



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID : 3CME  
Title : The Structure of CA and CCA-PHE-CAP-BIO Bound to the Large Ribosomal Subunit of Haloarcula Marismortui  
Authors : Simonovic, M.; Steitz, T.A.  
Deposited on : 2008-03-21  
Resolution : 2.95 Å(reported)

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

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

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

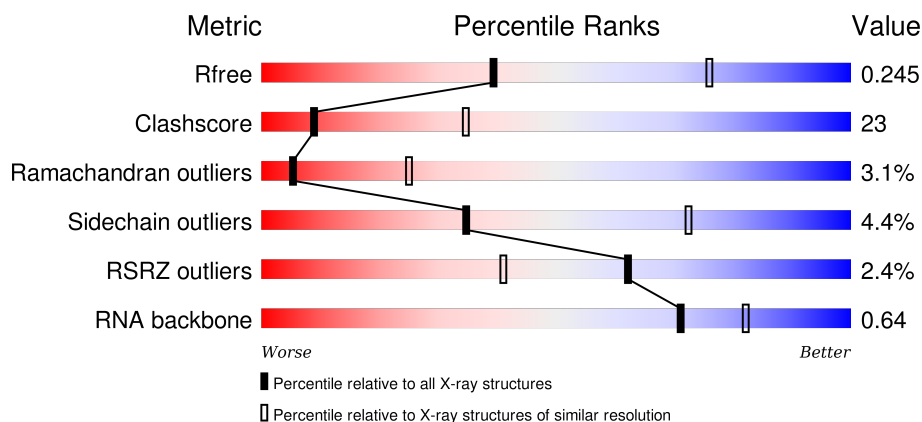
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>2%</div> <div> <div>43%</div> <div>48%</div> <div>7%</div> </div> </div>
2	B	338	<div> <div>41%</div> <div>53%</div> <div>6%</div> </div>
3	C	246	<div> <div>43%</div> <div>51%</div> <div>6%</div> </div>
4	D	177	<div> <div>18%</div> <div>25%</div> <div>46%</div> <div>7%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	240	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	
32	5	3	
33	6	3	

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
35	MG	0	8002	-	-	-	X
35	MG	0	8003	-	-	-	X
35	MG	0	8004	-	-	-	X
35	MG	0	8006	-	-	-	X
35	MG	0	8008	-	-	-	X
35	MG	0	8009	-	-	-	X
35	MG	0	8010	-	-	-	X
35	MG	0	8014	-	-	-	X
35	MG	0	8015	-	-	-	X
35	MG	0	8028	-	-	-	X
35	MG	0	8029	-	-	-	X
35	MG	0	8034	-	-	-	X
35	MG	0	8041	-	-	-	X
35	MG	0	8047	-	-	-	X
35	MG	0	8050	-	-	-	X
35	MG	0	8062	-	-	-	X
35	MG	0	8071	-	-	-	X
35	MG	0	8076	-	-	-	X
35	MG	0	8079	-	-	-	X
35	MG	0	8087	-	-	-	X
35	MG	A	8025	-	-	-	X
35	MG	A	8051	-	-	-	X
35	MG	B	8043	-	-	-	X
35	MG	C	8012	-	-	-	X
36	NA	0	8504	-	-	-	X
36	NA	0	8507	-	-	-	X
36	NA	0	8512	-	-	-	X
36	NA	0	8513	-	-	-	X
36	NA	0	8517	-	-	-	X
36	NA	0	8519	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	8520	-	-	-	X
36	NA	0	8521	-	-	-	X
36	NA	0	8523	-	-	-	X
36	NA	0	8527	-	-	-	X
36	NA	0	8528	-	-	-	X
36	NA	0	8530	-	-	-	X
36	NA	0	8533	-	-	-	X
36	NA	0	8534	-	-	-	X
36	NA	0	8535	-	-	-	X
36	NA	0	8542	-	-	-	X
36	NA	0	8547	-	-	-	X
36	NA	0	8550	-	-	-	X
36	NA	0	8552	-	-	-	X
36	NA	0	8553	-	-	-	X
36	NA	0	8556	-	-	-	X
36	NA	0	8557	-	-	-	X
36	NA	0	8559	-	-	-	X
36	NA	0	8560	-	-	-	X
36	NA	0	8562	-	-	-	X
36	NA	0	8563	-	-	-	X
36	NA	0	8565	-	-	-	X
36	NA	0	8567	-	-	-	X
36	NA	0	8568	-	-	-	X
36	NA	0	8569	-	-	-	X
36	NA	9	8572	-	-	-	X
36	NA	C	8503	-	-	-	X
37	SR	0	8904	-	-	-	X
37	SR	0	8910	-	-	-	X
37	SR	0	8948	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8981	-	-	-	X
37	SR	1	8913	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
37	SR	R	8912	-	-	-	X
38	CL	J	8801	-	-	X	-
38	CL	L	8814	-	-	X	-
39	K	0	8401	-	-	-	X
39	K	0	8402	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 99194 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1752	1072	351	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2624	1616	492	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1859	1130	344	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1093	685	194	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1356	840	223	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			889	551	140	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1281	798	239	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			518	323	80	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1119	696	198	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			993	609	188	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O		0	0	0
			1117	670	221	226				

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1557	943	332	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1444	895	261	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			864	529	160	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1135	683	228	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			734	450	140	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1148	713	208	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			640	389	110	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			949	568	179	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1195	737	208	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			653	402	128	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			572	343	112	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			754	458	152	137	7			

- Molecule 30 is a RNA chain called 50S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26345	10873	19054	2745			

- 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
			2595	1156	471	847	121			

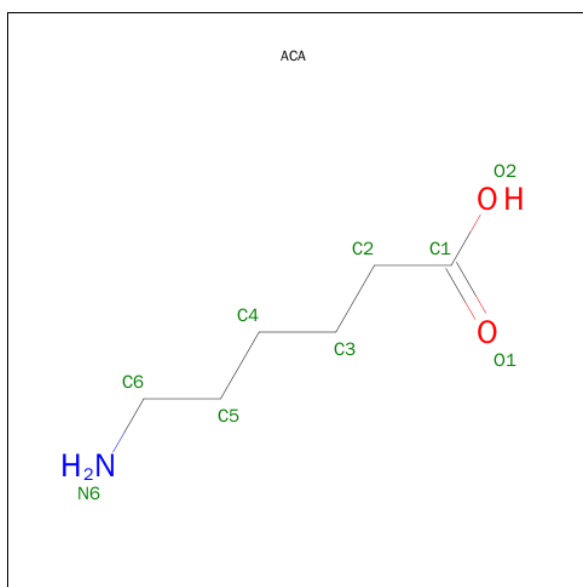
- Molecule 32 is a RNA chain called RNA (5'-R(\*C\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	2	Total	C	N	O	P	0	0	0
			39	19	8	11	1			

- Molecule 33 is a RNA chain called RNA (5'-R(\*CP\*CP\*(8AN))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			

- Molecule 34 is PHENYLALANINE (three-letter code: ACA, PHE) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>, C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	6	2	Total	C	N	O	0	0
			19	15	2	2		

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total	Mg	0	0
			82	82		
35	Y	1	Total	Mg	0	0
			1	1		
35	K	1	Total	Mg	0	0
			1	1		
35	B	2	Total	Mg	0	0
			2	2		
35	C	1	Total	Mg	0	0
			1	1		
35	A	3	Total	Mg	0	0
			3	3		
35	T	1	Total	Mg	0	0
			1	1		
35	2	1	Total	Mg	0	0
			1	1		
35	9	1	Total	Mg	0	0
			1	1		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	65	Total Na 65 65	0	0
36	J	1	Total Na 1 1	0	0
36	Q	1	Total Na 1 1	0	0
36	H	1	Total Na 1 1	0	0
36	C	1	Total Na 1 1	0	0
36	R	1	Total Na 1 1	0	0
36	9	3	Total Na 3 3	0	0
36	S	1	Total Na 1 1	0	0
36	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	87	Total Sr 87 87	0	0
37	Y	1	Total Sr 1 1	0	0
37	H	2	Total Sr 2 2	0	0
37	B	2	Total Sr 2 2	0	0
37	1	2	Total Sr 2 2	0	0
37	A	3	Total Sr 3 3	0	0
37	T	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	3	3	Total Sr 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	6	Total	Cl	0	0
			6	6		
38	J	4	Total	Cl	0	0
			4	4		
38	Q	1	Total	Cl	0	0
			1	1		
38	B	1	Total	Cl	0	0
			1	1		
38	A	1	Total	Cl	0	0
			1	1		
38	N	1	Total	Cl	0	0
			1	1		
38	O	1	Total	Cl	0	0
			1	1		
38	R	1	Total	Cl	0	0
			1	1		
38	Y	2	Total	Cl	0	0
			2	2		
38	L	2	Total	Cl	0	0
			2	2		
38	3	1	Total	Cl	0	0
			1	1		
38	M	1	Total	Cl	0	0
			1	1		

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total	K	0	0
			2	2		

- Molecule 40 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	O	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	Z	1	Total	Cd	0	0
			1	1		
40	1	1	Total	Cd	0	0
			1	1		
40	3	1	Total	Cd	0	0
			1	1		
40	U	1	Total	Cd	0	0
			1	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	9	138	Total	O	0	0
			138	138		
41	A	134	Total	O	0	0
			134	134		
41	B	156	Total	O	0	0
			156	156		
41	C	168	Total	O	0	0
			168	168		
41	D	49	Total	O	0	0
			49	49		
41	E	49	Total	O	0	0
			49	49		
41	F	31	Total	O	0	0
			31	31		
41	G	20	Total	O	0	0
			20	20		
41	H	78	Total	O	0	0
			78	78		
41	I	11	Total	O	0	0
			11	11		
41	J	58	Total	O	0	0
			58	58		
41	K	57	Total	O	0	0
			57	57		
41	L	91	Total	O	0	0
			91	91		
41	M	129	Total	O	0	0
			129	129		
41	N	68	Total	O	0	0
			68	68		

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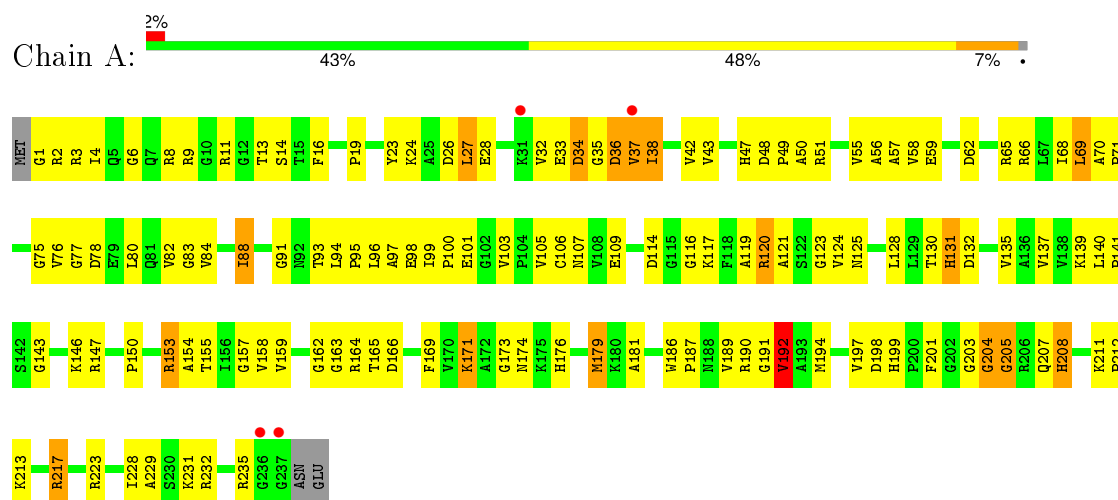
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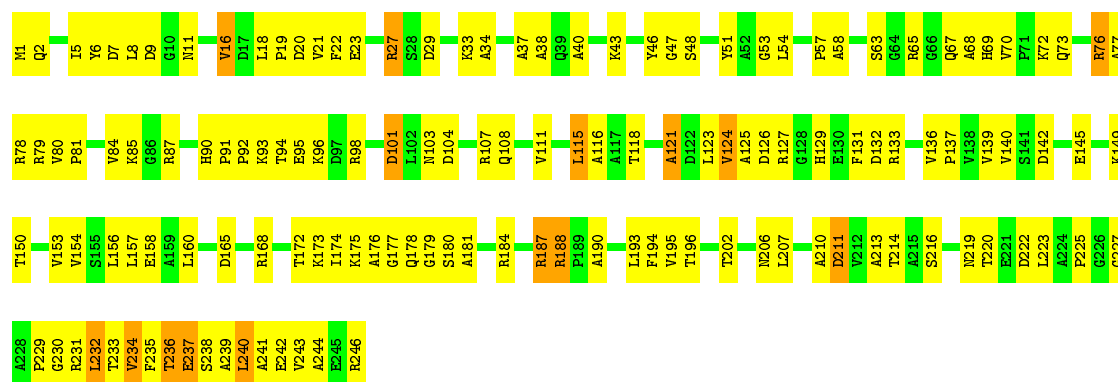
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	46	Total 46	O 46	0	0
41	P	72	Total 72	O 72	0	0
41	Q	52	Total 52	O 52	0	0
41	R	89	Total 89	O 89	0	0
41	S	35	Total 35	O 35	0	0
41	T	42	Total 42	O 42	0	0
41	U	29	Total 29	O 29	0	0
41	V	16	Total 16	O 16	0	0
41	W	75	Total 75	O 75	0	0
41	X	31	Total 31	O 31	0	0
41	Y	105	Total 105	O 105	0	0
41	Z	25	Total 25	O 25	0	0
41	0	5775	Total 5775	O 5775	0	0
41	1	57	Total 57	O 57	0	0
41	2	50	Total 50	O 50	0	0
41	3	66	Total 66	O 66	0	0
41	6	6	Total 6	O 6	0	0

