76	-	72,72,72,72	0
37	SR	0	9004	1/1	0.93	0.25	-	172,172,172,172	0
35	NA	0	8566	1/1	0.91	0.38	-	64,64,64,64	0
37	SR	0	8916	1/1	0.74	0.17	-	126,126,126,126	0
37	SR	0	8988	1/1	0.78	0.17	-	183,183,183,183	0
37	SR	0	8939	1/1	0.90	0.15	-	166,166,166,166	0
33	MG	0	8063	1/1	0.89	0.16	-	62,62,62,62	0
37	SR	9	8978	1/1	0.94	0.10	-	154,154,154,154	0
35	NA	0	8508	1/1	0.71	0.44	-	68,68,68,68	0
35	NA	0	8506	1/1	0.45	0.80	-	65,65,65,65	0
33	MG	0	8087	1/1	0.95	0.10	-	29,29,29,29	0
35	NA	0	8550	1/1	0.86	0.28	-	76,76,76,76	0
37	SR	0	8918	1/1	0.85	0.14	-	92,92,92,92	0
37	SR	0	9001	1/1	0.79	0.18	-	200,200,200,200	0
37	SR	0	8957	1/1	0.77	0.29	-	200,200,200,200	0
35	NA	0	8505	1/1	0.88	0.48	-	58,58,58,58	0
33	MG	0	8068	1/1	0.99	0.12	-	64,64,64,64	0
35	NA	B	8552	1/1	0.92	0.22	-	111,111,111,111	0
37	SR	3	8999	1/1	0.66	0.71	-	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	R	8912	1/1	0.96	0.16	-	93,93,93,93	0
33	MG	0	8023	1/1	0.94	0.18	-	41,41,41,41	0
35	NA	0	8502	1/1	0.70	0.39	-	53,53,53,53	0
37	SR	0	8963	1/1	0.92	0.12	-	146,146,146,146	0
37	SR	0	8968	1/1	0.60	0.15	-	180,180,180,180	0
37	SR	0	9002	1/1	0.42	0.12	-	169,169,169,169	0
37	SR	0	8926	1/1	0.79	0.16	-	127,127,127,127	0
35	NA	0	8525	1/1	0.85	0.26	-	67,67,67,67	0
35	NA	0	8501	1/1	0.89	0.24	-	41,41,41,41	0
33	MG	0	8071	1/1	0.74	0.30	-	67,67,67,67	0
37	SR	0	8959	1/1	0.39	0.37	-	194,194,194,194	0
37	SR	0	8984	1/1	0.84	0.07	-	118,118,118,118	0
37	SR	0	8964	1/1	0.81	0.08	-	160,160,160,160	0
37	SR	0	8928	1/1	0.92	0.12	-	148,148,148,148	0
37	SR	0	8954	1/1	0.93	0.15	-	108,108,108,108	0
33	MG	0	8026	1/1	0.87	0.20	-	39,39,39,39	0
37	SR	0	8906	1/1	0.95	0.21	-	64,64,64,64	0
35	NA	0	8526	1/1	0.94	0.13	-	40,40,40,40	0
33	MG	0	8037	1/1	0.99	0.10	-	67,67,67,67	0
35	NA	0	8541	1/1	0.82	0.38	-	65,65,65,65	0
33	MG	0	8031	1/1	0.82	0.62	-	77,77,77,77	0
37	SR	0	8915	1/1	0.74	0.14	-	131,131,131,131	0
37	SR	0	9007	1/1	0.79	0.38	-	200,200,200,200	0
37	SR	0	8986	1/1	0.53	0.84	-	200,200,200,200	0
35	NA	0	8509	1/1	0.62	0.58	-	90,90,90,90	0
37	SR	0	8927	1/1	0.77	0.16	-	176,176,176,176	0
33	MG	0	8022	1/1	0.94	0.07	-	56,56,56,56	0
33	MG	0	8032	1/1	0.92	0.16	-	66,66,66,66	0
33	MG	0	8073	1/1	0.73	0.09	-	70,70,70,70	0
33	MG	0	8067	1/1	0.97	0.17	-	33,33,33,33	0
37	SR	S	8961	1/1	0.90	0.12	-	150,150,150,150	0
37	SR	0	8931	1/1	0.89	0.09	-	147,147,147,147	0
37	SR	0	8967	1/1	0.92	0.07	-	164,164,164,164	0
37	SR	0	8942	1/1	0.86	0.21	-	139,139,139,139	0
37	SR	0	9000	1/1	0.52	1.08	-	200,200,200,200	0
37	SR	0	8940	1/1	0.96	0.16	-	110,110,110,110	0
35	NA	S	8510	1/1	0.83	0.12	-	56,56,56,56	0
37	SR	0	8996	1/1	0.96	0.22	-	200,200,200,200	0
37	SR	0	9006	1/1	0.80	0.13	-	190,190,190,190	0