### 3 Residue-property plots

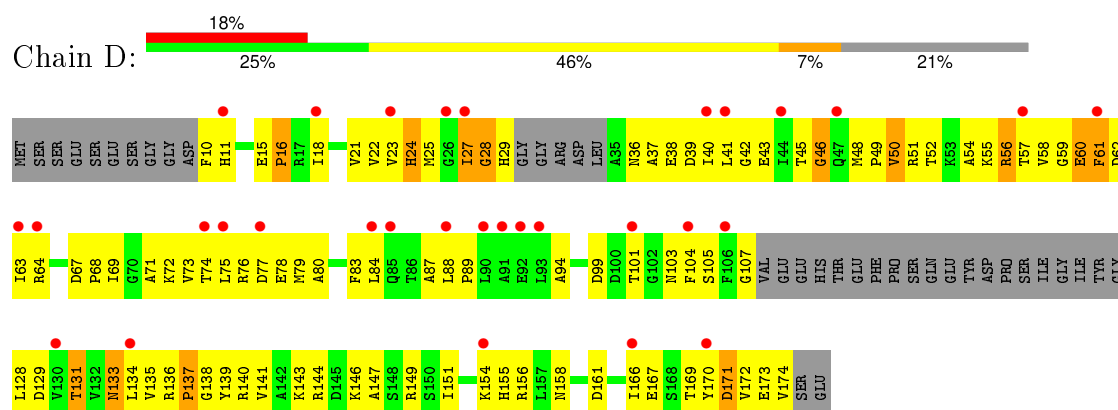
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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: 50S ribosomal protein L2P

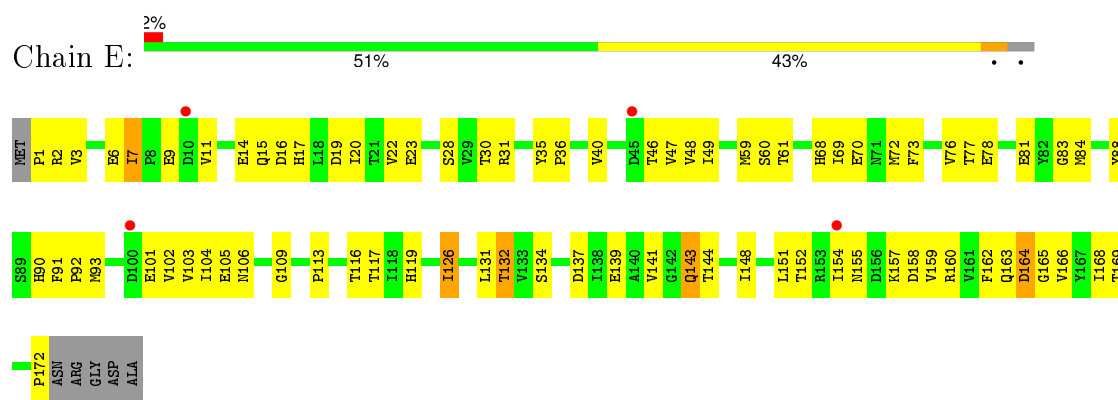




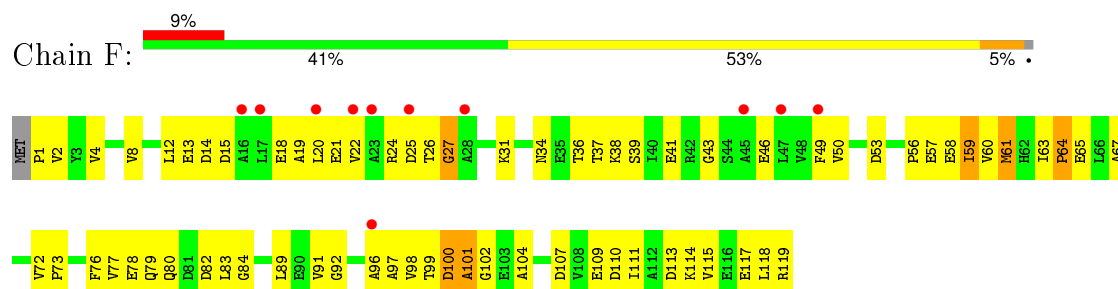
• Molecule 4: 50S ribosomal protein L5P



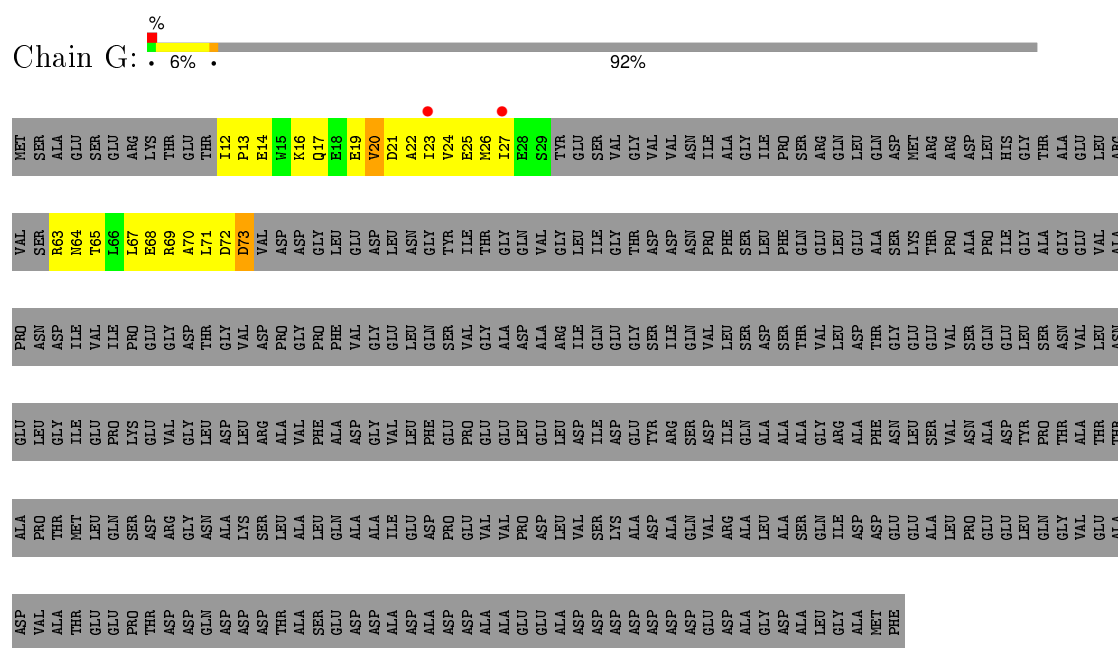
• Molecule 5: 50S ribosomal protein L6P



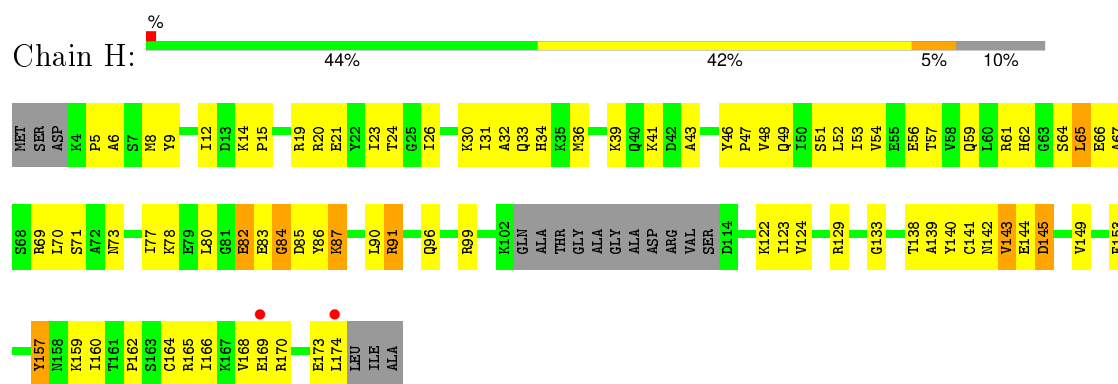
• Molecule 6: 50S ribosomal protein L7Ae



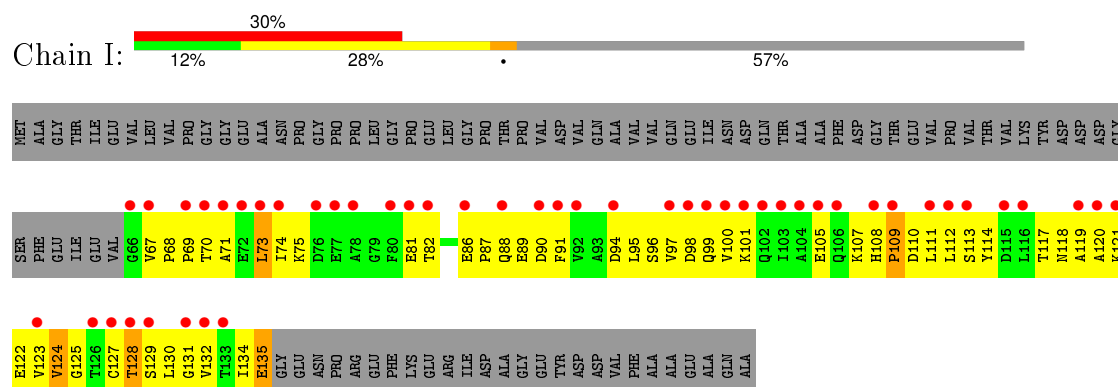
• Molecule 7: 50S ribosomal protein L10E



- Molecule 8: 50S ribosomal protein L10e

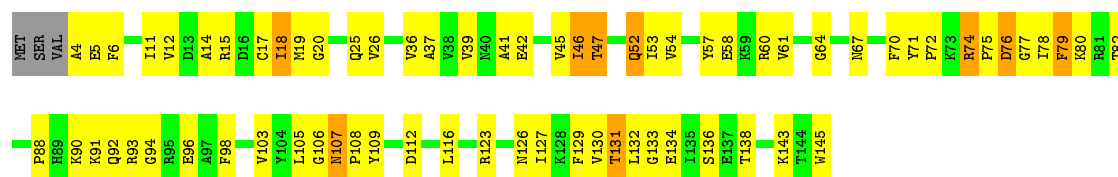


- Molecule 9: 50S ribosomal protein L11P



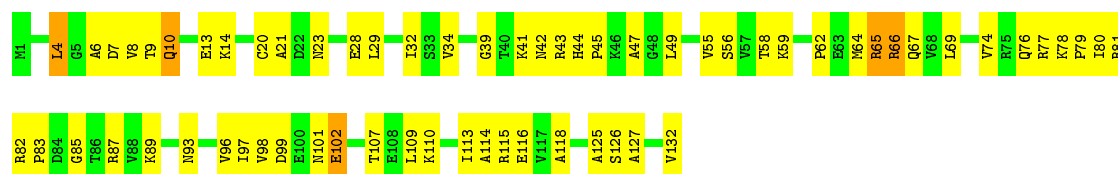
- Molecule 10: 50S ribosomal protein L13P





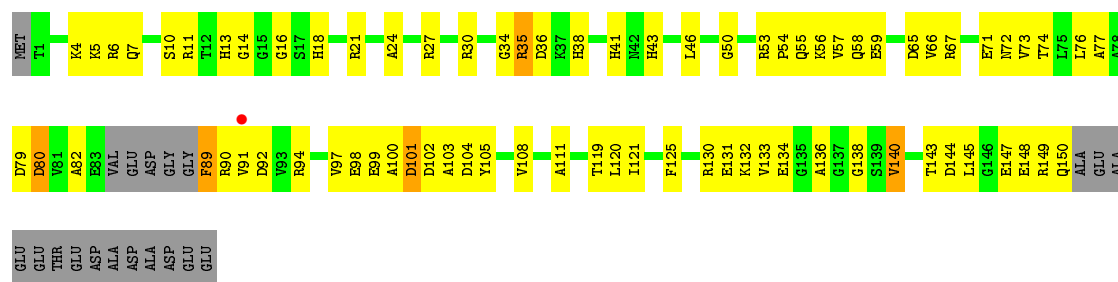
### • Molecule 11: 50S ribosomal protein L14P

Chain K: 52% 45%



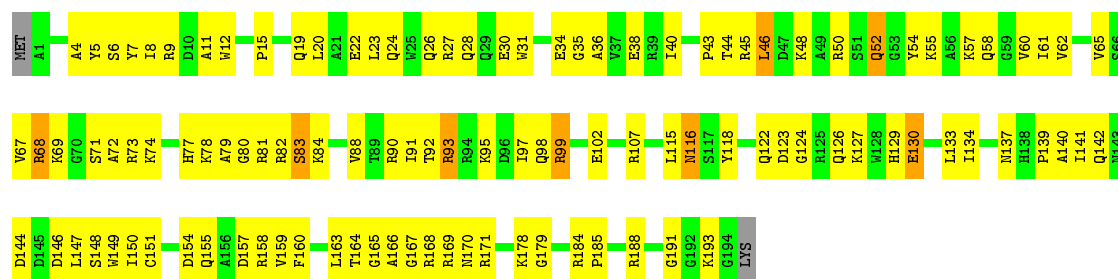
### • Molecule 12: 50S ribosomal protein L15P

Chain L: 42% 43% 12%



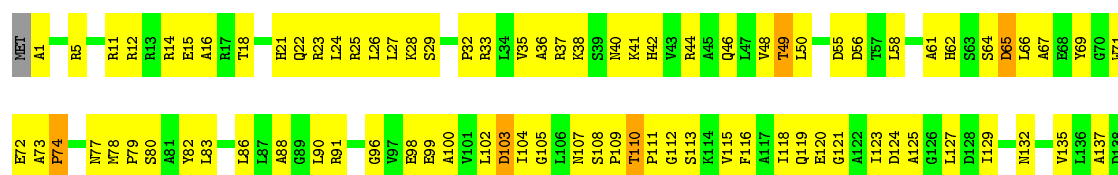
### • Molecule 13: 50S ribosomal protein L15e

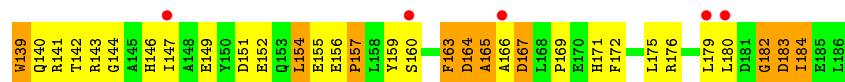
Chain M: 42% 53%



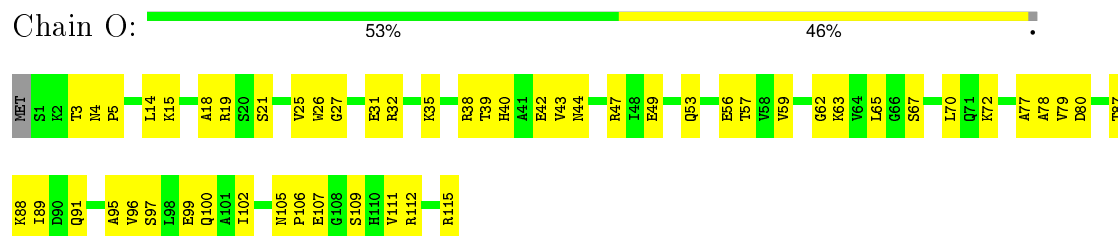
### • Molecule 14: 50S ribosomal protein L18P

Chain N: 3% 37% 54% 8%

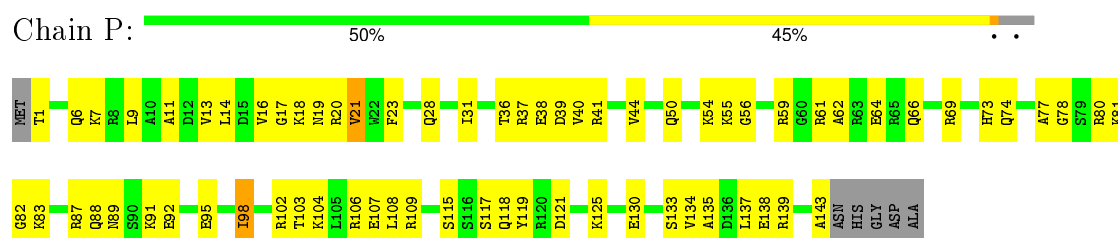




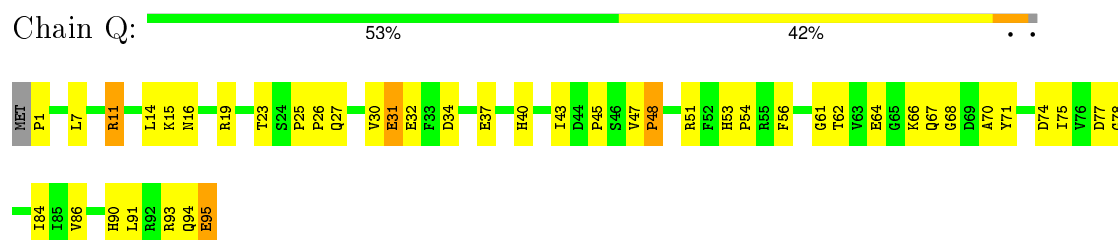
• Molecule 15: 50S ribosomal protein L18e



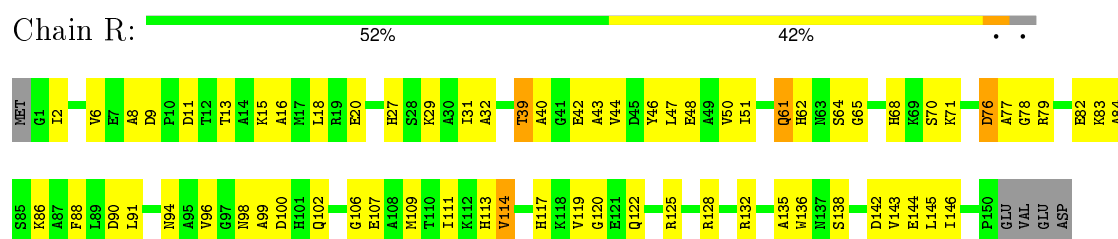
• Molecule 16: 50S ribosomal protein L19e



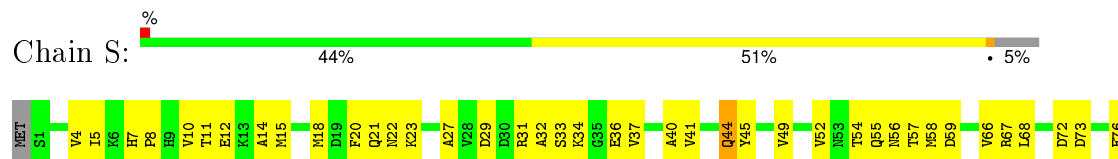
• Molecule 17: 50S ribosomal protein L21e

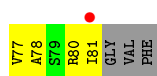


• Molecule 18: 50S ribosomal protein L22P

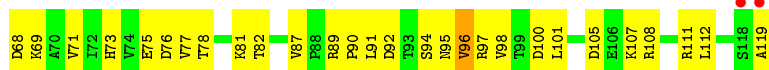
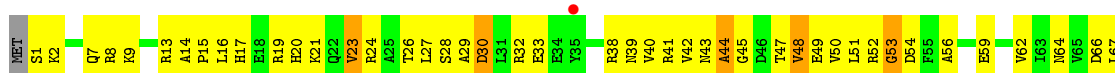


• Molecule 19: 50S ribosomal protein L23P

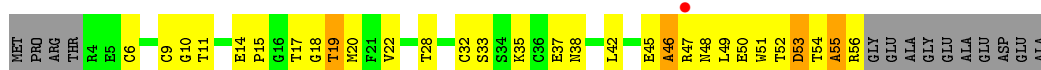




- Molecule 20: 50S ribosomal protein L24P



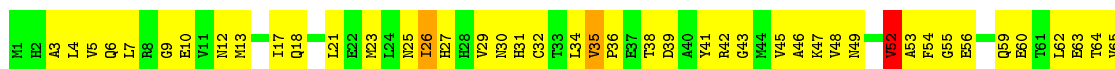
- Molecule 21: 50S ribosomal protein L24e



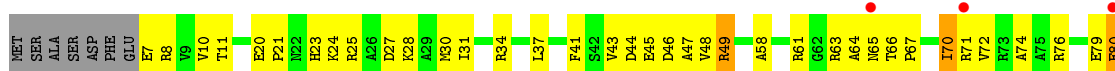
- Molecule 22: 50S ribosomal protein L29P

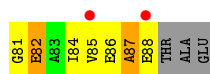


- Molecule 23: 50S ribosomal protein L30P

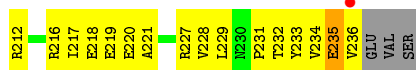
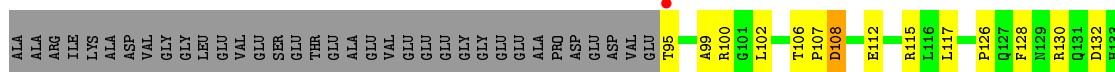
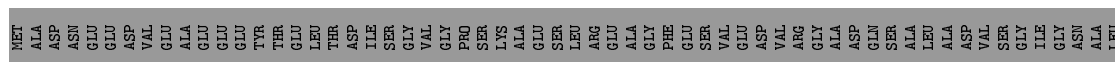
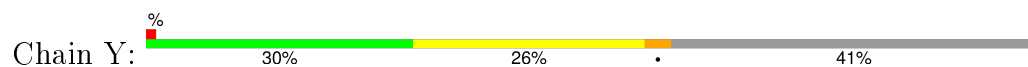


- Molecule 24: 50S ribosomal protein L31e

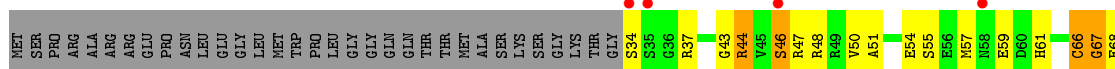
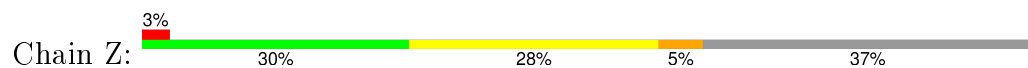




- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae



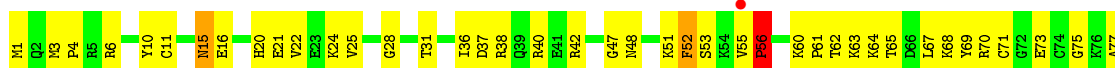
- Molecule 27: 50S ribosomal protein L37e