37	SR	0	8990	1/1	0.98	0.19	-	108,108,108,108	0
37	SR	9	9003	1/1	0.64	0.06	-	195,195,195,195	0
36	CL	N	8807	1/1	0.89	0.29	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8570	1/1	0.69	0.26	-	61,61,61,61	0
33	MG	0	8081	1/1	0.63	0.59	-	80,80,80,80	0
33	MG	0	8035	1/1	0.94	0.25	-	52,52,52,52	0
33	MG	0	8075	1/1	0.30	0.14	-	64,64,64,64	0
33	MG	0	8020	1/1	0.83	0.15	-	56,56,56,56	0
33	MG	0	8036	1/1	0.79	0.16	-	59,59,59,59	0
33	MG	0	8066	1/1	0.56	0.24	-	75,75,75,75	0
33	MG	0	8055	1/1	0.63	0.54	-	87,87,87,87	0
37	SR	0	8914	1/1	0.88	0.15	-	109,109,109,109	0
37	SR	0	8909	1/1	0.96	0.18	-	105,105,105,105	0
35	NA	H	8518	1/1	0.65	0.77	-	92,92,92,92	0
35	NA	0	8531	1/1	0.74	0.18	-	45,45,45,45	0
37	SR	0	8919	1/1	0.88	0.09	-	81,81,81,81	0
33	MG	0	8027	1/1	0.98	0.08	-	47,47,47,47	0
37	SR	0	8901	1/1	0.91	0.15	-	78,78,78,78	0
37	SR	0	8922	1/1	0.74	0.64	-	182,182,182,182	0
37	SR	1	8952	1/1	0.94	0.16	-	81,81,81,81	0
33	MG	0	8092	1/1	0.69	0.48	-	133,133,133,133	0
33	MG	0	8064	1/1	0.80	0.29	-	53,53,53,53	0
35	NA	0	8551	1/1	0.48	0.79	-	86,86,86,86	0
36	CL	0	8814	1/1	0.97	0.17	-	55,55,55,55	0
37	SR	F	9005	1/1	0.61	0.07	-	153,153,153,153	0
35	NA	0	8514	1/1	0.95	0.56	-	38,38,38,38	0
35	NA	0	8571	1/1	0.70	0.35	-	101,101,101,101	0
37	SR	3	8932	1/1	-0.02	0.28	-	184,184,184,184	0
37	SR	0	8976	1/1	0.78	0.38	-	200,200,200,200	0
33	MG	0	8085	1/1	0.93	0.13	-	73,73,73,73	0
37	SR	0	9008	1/1	0.93	0.16	-	107,107,107,107	0
35	NA	0	8560	1/1	0.78	0.80	-	61,61,61,61	0
33	MG	K	8054	1/1	0.72	0.19	-	29,29,29,29	0
33	MG	0	8046	1/1	0.85	0.13	-	46,46,46,46	0
37	SR	0	8933	1/1	0.83	0.06	-	122,122,122,122	0
36	CL	3	8804	1/1	0.08	0.58	-	121,121,121,121	0
37	SR	0	8937	1/1	0.93	0.10	-	116,116,116,116	0
33	MG	0	8005	1/1	0.90	0.31	-	46,46,46,46	0
37	SR	0	8997	1/1	0.79	0.74	-	200,200,200,200	0
33	MG	0	8056	1/1	0.81	0.13	-	44,44,44,44	0
33	MG	0	8093	1/1	0.59	0.11	-	29,29,29,29	0
33	MG	B	8042	1/1	0.92	0.47	-	121,121,121,121	0
37	SR	0	8956	1/1	0.88	0.09	-	154,154,154,154	0
37	SR	0	8998	1/1	0.95	0.21	-	196,196,196,196	0
37	SR	0	8995	1/1	0.86	0.45	-	191,191,191,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8567	1/1	0.78	0.81	-	57,57,57,57	0
35	NA	0	8558	1/1	0.70	0.58	-	60,60,60,60	0
36	CL	0	8817	1/1	0.95	0.34	-	80,80,80,80	0
37	SR	0	8913	1/1	0.89	0.77	-	181,181,181,181	0
33	MG	0	8024	1/1	0.79	0.24	-	55,55,55,55	0
37	SR	0	8981	1/1	0.94	0.28	-	198,198,198,198	0
37	SR	0	8994	1/1	0.97	0.59	-	200,200,200,200	0
37	SR	0	8921	1/1	0.92	0.16	-	98,98,98,98	0
33	MG	0	8091	1/1	0.78	0.10	-	111,111,111,111	0
37	SR	0	8925	1/1	0.97	0.10	-	99,99,99,99	0
33	MG	0	8079	1/1	0.87	0.41	-	76,76,76,76	0
36	CL	R	8806	1/1	0.95	0.08	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.