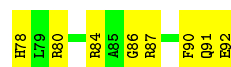


- Molecule 28: 50S ribosomal protein L39e

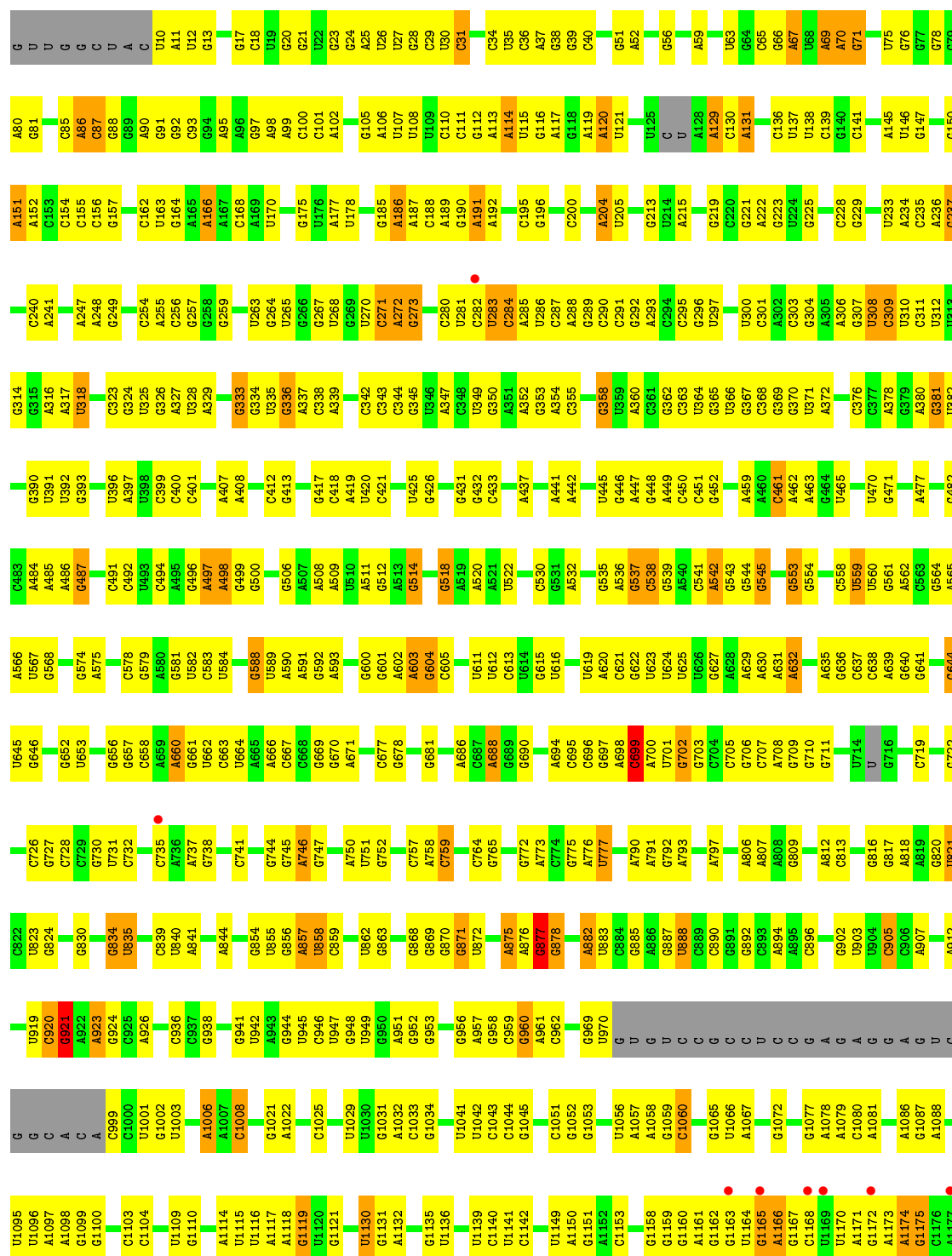


- Molecule 29: 50S ribosomal protein L44E

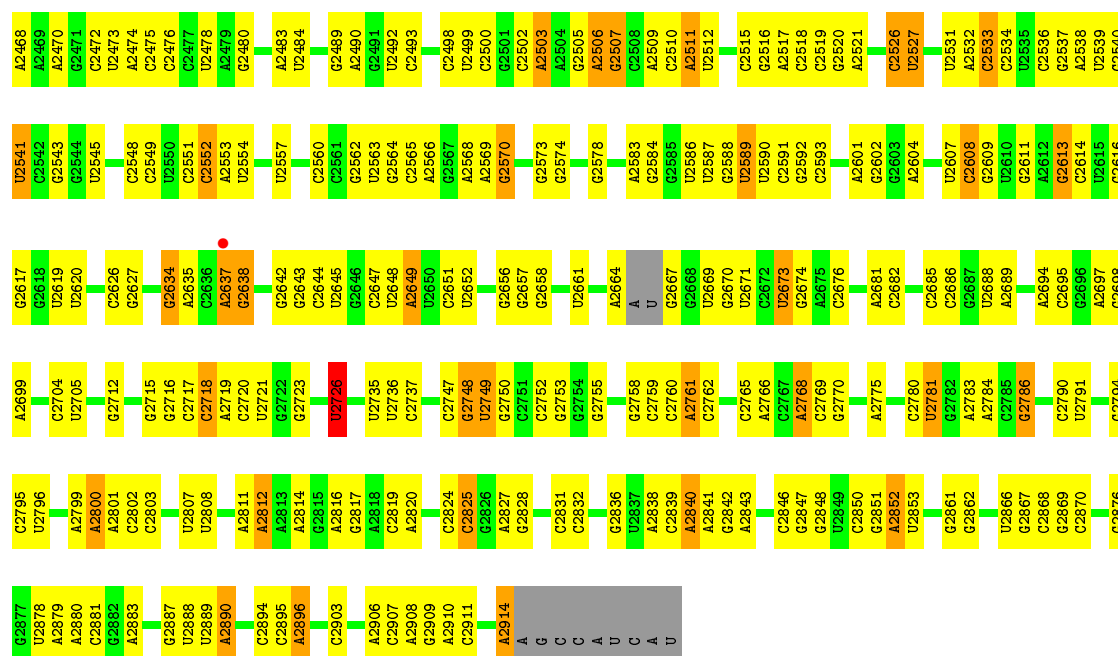




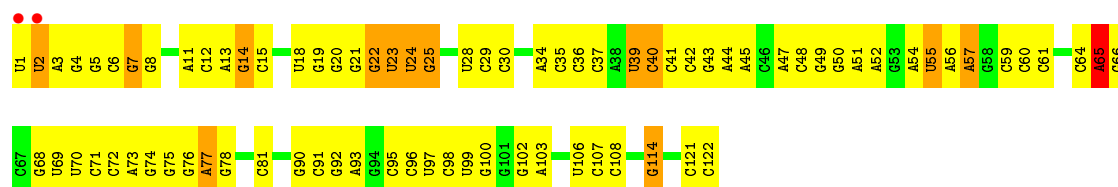
• Molecule 30: 50S RIBOSOMAL RNA



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C2508	C2428	C	C	C	C2066	C2066	U1896	C1823		C1658		A1297	
C2509	C2429	C	C	C	U1982	U1982	C1897	C1824		C1659		A1298	
C2510	C2430	C	C	C	U1983	U1983	C1898	C1825		C1660		A1299	
C2511	C2431	C	C	C	U198								



• Molecule 31: 5S RIBOSOMAL RNA



• Molecule 32: RNA (5'-R(\*C\*CP\*A)-3')



• Molecule 33: RNA (5'-R(\*CP\*CP\*(8AN))-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.79 Å   297.78 Å   572.59 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.82 – 2.95 85.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.82-2.95) 90.2 (85.07-2.39)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.198   ,   0.255 0.193   ,   0.245	Depositor DCC
$R_{free}$ test set	3661 reflections (1.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 83.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 667135 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	99194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: ACA, OMG, 8AN, CL, SR, NA, K, MG, CD, OMU, UR3, 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	A	0.37	0/1784	0.67	0/2403
2	B	0.36	0/2687	0.68	0/3644
3	C	0.38	0/1883	0.65	0/2547
4	D	0.33	0/1109	0.58	0/1493
5	E	0.35	0/1380	0.61	0/1875
6	F	0.36	0/899	0.60	0/1219
7	G	0.30	0/241	0.51	0/324
8	H	0.36	0/1300	0.67	0/1738
9	I	0.29	0/524	0.54	0/711
10	J	0.38	0/1134	0.62	0/1525
11	K	0.39	0/1002	0.68	0/1346
12	L	0.34	0/1128	0.65	0/1504
13	M	0.38	0/1580	0.61	0/2111
14	N	0.31	0/1472	0.66	1/1994 (0.1%)
15	O	0.35	0/872	0.64	0/1176
16	P	0.37	0/1145	0.56	0/1524
17	Q	0.36	0/747	0.68	0/1001
18	R	0.39	0/1170	0.66	0/1574
19	S	0.37	0/646	0.60	1/870 (0.1%)
20	T	0.35	0/956	0.64	0/1284
21	U	0.36	0/417	0.64	0/562
22	V	0.29	0/502	0.57	0/675
23	W	0.39	0/1217	1.24	2/1650 (0.1%)
24	X	0.35	0/662	0.61	0/890
25	Y	0.37	0/1146	0.65	0/1536
26	Z	0.36	0/582	0.62	0/776
27	1	0.41	0/438	0.62	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.40	0/769	0.61	0/1019
30	0	0.42	1/65948 (0.0%)	0.69	18/102852 (0.0%)
31	9	0.37	0/2894	0.71	0/4509
32	5	0.45	0/43	0.61	0/65

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	6	0.38	0/40	0.60	0/60
All	All	0.40	1/98718 (0.0%)	0.69	22/147564 (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
23	W	0	1
30	0	0	39
31	9	0	2
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	1942	A	O3'-P	-6.61	1.53	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	36.02	168.52	110.90
23	W	52	VAL	CA-CB-CG2	-23.54	75.59	110.90
30	0	1942	A	C5'-C4'-C3'	7.03	127.25	116.00
30	0	1942	A	OP2-P-O3'	6.73	120.00	105.20
30	0	1942	A	C5'-C4'-O4'	6.64	117.07	109.10
30	0	2467	A	C1'-O4'-C4'	-6.45	104.74	109.90
30	0	2291	A	N9-C1'-C2'	6.25	122.13	114.00
30	0	2726	U	N1-C1'-C2'	5.77	121.51	114.00
30	0	921	G	N9-C1'-C2'	5.53	121.19	114.00
30	0	1979	G	N9-C1'-C2'	5.44	121.07	114.00
30	0	1819	G	C5'-C4'-C3'	5.33	124.53	116.00
30	0	1942	A	C1'-O4'-C4'	-5.31	105.65	109.90
30	0	2313	C	C5'-C4'-C3'	5.24	124.39	116.00
30	0	1979	G	C2'-C3'-O3'	5.19	122.00	113.70
30	0	1701	A	C5'-C4'-C3'	5.18	124.29	116.00
14	N	163	PHE	N-CA-C	-5.18	97.02	111.00
19	S	27	ALA	N-CA-C	-5.17	97.04	111.00
30	0	1941	A	O3'-P-O5'	5.15	113.78	104.00
30	0	1504	A	C1'-O4'-C4'	-5.11	105.81	109.90
30	0	1504	A	N9-C1'-C2'	5.11	120.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	699	C	C1'-O4'-C4'	-5.06	105.85	109.90
30	0	2301	A	N9-C1'-C2'	5.02	120.53	114.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1309	U	Sidechain
30	0	1340	G	Sidechain
30	0	1358	A	Sidechain
30	0	1359	U	Sidechain
30	0	1380	U	Sidechain
30	0	1417	G	Sidechain
30	0	1635	U	Sidechain
30	0	1741	U	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1855	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	2043	U	Sidechain
30	0	2046	G	Sidechain
30	0	2065	C	Sidechain
30	0	2316	G	Sidechain
30	0	2478	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2557	U	Sidechain
30	0	2673	U	Sidechain
30	0	2781	U	Sidechain
30	0	2790	C	Sidechain
30	0	2840	A	Sidechain
30	0	333	G	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
30	0	63	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	688	A	Sidechain
30	0	722	G	Sidechain
30	0	877	G	Sidechain
30	0	888	U	Sidechain
31	9	65	A	Sidechain
31	9	90	G	Sidechain
23	W	90	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	1764	160	0
2	B	2624	0	2530	225	0
3	C	1859	0	1811	154	0
4	D	1093	0	1083	102	0
5	E	1356	0	1264	81	0
6	F	889	0	841	68	0
7	G	240	0	231	30	0
8	H	1281	0	1290	86	0
9	I	518	0	495	67	0
10	J	1119	0	1096	87	0
11	K	993	0	1025	77	0
12	L	1117	0	1071	85	0
13	M	1557	0	1571	130	0
14	N	1444	0	1399	140	0
15	O	864	0	868	60	0
16	P	1135	0	1120	68	0
17	Q	734	0	726	50	0
18	R	1148	0	1119	81	0
19	S	640	0	600	36	0
20	T	949	0	922	88	0
21	U	410	0	364	38	0
22	V	499	0	511	49	0
23	W	1195	0	1135	118	0
24	X	653	0	651	50	0
25	Y	1130	0	1133	82	0
26	Z	572	0	529	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	1	431	0	426	43	0
28	2	396	0	413	30	0
29	3	754	0	726	58	0
30	0	59017	0	29809	1406	0
31	9	2595	0	1322	96	0
32	5	39	0	24	3	0
33	6	59	0	35	6	0
34	6	19	0	20	0	0
35	0	82	0	0	0	0
35	2	1	0	0	0	0
35	9	1	0	0	0	0
35	A	3	0	0	0	0
35	B	2	0	0	0	0
35	C	1	0	0	0	0
35	K	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	65	0	0	0	0
36	9	3	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	87	0	0	1	0
37	1	2	0	0	0	0
37	3	3	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	2	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	T	2	0	0	0	0
37	Y	1	0	0	0	0
38	0	6	0	0	1	0
38	3	1	0	0	0	0
38	A	1	0	0	0	0
38	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	J	4	0	0	4	0
38	L	2	0	0	2	0
38	M	1	0	0	1	0
38	N	1	0	0	0	0
38	O	1	0	0	1	0
38	Q	1	0	0	1	0
38	R	1	0	0	0	0
38	Y	2	0	0	0	0
39	0	2	0	0	0	0
40	1	1	0	0	0	0
40	3	1	0	0	0	0
40	O	1	0	0	0	0
40	U	1	0	0	0	0
40	Z	1	0	0	0	0
41	0	5775	0	0	197	0
41	1	57	0	0	3	0
41	2	50	0	0	2	0
41	3	66	0	0	7	0
41	6	6	0	0	4	0
41	9	138	0	0	12	0
41	A	134	0	0	19	0
41	B	156	0	0	21	0
41	C	168	0	0	21	0
41	D	49	0	0	6	0
41	E	49	0	0	5	0
41	F	31	0	0	3	0
41	G	20	0	0	2	0
41	H	78	0	0	9	0
41	I	11	0	0	3	0
41	J	58	0	0	2	0
41	K	57	0	0	3	0
41	L	91	0	0	11	0
41	M	129	0	0	5	0
41	N	68	0	0	14	0
41	O	46	0	0	6	0
41	P	72	0	0	7	0
41	Q	52	0	0	3	0
41	R	89	0	0	5	0
41	S	35	0	0	1	0
41	T	42	0	0	5	0
41	U	29	0	0	3	0
41	V	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	W	75	0	0	10	0
41	X	31	0	0	5	0
41	Y	105	0	0	5	0
41	Z	25	0	0	6	0
All	All	99194	0	59924	3515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (3515) 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)
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.27	1.15
3:C:236:THR:HG22	3:C:239:ALA:H	1.00	1.13
37:O:8979:SR:SR	41:O:4399:HOH:O	0.84	1.13
14:N:37:ARG:HH12	31:9:6:C:H5''	1.10	1.09
30:0:870:G:H2'	30:0:871:G:H5''	1.30	1.08
14:N:37:ARG:NH1	31:9:6:C:H5''	1.69	1.07
31:9:76:G:H3'	31:9:77:A:H5''	1.29	1.07
10:J:52:GLN:HE22	30:0:1119:G:H2'	0.96	1.05
30:0:871:G:H5'	30:0:871:G:H8	1.17	1.05
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.39	1.05
6:F:91:VAL:HG12	6:F:92:GLY:H	1.18	1.05
30:0:1160:G:H5'	30:0:1161:A:H5'	1.39	1.04
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.39	1.04
22:V:1:THR:HG23	22:V:2:VAL:H	1.18	1.04
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.73	1.03
24:X:28:LYS:HD2	24:X:31:ILE:HD12	1.41	1.03
13:M:164:THR:HG22	13:M:166:ALA:H	1.18	1.03
10:J:82:THR:HG23	30:0:1242:A:H5'	1.40	1.03
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.41	1.03
30:0:871:G:C8	30:0:871:G:H5'	1.93	1.02
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.37	1.02
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.18	1.02
30:0:541:C:H2'	30:0:542:A:H5''	1.42	1.02
11:K:10:GLN:NE2	11:K:10:GLN:H	1.58	1.01
3:C:1:MET:HG2	3:C:2:GLN:H	1.25	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.05	0.98
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.42	0.98
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.45	0.98
30:0:2586:U:H3	30:0:2592:G:H22	1.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.06	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.29	0.96
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.48	0.96
2:B:36:PRO:HG3	2:B:169:GLY:H	1.30	0.95
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.43	0.95
30:0:2717:C:H2'	30:0:2718:C:H5''	1.47	0.95
14:N:144:GLY:O	14:N:147:ILE:HG22	1.66	0.95
30:0:1451:C:H5'	30:0:1505:U:C5	2.01	0.95
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.44	0.94
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.49	0.94
4:D:57:THR:HG23	4:D:63:ILE:HA	1.50	0.94
4:D:172:VAL:HG12	4:D:173:GLU:H	1.32	0.94
31:9:56:A:H2'	31:9:57:A:H5''	1.49	0.93
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.51	0.93
30:0:541:C:C2'	30:0:542:A:H5''	1.97	0.93
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.49	0.93
30:0:2506:A:HO2'	30:0:2507:G:H8	1.04	0.93
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.49	0.92
3:C:236:THR:HG22	3:C:239:ALA:N	1.85	0.92
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.52	0.91
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.50	0.91
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.04	0.91
18:R:39:THR:HB	18:R:42:GLU:HG3	1.50	0.90
2:B:179:LEU:O	2:B:183:GLU:HG2	1.71	0.90
30:0:506:G:H22	30:0:509:A:H5'	1.34	0.90
2:B:206:THR:HG21	30:0:2716:G:H5''	1.51	0.90
8:H:30:LYS:H	8:H:62:HIS:HD2	1.17	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.88
11:K:39:GLY:HA2	41:K:4183:HOH:O	1.73	0.88
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.53	0.88
3:C:233:THR:HG22	3:C:234:VAL:H	1.38	0.88
30:0:2005:G:H3'	30:0:2005:G:OP2	1.74	0.88
11:K:87:ARG:HB2	21:U:19:THR:HG23	1.53	0.88
11:K:10:GLN:H	11:K:10:GLN:HE21	1.19	0.88
3:C:236:THR:HG21	41:C:8580:HOH:O	1.74	0.88
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.54	0.87
13:M:164:THR:HG22	13:M:166:ALA:N	1.89	0.87
30:0:2291:A:C8	30:0:2309:C:H5'	2.09	0.87
5:E:15:GLN:HG2	5:E:19:ASP:O	1.74	0.87
1:A:153:ARG:CB	1:A:153:ARG:HH11	1.86	0.87
15:O:3:THR:HB	30:0:656:G:H5'	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:HG2	3:C:27:ARG:HH11	1.37	0.86
21:U:9:CYS:HA	21:U:52:THR:HG23	1.57	0.86
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.57	0.86
3:C:72:LYS:HG2	3:C:77:ALA:HA	1.56	0.86
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.05	0.86
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.56	0.86
30:0:1451:C:H5'	30:0:1505:U:H5	1.34	0.86
30:0:1559:A:H1'	41:0:6702:HOH:O	1.74	0.86
30:0:870:G:C2'	30:0:871:G:H5''	2.05	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD3	1.40	0.86
16:P:103:THR:HA	16:P:106:ARG:NH1	1.91	0.85
30:0:681:G:N3	30:0:681:G:H5'	1.91	0.85
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.85
1:A:109:GLU:HG2	1:A:116:GLY:H	1.42	0.85
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.56	0.85
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.58	0.85
4:D:25:MET:HE1	4:D:41:LEU:HG	1.57	0.85
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.58	0.85
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.73	0.85
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.58	0.85
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.55	0.85
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.40	0.84
20:T:28:SER:HA	20:T:97:ARG:HD3	1.59	0.84
12:L:55:GLN:HA	12:L:58:GLN:HE21	1.38	0.84
19:S:10:VAL:HG11	22:V:36:ALA:HB2	1.59	0.84
1:A:153:ARG:NH1	1:A:153:ARG:HB2	1.93	0.84
30:0:2717:C:C2'	30:0:2718:C:H5''	2.07	0.84
28:2:41:HIS:H	28:2:45:ASN:HD22	1.20	0.84
24:X:49:ARG:HG3	24:X:49:ARG:O	1.75	0.84
30:0:2812:A:H2	30:0:2814:A:H62	1.22	0.84
15:O:42:GLU:HB2	41:O:2176:HOH:O	1.77	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.41	0.84
31:9:29:C:H2'	31:9:30:C:H5'	1.59	0.84
30:0:1603:A:H5'	30:0:1605:G:O4'	1.77	0.84
30:0:1116:U:O2'	30:0:1118:A:H2	1.61	0.83
6:F:12:LEU:HD21	6:F:111:ILE:HG23	1.58	0.83
41:Z:8705:HOH:O	30:0:1886:A:H4'	1.78	0.83
12:L:35:ARG:HH11	12:L:35:ARG:HB2	1.41	0.83
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.60	0.83
30:0:1160:G:C5'	30:0:1161:A:H5'	2.07	0.83
32:5:75:C:H3'	32:5:76:A:H8	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:52:THR:HG22	21:U:54:THR:H	1.44	0.83
30:0:1184:C:H1'	41:0:9264:HOH:O	1.79	0.83
6:F:91:VAL:HG12	6:F:92:GLY:N	1.94	0.82
14:N:113:SER:HB2	41:N:8857:HOH:O	1.79	0.82
29:3:6:ARG:NH1	29:3:21:GLU:HG3	1.94	0.82
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.62	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.83	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.78	0.81
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.62	0.81
29:3:48:ASN:HD21	30:0:2468:A:H61	1.28	0.81
10:J:52:GLN:HG3	10:J:53:ILE:N	1.94	0.81
2:B:162:MET:HE1	2:B:310:ARG:HD2	1.63	0.81
15:O:21:SER:OG	15:O:106:PRO:HB2	1.80	0.81
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.43	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:1679:C:H5'	41:0:3235:HOH:O	1.78	0.81
16:P:38:GLU:HA	16:P:41:ARG:HD2	1.63	0.81
27:1:20:ARG:HG2	30:0:111:C:O2'	1.81	0.81
9:I:73:LEU:HD12	9:I:107:LYS:NZ	1.96	0.81
30:0:271:C:H41	30:0:378:A:H2	1.27	0.81
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.62	0.81
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.63	0.80
30:0:877:G:H5'	30:0:878:G:OP1	1.81	0.80
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.63	0.80
7:G:23:ILE:HD13	7:G:67:LEU:HD23	1.63	0.80
3:C:225:PRO:O	30:0:1308:A:H4'	1.82	0.80
18:R:99:ALA:HB1	18:R:109:MET:CE	2.12	0.80
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.64	0.80
30:0:1625:U:H4'	41:0:5524:HOH:O	1.80	0.80
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.61	0.80
3:C:103:ASN:ND2	30:0:663:C:H5''	1.95	0.80
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.63	0.80
30:0:1160:G:H5'	30:0:1161:A:C5'	2.12	0.80
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.64	0.80
18:R:18:LEU:HD12	18:R:143:VAL:HG11	1.63	0.80
30:0:2420:G:O2'	30:0:2421:G:H5'	1.82	0.79
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.62	0.79
1:A:26:ASP:HB2	41:0:4577:HOH:O	1.81	0.79
8:H:30:LYS:H	8:H:62:HIS:CD2	2.01	0.79
27:1:16:HIS:HD2	30:0:470:U:O2'	1.65	0.79
19:S:73:ASP:OD1	19:S:76:GLU:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:114:VAL:HB	18:R:145:LEU:HD12	1.64	0.79
30:0:1377:C:H6	30:0:1377:C:H5'	1.45	0.79
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.63	0.79
18:R:132:ARG:NH2	30:0:2055:A:H4'	1.98	0.79
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.79
21:U:14:GLU:O	21:U:17:THR:HB	1.83	0.78
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.23	0.78
30:0:2042:U:H1'	41:0:9124:HOH:O	1.82	0.78
23:W:80:ASP:O	23:W:84:VAL:HG23	1.84	0.78
1:A:33:GLU:H	1:A:33:GLU:CD	1.86	0.78
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.78
14:N:164:ASP:CG	14:N:167:ASP:HA	2.04	0.78
13:M:171:ARG:HD3	30:0:156:C:H5''	1.64	0.78
22:V:50:ARG:NH1	30:0:56:G:H5''	1.99	0.78
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.66	0.78
16:P:115:SER:OG	16:P:118:GLN:HG3	1.84	0.78
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.64	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.63	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.78
6:F:58:GLU:CD	13:M:27:ARG:HH22	1.87	0.78
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.64	0.78
12:L:92:ASP:HA	12:L:121:ILE:HB	1.66	0.78
1:A:199:HIS:CD2	1:A:201:PHE:H	2.02	0.78
18:R:39:THR:HG23	18:R:107:GLU:O	1.83	0.78
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.82	0.77
2:B:162:MET:CE	2:B:310:ARG:HD2	2.14	0.77
14:N:40:ASN:HD21	31:9:28:U:H5''	1.49	0.77
14:N:40:ASN:ND2	31:9:28:U:H5''	2.00	0.77
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.15	0.77
1:A:179:MET:HA	1:A:179:MET:CE	2.14	0.77
2:B:275:GLY:O	2:B:291:ASP:HA	1.84	0.77
23:W:137:GLN:HE21	23:W:141:HIS:CE1	1.98	0.77
3:C:27:ARG:HG2	3:C:27:ARG:NH1	1.95	0.77
1:A:191:GLY:HA2	1:A:194:MET:CE	2.14	0.77
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.48	0.77
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.67	0.77
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.67	0.76
22:V:12:THR:HG22	22:V:15:GLU:CG	2.16	0.76
1:A:66:ARG:HH11	1:A:66:ARG:HB2	1.50	0.76
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.66	0.76
30:0:541:C:H2'	30:0:542:A:C5'	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1835:U:H5	30:0:1840:A:N7	1.83	0.76
7:G:64:ASN:O	7:G:68:GLU:HG3	1.86	0.76
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.65	0.76
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.19	0.76
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.49	0.76
2:B:267:LYS:HD3	41:0:3465:HOH:O	1.85	0.76
12:L:90:ARG:HA	12:L:119:THR:HB	1.67	0.76
10:J:131:THR:HG22	10:J:134:GLU:H	1.51	0.76
30:0:2661:U:H3	30:0:2812:A:H62	1.32	0.76
3:C:236:THR:H	3:C:239:ALA:HB3	1.51	0.76
30:0:1116:U:H3	30:0:1246:A:H62	1.32	0.76
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.21	0.76
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.69	0.75
13:M:80:GLY:O	13:M:81:ARG:HD2	1.86	0.75
30:0:871:G:C5'	30:0:871:G:H8	1.95	0.75
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.07	0.75
30:0:1118:A:H8	30:0:1119:G:H5''	1.51	0.75
32:5:75:C:H3'	32:5:76:A:C8	2.21	0.75
24:X:43:VAL:HG12	24:X:44:ASP:H	1.51	0.75
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.16	0.75
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.66	0.75
30:0:1730:G:H5'	30:0:1731:C:C5	2.22	0.75
1:A:203:GLY:HA2	41:0:3401:HOH:O	1.87	0.75
30:0:2578:G:H5'	30:0:2578:G:H8	1.50	0.75
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.69	0.75
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.74
4:D:170:TYR:O	4:D:171:ASP:HB3	1.87	0.74
22:V:1:THR:HG23	22:V:2:VAL:N	1.99	0.74
15:O:57:THR:O	15:O:111:VAL:HG23	1.87	0.74
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.68	0.74
3:C:180:SER:HB2	41:C:8643:HOH:O	1.86	0.74
4:D:105:SER:HB2	4:D:131:THR:HG23	1.70	0.74
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.69	0.74
30:0:530:C:H4'	30:0:612:U:H4'	1.69	0.74
30:0:625:U:H3'	41:0:4150:HOH:O	1.87	0.74
9:I:101:LYS:O	9:I:105:GLU:HG3	1.87	0.74
22:V:12:THR:HG22	22:V:15:GLU:OE2	1.87	0.74
24:X:61:ARG:HB2	24:X:65:ASN:HB2	1.69	0.74
30:0:1206:U:H5'	30:0:1206:U:H6	1.51	0.74
14:N:169:PRO:O	14:N:172:PHE:HB3	1.88	0.74
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:292:G:H2'	30:0:358:G:N2	2.02	0.74
25:Y:189:ASN:CA	25:Y:217:ILE:HD11	2.16	0.74
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.22	0.74
7:G:12:ILE:HG23	41:0:6301:HOH:O	1.88	0.74
14:N:119:GLN:O	14:N:123:ILE:HG13	1.87	0.74
14:N:86:LEU:O	14:N:90:LEU:HG	1.88	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.52	0.74
30:0:1878:G:H5'	41:0:5236:HOH:O	1.87	0.73
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.18	0.73
30:0:1452:G:H1'	38:0:8803:CL:CL	2.25	0.73
30:0:2073:G:H5''	41:0:4699:HOH:O	1.88	0.73
2:B:27:ASN:HD21	30:0:2807:U:P	2.11	0.73
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.71	0.73
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.52	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.87	0.73
18:R:82:GLU:HG3	18:R:83:LYS:N	2.04	0.73
30:0:1119:G:N2	30:0:1246:A:C2	2.56	0.73
41:M:8871:HOH:O	30:0:381:G:H5''	1.89	0.73
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.53	0.73
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.71	0.73
24:X:72:VAL:HG22	24:X:85:VAL:CG1	2.19	0.72
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.70	0.72
4:D:57:THR:HA	41:D:5728:HOH:O	1.89	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.70	0.72
31:9:50:G:H2'	31:9:51:A:C8	2.24	0.72
18:R:39:THR:HB	18:R:42:GLU:CG	2.18	0.72
14:N:110:THR:HB	14:N:113:SER:OG	1.89	0.72
14:N:112:GLY:HA2	14:N:137:ALA:H	1.54	0.72
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.71	0.72
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.24	0.72
30:0:78:G:N3	30:0:78:G:N2	2.37	0.72
10:J:77:GLY:HA2	10:J:80:LYS:H	1.54	0.72
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.54	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.38	0.72
20:T:2:LYS:HG2	30:0:447:A:OP1	1.90	0.72
30:0:558:C:H2'	30:0:559:U:H5''	1.71	0.72
27:1:1:THR:HA	41:1:435:HOH:O	1.89	0.72
12:L:143:THR:HG22	12:L:145:LEU:H	1.55	0.72
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:LEU:HA	41:B:9050:HOH:O	1.90	0.72
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.72	0.71
30:0:855:U:H3'	41:0:4510:HOH:O	1.89	0.71
30:0:558:C:C2'	30:0:559:U:H5''	2.19	0.71
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.71	0.71
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.70	0.71
6:F:96:ALA:HA	41:F:3111:HOH:O	1.88	0.71
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.73	0.71
30:0:2356:A:H2'	30:0:2357:G:O4'	1.91	0.71
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.04	0.71
30:0:2296:C:H2'	30:0:2297:U:H6	1.55	0.71
22:V:12:THR:CG2	22:V:15:GLU:HG3	2.20	0.71
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.71
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.36	0.71
30:0:1838:U:O2'	30:0:2644:C:H5'	1.90	0.71
30:0:1667:A:H5'	30:0:1667:A:C8	2.25	0.71
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.70	0.71
18:R:82:GLU:HG3	18:R:83:LYS:H	1.55	0.71
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.56	0.71
22:V:39:ALA:N	22:V:40:PRO:HD2	2.05	0.71
22:V:1:THR:CG2	22:V:2:VAL:H	2.00	0.70
6:F:58:GLU:HA	6:F:61:MET:CE	2.21	0.70
24:X:49:ARG:HG2	24:X:84:ILE:HG12	1.72	0.70
18:R:6:VAL:HG21	18:R:113:HIS:CD2	2.25	0.70
30:0:1701:A:H4'	30:0:1702:U:H5''	1.72	0.70
3:C:194:PHE:HA	3:C:234:VAL:HG13	1.73	0.70
1:A:36:ASP:O	1:A:38:ILE:N	2.23	0.70
30:0:1372:A:H3'	41:0:7993:HOH:O	1.91	0.70
17:Q:66:LYS:HB2	17:Q:70:ALA:O	1.91	0.70
30:0:1474:C:C6	30:0:1474:C:H5'	2.24	0.70
14:N:164:ASP:OD1	14:N:167:ASP:HA	1.91	0.70
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.71	0.70
14:N:11:ARG:HD3	31:9:114:G:O6	1.91	0.70
14:N:132:ASN:O	14:N:135:VAL:HG12	1.92	0.70
3:C:1:MET:HG2	3:C:2:GLN:N	2.04	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.89	0.70
30:0:2851:G:O2'	30:0:2852:A:H5'	1.90	0.70
20:T:54:ASP:OD2	30:0:316:A:H5'	1.90	0.70
30:0:2908:A:H2'	30:0:2909:G:O4'	1.92	0.70
5:E:84:MET:HG2	5:E:168:ILE:HA	1.73	0.70
27:1:9:GLY:HA2	30:0:1687:C:O2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.73	0.70
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.72	0.70
18:R:128:ARG:NH2	30:0:2054:A:N3	2.39	0.70
3:C:27:ARG:CG	3:C:27:ARG:HH11	2.05	0.70
13:M:164:THR:CG2	13:M:166:ALA:H	2.02	0.69
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.73	0.69
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.69
13:M:57:LYS:HE2	13:M:140:ALA:O	1.92	0.69
3:C:84:VAL:HG12	3:C:85:LYS:HG2	1.72	0.69
8:H:36:MET:HB3	8:H:73:ASN:ND2	2.07	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.27	0.69
30:0:1829:A:H2'	30:0:1830:C:H5'	1.74	0.69
30:0:236:A:H4'	30:0:237:G:H5'	1.74	0.69
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.69
30:0:1634:G:H3'	41:0:4766:HOH:O	1.92	0.69
3:C:233:THR:HG22	3:C:234:VAL:N	2.07	0.69
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.23	0.69
8:H:31:ILE:HA	8:H:66:GLU:OE1	1.93	0.69
26:Z:46:SER:O	26:Z:50:VAL:HG23	1.92	0.69
31:9:75:G:H1	31:9:106:U:H3	1.39	0.69
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.74	0.69
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.23	0.69
25:Y:117:LEU:HD13	25:Y:174:VAL:HG11	1.73	0.69
30:0:2637:A:H4'	30:0:2638:G:C5'	2.23	0.69
30:0:1205:U:H2'	30:0:1206:U:C5'	2.22	0.69
13:M:24:GLN:NE2	13:M:27:ARG:HD2	2.07	0.69
2:B:175:LEU:O	2:B:175:LEU:HD23	1.93	0.69
25:Y:234:VAL:HG12	25:Y:235:GLU:H	1.56	0.69
30:0:2102:G:H2'	41:0:9555:HOH:O	1.93	0.69
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.74	0.69
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.08	0.69
30:0:2004:U:H2'	30:0:2004:U:O2	1.93	0.69
30:0:2387:U:H2'	30:0:2388:C:C6	2.28	0.69
23:W:52:VAL:HG23	23:W:53:ALA:N	1.64	0.69
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.22	0.69
22:V:11:MET:HB3	22:V:15:GLU:HB2	1.73	0.68
1:A:199:HIS:HD2	1:A:201:PHE:H	1.38	0.68
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.09	0.68
24:X:25:ARG:HD3	24:X:64:ALA:O	1.93	0.68
17:Q:16:ASN:HD21	17:Q:45:PRO:HD2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
2:B:229:ARG:HD2	41:B:8991:HOH:O	1.93	0.68
3:C:193:LEU:HD13	3:C:222:ASP:HB2	1.76	0.68
30:0:2247:C:H2'	30:0:2248:C:H6	1.59	0.68
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.76	0.68
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.23	0.68
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.23	0.68
23:W:38:THR:HG22	23:W:39:ASP:N	2.09	0.68
1:A:139:LYS:HE2	1:A:143:GLY:HA2	1.76	0.68
10:J:4:ALA:O	10:J:5:GLU:HB2	1.94	0.68
16:P:139:ARG:HH11	16:P:139:ARG:HG3	1.58	0.68
30:0:1300:G:H1'	41:0:5541:HOH:O	1.91	0.68
30:0:304:G:H1'	30:0:347:A:N6	2.08	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.86	0.68
14:N:5:ARG:NH1	30:0:962:C:H1'	2.09	0.68
8:H:6:ALA:HB3	30:0:2521:A:OP2	1.94	0.68
4:D:135:VAL:HG21	4:D:139:TYR:CG	2.28	0.68
6:F:14:ASP:O	6:F:18:GLU:HG3	1.94	0.68
30:0:2851:G:C2'	30:0:2852:A:H5'	2.24	0.68
23:W:13:MET:CE	23:W:17:ILE:HG22	2.24	0.68
30:0:558:C:H2'	30:0:559:U:C5'	2.24	0.68
3:C:153:VAL:O	3:C:157:LEU:HG	1.94	0.68
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.87	0.68
30:0:282:C:O2'	30:0:283:U:H5'	1.93	0.68
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.75	0.68
2:B:214:PRO:HD2	41:0:2996:HOH:O	1.92	0.68
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.67
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.67
25:Y:170:SER:OG	25:Y:175:ARG:HG3	1.94	0.67
23:W:84:VAL:HG12	41:W:6679:HOH:O	1.94	0.67
30:0:2588:OMG:HN21	32:5:76:A:H2	1.40	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.59	0.67
6:F:83:LEU:HD11	6:F:96:ALA:HB3	1.76	0.67
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.76	0.67
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.76	0.67
22:V:1:THR:HB	30:0:93:C:H5''	1.77	0.67
29:3:25:VAL:HG13	29:3:68:LYS:HE3	1.75	0.67
12:L:6:ARG:HD3	30:0:1299:G:O6	1.94	0.67
22:V:56:ILE:O	22:V:60:GLN:HG3	1.93	0.67
10:J:54:VAL:O	10:J:58:GLU:HG3	1.95	0.67
18:R:117:HIS:HD2	30:0:20:G:H21	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:ILE:HD11	4:D:37:ALA:CB	2.25	0.67
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
21:U:11:THR:HG22	21:U:53:ASP:HB2	1.77	0.67
3:C:211:ASP:HB2	3:C:231:ARG:HH22	1.60	0.67
2:B:74:ILE:HG22	2:B:76:THR:HG23	1.76	0.67
1:A:201:PHE:HA	41:A:9065:HOH:O	1.94	0.67
30:0:2073:G:OP2	30:0:2490:A:H5'	1.94	0.67
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.76	0.67
31:9:18:U:H2'	31:9:19:G:H8	1.59	0.67
2:B:321:PRO:HA	41:B:9136:HOH:O	1.94	0.67
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.25	0.67
8:H:48:VAL:HA	8:H:170:ARG:O	1.94	0.67
5:E:101:GLU:HB3	5:E:117:THR:HA	1.75	0.67
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.23	0.67
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.77	0.67
31:9:49:G:H5''	41:9:9086:HOH:O	1.95	0.67
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.67
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.67
11:K:41:LYS:HE2	11:K:42:ASN:HD21	1.60	0.67
30:0:1058:A:H2'	30:0:1060:C:C5'	2.25	0.67
1:A:103:VAL:O	1:A:105:VAL:HG23	1.95	0.67
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.41	0.67
30:0:1730:G:H5'	30:0:1731:C:C6	2.30	0.67
3:C:174:ILE:CD1	30:0:338:C:H4'	2.25	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.67
30:0:451:C:O2'	30:0:452:G:H5'	1.95	0.67
30:0:2047:C:H5'	41:0:3722:HOH:O	1.95	0.67
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.25	0.66
30:0:2102:G:H1'	41:0:6120:HOH:O	1.94	0.66
23:W:122:ARG:NH2	23:W:154:ARG:HB3	2.10	0.66
5:E:23:GLU:HG2	5:E:28:SER:CB	2.25	0.66
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	0.66
18:R:16:ALA:HB1	18:R:94:ASN:HD22	1.60	0.66
30:0:1766:U:O2	30:0:1778:A:H5'	1.95	0.66
2:B:235:ARG:HD3	30:0:2091:G:O3'	1.95	0.66
12:L:55:GLN:HA	12:L:58:GLN:NE2	2.07	0.66
27:1:16:HIS:HE1	30:0:775:G:OP1	1.79	0.66
30:0:1461:U:H2'	30:0:1462:C:C6	2.31	0.66
3:C:236:THR:CG2	3:C:239:ALA:H	1.93	0.66
30:0:1666:C:O2'	30:0:1667:A:H5''	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:9:LYS:HD2	41:0:4631:HOH:O	1.96	0.66
4:D:131:THR:HG21	30:0:2348:C:H1'	1.77	0.66
18:R:68:HIS:CD2	18:R:76:ASP:HB2	2.30	0.66
22:V:26:GLU:OE2	22:V:45:ARG:HD3	1.95	0.66
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.10	0.66
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.66
6:F:26:THR:HG21	6:F:102:GLY:C	2.16	0.66
13:M:31:TRP:HA	13:M:34:GLU:HG3	1.78	0.66
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.75	0.66
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.66
30:0:2769:C:H2'	30:0:2770:G:O4'	1.95	0.66
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.76	0.66
30:0:1666:C:H2'	30:0:1667:A:H5'	1.78	0.66
21:U:45:GLU:HB2	21:U:48:ASN:HD22	1.60	0.66
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.78	0.66
24:X:80:GLU:HB3	41:X:5564:HOH:O	1.96	0.66
2:B:211:THR:HG23	30:0:2840:A:OP1	1.96	0.66
14:N:36:ALA:HB1	14:N:118:ILE:HD12	1.77	0.66
30:0:1171:A:H2'	30:0:1172:G:H5'	1.78	0.66
30:0:1118:A:H3'	30:0:1118:A:C8	2.30	0.66
20:T:48:VAL:HG23	20:T:98:VAL:HA	1.78	0.66
30:0:946:C:H2'	30:0:947:U:H6	1.61	0.66
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.77	0.66
3:C:246:ARG:NH1	3:C:246:ARG:HB3	2.11	0.66
18:R:39:THR:CB	18:R:42:GLU:HG3	2.24	0.65
1:A:33:GLU:O	1:A:34:ASP:HB2	1.95	0.65
25:Y:235:GLU:CD	25:Y:235:GLU:H	1.98	0.65
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.77	0.65
33:6:76:8AN:C2	41:6:82:HOH:O	2.44	0.65
3:C:111:VAL:HB	41:C:8521:HOH:O	1.95	0.65
10:J:25:GLN:HE22	10:J:116:LEU:HB3	1.61	0.65
1:A:88:ILE:HG22	1:A:88:ILE:O	1.96	0.65
3:C:156:LEU:O	3:C:160:LEU:HG	1.96	0.65
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.19	0.65
4:D:173:GLU:O	4:D:174:VAL:O	2.13	0.65
10:J:19:MET:HE2	10:J:79:PHE:HA	1.77	0.65
21:U:45:GLU:HB2	21:U:48:ASN:ND2	2.11	0.65
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.27	0.65
8:H:5:PRO:O	8:H:8:MET:HB2	1.95	0.65
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:23:U:O2'	31:9:24:U:H4'	1.95	0.65
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.79	0.65
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.79	0.65
31:9:76:G:C3'	31:9:77:A:H5''	2.16	0.65
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.27	0.65
1:A:207:GLN:HA	41:A:9036:HOH:O	1.95	0.65
19:S:22:ASN:ND2	19:S:68:LEU:HB2	2.12	0.65
3:C:242:GLU:HG3	41:C:8587:HOH:O	1.95	0.65
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.25	0.65
10:J:76:ASP:HA	41:J:5907:HOH:O	1.97	0.65
6:F:84:GLY:O	6:F:89:LEU:HB2	1.95	0.65
30:0:1201:C:H5''	41:0:7064:HOH:O	1.96	0.65
23:W:139:GLY:O	23:W:141:HIS:HD2	1.79	0.65
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.11	0.65
16:P:121:ASP:O	16:P:125:LYS:HG3	1.96	0.65
30:0:168:C:H5''	41:0:3347:HOH:O	1.96	0.65
14:N:78:MET:HB2	14:N:146:HIS:CE1	2.32	0.65
9:I:127:CYS:C	9:I:129:SER:H	2.00	0.65
30:0:2387:U:H2'	30:0:2388:C:H6	1.61	0.65
9:I:82:THR:HG23	30:0:1168:C:H5''	1.79	0.65
6:F:27:GLY:HA3	6:F:101:ALA:O	1.97	0.65
6:F:46:GLU:O	6:F:73:PRO:HD2	1.97	0.65
30:0:506:G:H22	30:0:509:A:C5'	2.07	0.64
31:9:13:A:O2'	31:9:14:G:H5''	1.97	0.64
30:0:545:G:C8	30:0:545:G:H5'	2.29	0.64
2:B:77:PRO:HA	2:B:293:PRO:HB2	1.79	0.64
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.79	0.64
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.79	0.64
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.79	0.64
30:0:1118:A:H3'	30:0:1118:A:H8	1.62	0.64
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.64
28:2:41:HIS:CD2	28:2:44:ARG:H	2.14	0.64
21:U:6:CYS:O	21:U:10:GLY:HA2	1.98	0.64
30:0:1136:U:H2'	41:0:5826:HOH:O	1.96	0.64
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.28	0.64
20:T:48:VAL:CG2	20:T:96:VAL:HG13	2.28	0.64
30:0:2637:A:H4'	30:0:2638:G:H5'	1.79	0.64
3:C:5:ILE:HD11	3:C:16:VAL:HG22	1.79	0.64
27:1:28:HIS:HD2	27:1:30:LYS:H	1.45	0.64
30:0:660:A:H4'	30:0:661:G:O5'	1.98	0.64
17:Q:95:GLU:HA	30:0:949:U:H4'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:37:THR:O	6:F:41:GLU:HG3	1.97	0.64
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.80	0.64
14:N:182:GLY:O	14:N:184:ILE:HG22	1.97	0.64
6:F:57:GLU:O	6:F:61:MET:HG3	1.98	0.64
15:O:65:LEU:HD13	30:0:746:A:C6	2.32	0.64
30:0:2540:G:O2'	30:0:2541:U:H5''	1.98	0.64
14:N:160:SER:HB3	31:9:51:A:H5'	1.80	0.64
16:P:7:LYS:HD3	16:P:23:PHE:CZ	2.32	0.64
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.80	0.64
19:S:33:SER:O	19:S:37:VAL:HG23	1.97	0.64
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.45	0.64
13:M:68:ARG:HD3	13:M:68:ARG:O	1.98	0.64
8:H:14:LYS:HE2	41:0:4718:HOH:O	1.98	0.64
21:U:9:CYS:SG	21:U:11:THR:HG23	2.38	0.64
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	1.79	0.64
2:B:211:THR:HG21	41:0:9253:HOH:O	1.98	0.64
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.79	0.64
31:9:2:U:OP2	31:9:3:A:H5'	1.96	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.56	0.64
9:I:110:ASP:O	30:0:1163:G:H5'	1.98	0.64
30:0:316:A:N3	30:0:336:G:O2'	2.31	0.64
16:P:1:THR:O	30:0:1396:C:H1'	1.97	0.64
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.11	0.64
22:V:50:ARG:HH12	30:0:56:G:H5''	1.60	0.64
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.63	0.64
2:B:62:ARG:HA	2:B:65:MET:CE	2.28	0.64
3:C:246:ARG:HH11	3:C:246:ARG:HB3	1.63	0.63
20:T:16:LEU:HB2	30:0:100:C:H4'	1.80	0.63
9:I:96:SER:HB3	9:I:99:GLN:HE21	1.61	0.63
31:9:59:C:H2'	31:9:60:C:C6	2.33	0.63
10:J:90:LYS:HB2	38:J:8802:CL:CL	2.35	0.63
6:F:91:VAL:CG1	6:F:92:GLY:H	2.02	0.63
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.62	0.63
6:F:58:GLU:HA	6:F:61:MET:HE2	1.79	0.63
31:9:29:C:C2'	31:9:30:C:H5'	2.29	0.63
29:3:73:GLU:HB3	41:3:9050:HOH:O	1.97	0.63
18:R:51:ILE:HD13	18:R:86:LYS:HG2	1.79	0.63
1:A:11:ARG:NH1	41:A:9044:HOH:O	2.31	0.63
29:3:62:THR:HB	41:3:9041:HOH:O	1.98	0.63
2:B:139:ASP:OD2	2:B:165:ARG:HD2	1.97	0.63
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:32:ARG:HD3	15:O:32:ARG:O	1.98	0.63
12:L:67:ARG:O	12:L:71:GLU:HG3	1.99	0.63
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.80	0.63
30:O:1042:U:O2'	30:O:1043:C:H5'	1.98	0.63
11:K:125:ALA:C	11:K:127:ALA:H	2.02	0.63
30:O:1189:A:H3'	41:O:9471:HOH:O	1.98	0.63
23:W:88:THR:HB	41:W:6679:HOH:O	1.99	0.63
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.81	0.63
21:U:14:GLU:OE1	21:U:15:PRO:HD2	1.98	0.63
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.61	0.63
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.29	0.63
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.34	0.63
1:A:8:ARG:HG2	41:A:9031:HOH:O	1.96	0.63
3:C:104:ASP:O	3:C:108:GLN:HG3	1.98	0.63
7:G:16:LYS:O	7:G:20:VAL:HG23	1.98	0.63
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.34	0.63
30:O:1183:C:H2'	41:O:7072:HOH:O	1.99	0.63
1:A:179:MET:HA	1:A:179:MET:HE3	1.80	0.63
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.64	0.63
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	1.98	0.63
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.81	0.63
1:A:121:ALA:O	1:A:124:VAL:HG22	1.99	0.63
30:O:2106:C:H5'	30:O:2284:G:H21	1.64	0.63
20:T:50:VAL:HG12	20:T:56:ALA:HA	1.81	0.63
30:O:463:A:H5'	30:O:465:U:O4'	1.99	0.63
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.63
30:O:95:A:H5''	30:O:97:G:O4'	1.99	0.62
30:O:151:A:H2'	30:O:152:A:O4'	1.99	0.62
7:G:69:ARG:NH2	30:O:1150:A:N7	2.47	0.62
30:O:858:U:H2'	30:O:859:C:H6	1.64	0.62
2:B:150:ALA:O	2:B:152:PRO:HD3	1.98	0.62
2:B:97:LEU:O	2:B:98:THR:HG23	1.99	0.62
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.17	0.62
20:T:49:GLU:OE2	20:T:97:ARG:NH1	2.32	0.62
12:L:35:ARG:HD3	12:L:35:ARG:C	2.20	0.62
13:M:171:ARG:CD	30:O:156:C:H5''	2.28	0.62
23:W:46:ALA:O	23:W:49:ASN:HB2	1.99	0.62
22:V:13:PRO:HA	22:V:16:ARG:NH1	2.14	0.62
30:O:871:G:C8	30:O:871:G:C5'	2.74	0.62
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.81	0.62
10:J:130:VAL:HG12	10:J:131:THR:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:281:U:H2'	30:0:282:C:O4'	1.98	0.62
30:0:2362:A:H2'	30:0:2363:G:C8	2.34	0.62
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.78	0.62
12:L:7:GLN:HG3	38:L:8814:CL:CL	2.37	0.62
30:0:603:A:H4'	30:0:604:G:O5'	2.00	0.62
20:T:48:VAL:HG21	20:T:96:VAL:HG13	1.80	0.62
30:0:280:C:H2'	30:0:281:U:O4'	1.99	0.62
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.79	0.62
30:0:1058:A:H2'	30:0:1060:C:H5''	1.80	0.62
30:0:726:C:H2'	30:0:727:G:O4'	2.00	0.62
31:9:98:C:H2'	31:9:99:U:H6	1.64	0.62
30:0:1218:U:H2'	30:0:1219:U:C6	2.34	0.62
30:0:2266:A:H2'	30:0:2267:G:C8	2.35	0.62
30:0:790:A:H1'	30:0:1710:A:H2'	1.82	0.62
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.29	0.62
31:9:73:A:H61	31:9:108:C:H42	1.48	0.62
20:T:19:ARG:HD3	20:T:67:LEU:O	2.00	0.62
4:D:64:ARG:NE	4:D:67:ASP:HB3	2.15	0.62
16:P:143:ALA:HA	41:P:5521:HOH:O	1.99	0.62
12:L:66:VAL:HG23	12:L:67:ARG:N	2.14	0.62
30:0:204:A:H2'	30:0:205:U:H5'	1.82	0.62
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.80	0.62
30:0:241:A:C2	30:0:378:A:H4'	2.35	0.62
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.82	0.62
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.35	0.62
30:0:1406:A:H4'	30:0:1407:A:H5''	1.82	0.62
4:D:25:MET:CE	4:D:37:ALA:HB1	2.23	0.62
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.81	0.62
30:0:2106:C:H1'	30:0:2484:U:O2	2.00	0.62
30:0:59:A:H5'	41:0:5197:HOH:O	1.98	0.62
3:C:214:THR:HG22	3:C:216:SER:H	1.64	0.62
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.65	0.62
5:E:131:LEU:HD12	5:E:166:VAL:HG11	1.81	0.62
27:1:25:LYS:O	27:1:25:LYS:HG2	2.00	0.62
16:P:9:LEU:O	16:P:13:VAL:HG12	2.00	0.62
5:E:36:PRO:HD3	10:J:127:ILE:CD1	2.30	0.62
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.80	0.61
5:E:144:THR:O	5:E:148:ILE:HG13	1.99	0.61
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.35	0.61
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.00	0.61
29:3:6:ARG:HH11	29:3:21:GLU:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2766:A:H5'	41:0:3465:HOH:O	1.99	0.61
31:9:14:G:C8	31:9:14:G:H5'	2.35	0.61
30:0:951:A:H2'	30:0:952:G:H5'	1.81	0.61
30:0:564:G:H1'	41:0:7141:HOH:O	1.99	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.29	0.61
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.61
30:0:946:C:H2'	30:0:947:U:C6	2.34	0.61
30:0:2866:U:H4'	30:0:2867:G:H5'	1.81	0.61
31:9:64:C:H2'	31:9:65:A:H5'	1.82	0.61
14:N:147:ILE:HD12	41:9:9086:HOH:O	2.00	0.61
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.33	0.61
30:0:2533:C:H5'	30:0:2533:C:H6	1.65	0.61
30:0:589:U:H2'	30:0:590:A:H8	1.64	0.61
12:L:53:ARG:HD2	30:0:2441:U:H4'	1.82	0.61
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.83	0.61
3:C:101:ASP:HB2	30:0:750:A:O3'	2.01	0.61
30:0:1976:G:O2'	30:0:1977:U:H5'	2.01	0.61
12:L:125:PHE:CZ	12:L:140:VAL:HG22	2.35	0.61
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.00	0.61
30:0:1461:U:H2'	30:0:1462:C:H6	1.65	0.61
16:P:121:ASP:OD1	16:P:125:LYS:HE3	1.99	0.61
30:0:494:C:H2'	30:0:496:G:OP2	2.00	0.61
18:R:29:LYS:HB3	41:R:8939:HOH:O	1.99	0.61
30:0:247:A:H2'	41:0:4794:HOH:O	2.00	0.61
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.61
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.35	0.61
13:M:61:ILE:N	13:M:61:ILE:HD12	2.15	0.61
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.64	0.61
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.61
1:A:19:PRO:HG2	1:A:23:TYR:CE2	2.35	0.61
29:3:65:THR:CG2	29:3:67:LEU:HG	2.31	0.61
18:R:46:TYR:HD2	18:R:47:LEU:HD23	1.65	0.61
13:M:9:ARG:HD2	30:0:380:A:OP2	2.00	0.61
3:C:121:ALA:N	3:C:136:VAL:HG11	2.15	0.61
30:0:185:G:H4'	30:0:186:A:H4'	1.81	0.61
25:Y:148:GLY:O	25:Y:154:ARG:HD3	2.01	0.61
7:G:12:ILE:HG22	7:G:17:GLN:NE2	2.16	0.61
14:N:112:GLY:HA2	14:N:137:ALA:N	2.15	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.31	0.61
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.81	0.61
30:0:2896:A:N3	30:0:2896:A:H2'	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2735:U:H2'	30:0:2736:U:C6	2.36	0.61
30:0:1528:A:H2'	30:0:1529:G:O4'	2.00	0.61
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.82	0.61
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.65	0.61
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.30	0.61
30:0:120:A:H2'	30:0:120:A:N3	2.15	0.61
3:C:51:TYR:CE1	27:1:56:GLU:HB2	2.35	0.61
30:0:2795:C:O2'	30:0:2796:U:H5'	2.00	0.61
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.83	0.61
10:J:127:ILE:N	38:J:8801:CL:CL	2.66	0.61
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.29	0.61
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.83	0.61
23:W:48:VAL:HG12	23:W:48:VAL:O	2.00	0.60
21:U:9:CYS:HA	21:U:52:THR:CG2	2.30	0.60
5:E:35:TYR:HA	10:J:127:ILE:HD11	1.83	0.60
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.66	0.60
2:B:42:ALA:HB2	2:B:162:MET:HE1	1.83	0.60
5:E:166:VAL:HG12	41:E:3134:HOH:O	2.00	0.60
14:N:48:VAL:HG13	14:N:55:ASP:HB3	1.83	0.60
30:0:2534:C:H1'	41:0:4385:HOH:O	2.00	0.60
13:M:22:GLU:O	13:M:26:GLN:HG3	2.01	0.60
30:0:536:A:H3'	41:0:5901:HOH:O	2.00	0.60
30:0:664:U:O4	30:0:681:G:H5''	2.00	0.60
2:B:75:GLU:C	2:B:77:PRO:HD3	2.22	0.60
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.65	0.60
7:G:67:LEU:O	7:G:71:LEU:HG	2.01	0.60
11:K:113:ILE:HG22	11:K:114:ALA:N	2.16	0.60
2:B:279:THR:HG22	2:B:280:VAL:H	1.64	0.60
2:B:16:ARG:HD3	41:B:9081:HOH:O	2.01	0.60
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.60
15:O:59:VAL:CG2	15:O:111:VAL:HG21	2.32	0.60
23:W:13:MET:HE2	23:W:17:ILE:HG22	1.83	0.60
19:S:37:VAL:O	19:S:41:VAL:HG23	2.01	0.60
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.15	0.60
1:A:130:THR:HB	1:A:137:VAL:HB	1.84	0.60
21:U:17:THR:CG2	21:U:18:GLY:N	2.64	0.60
1:A:84:VAL:O	1:A:98:GLU:HG3	2.01	0.60
30:0:1931:A:H2'	30:0:1932:G:H5'	1.83	0.60
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	1.84	0.60
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.60
23:W:85:ALA:HB2	23:W:91:ASP:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:165:GLY:O	13:M:169:ARG:HB2	2.02	0.60
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.60
31:9:20:G:O2'	31:9:21:G:H5'	2.02	0.60
7:G:20:VAL:O	7:G:24:VAL:HG23	2.02	0.60
3:C:7:ASP:OD2	3:C:9:ASP:HB2	2.01	0.60
30:0:1209:C:H2'	30:0:1210:G:H8	1.66	0.60
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.16	0.60
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.32	0.60
30:0:2296:C:H2'	30:0:2297:U:C6	2.37	0.60
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.83	0.60
30:0:1909:A:N1	30:0:2128:G:H1'	2.17	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.83	0.60
30:0:1416:G:C2'	30:0:1417:G:H5'	2.32	0.60
21:U:11:THR:HG22	21:U:53:ASP:CB	2.31	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.32	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.17	0.60
22:V:29:ASN:O	22:V:33:VAL:HG23	2.02	0.60
2:B:238:ASN:HD22	2:B:240:GLY:H	1.49	0.60
30:0:2472:C:O2'	30:0:2634:G:H4'	2.00	0.60
3:C:211:ASP:HB2	3:C:231:ARG:NH2	2.17	0.60
2:B:175:LEU:C	2:B:175:LEU:HD23	2.22	0.60
22:V:5:VAL:HG12	22:V:9:ARG:NH1	2.17	0.60
30:0:2816:A:H5''	30:0:2817:G:H5'	1.83	0.60
25:Y:208:LYS:NZ	30:0:1343:C:H1'	2.17	0.60
2:B:162:MET:HE3	2:B:310:ARG:HH11	1.67	0.59
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.59
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.01	0.59
14:N:152:GLU:C	14:N:154:LEU:H	2.05	0.59
30:0:2748:G:H2'	41:0:9338:HOH:O	2.01	0.59
5:E:132:THR:HB	41:E:2227:HOH:O	2.03	0.59
2:B:26:PHE:HD1	2:B:310:ARG:HH21	1.50	0.59
11:K:41:LYS:HE2	11:K:42:ASN:ND2	2.17	0.59
20:T:8:ARG:NH1	30:0:31:C:OP2	2.35	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.37	0.59
1:A:33:GLU:CD	1:A:33:GLU:N	2.55	0.59
20:T:76:ASP:C	20:T:78:THR:HG23	2.23	0.59
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.67	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.67	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.83	0.59
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.84	0.59
12:L:148:GLU:HA	41:L:9037:HOH:O	2.00	0.59
30:0:336:G:H5''	41:0:4601:HOH:O	2.02	0.59
30:0:1883:U:H5''	30:0:2013:G:OP2	2.01	0.59
30:0:969:G:H1	30:0:999:C:H42	1.50	0.59
14:N:77:ASN:C	14:N:80:SER:HB3	2.23	0.59
30:0:530:C:C4'	30:0:612:U:H4'	2.32	0.59
30:0:1172:G:H1'	41:0:5831:HOH:O	2.01	0.59
30:0:1545:C:H2'	30:0:1546:G:O4'	2.02	0.59
30:0:459:A:H4'	41:0:3355:HOH:O	2.03	0.59
1:A:82:VAL:HG22	1:A:93:THR:HB	1.83	0.59
30:0:248:A:H5'	30:0:249:G:OP2	2.03	0.59
24:X:72:VAL:HG22	24:X:85:VAL:HG11	1.84	0.59
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.00	0.59
30:0:2326:C:H4'	30:0:2412:G:C4'	2.33	0.59
9:I:108:HIS:N	9:I:109:PRO:HD2	2.17	0.59
3:C:154:VAL:O	3:C:158:GLU:HG3	2.03	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.59
30:0:1416:G:H2'	30:0:1417:G:H5'	1.85	0.59
14:N:149:GLU:HA	14:N:152:GLU:HB2	1.83	0.59
30:0:1555:G:H4'	30:0:1630:A:H2	1.67	0.59
8:H:54:VAL:HG13	8:H:162:PRO:CG	2.32	0.59
5:E:152:THR:HG21	5:E:165:GLY:HA2	1.84	0.59
30:0:834:G:H3'	30:0:835:U:H4'	1.83	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.18	0.59
12:L:27:ARG:NH2	12:L:30:ARG:HG2	2.17	0.59
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.02	0.59
12:L:35:ARG:NH1	12:L:35:ARG:HB2	2.13	0.59
25:Y:117:LEU:HD13	25:Y:174:VAL:CG1	2.33	0.59
12:L:71:GLU:HG2	30:0:700:A:C2	2.38	0.59
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.03	0.59
30:0:625:U:H5''	30:0:1044:C:N4	2.17	0.59
30:0:1634:G:H2'	30:0:1635:U:C6	2.38	0.59
30:0:1735:C:O2'	30:0:1736:A:H5'	2.02	0.59
9:I:121:LYS:HD3	30:0:1185:U:OP1	2.02	0.59
18:R:77:ALA:O	18:R:78:GLY:CA	2.51	0.59
30:0:213:G:N2	30:0:225:G:H2'	2.18	0.59
4:D:38:GLU:OE2	4:D:51:ARG:NE	2.35	0.59
11:K:10:GLN:N	11:K:10:GLN:NE2	2.37	0.58
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.18	0.58
18:R:106:GLY:HA2	18:R:109:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.32	0.58
17:Q:25:PRO:HB2	41:9:9077:HOH:O	2.03	0.58
30:0:559:U:H6	30:0:559:U:H5'	1.66	0.58
20:T:43:ASN:C	20:T:45:GLY:H	2.06	0.58
28:2:25:VAL:O	28:2:29:THR:HG23	2.02	0.58
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.03	0.58
8:H:80:LEU:HD21	8:H:145:ASP:HB3	1.85	0.58
14:N:71:TRP:HB2	41:N:8838:HOH:O	2.04	0.58
14:N:86:LEU:HD21	14:N:180:LEU:HD12	1.85	0.58
23:W:122:ARG:NH1	23:W:152:ALA:O	2.35	0.58
25:Y:165:GLU:HB3	41:0:7515:HOH:O	2.03	0.58
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.58
11:K:43:ARG:NH1	30:0:2712:G:OP1	2.35	0.58
1:A:66:ARG:NH1	1:A:66:ARG:HB2	2.16	0.58
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.03	0.58
30:0:958:G:O2'	30:0:959:C:H5'	2.03	0.58
30:0:1187:U:O2'	30:0:1189:A:H2	1.86	0.58
24:X:47:ALA:HB1	24:X:82:GLU:CB	2.32	0.58
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.17	0.58
30:0:1829:A:C2'	30:0:1830:C:H5'	2.33	0.58
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.33	0.58
16:P:16:VAL:HG13	16:P:20:ARG:NH1	2.18	0.58
1:A:55:VAL:HG23	1:A:68:ILE:O	2.03	0.58
30:0:2392:C:H4'	41:0:5133:HOH:O	2.03	0.58
14:N:139:TRP:CE3	14:N:139:TRP:HA	2.37	0.58
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.58
14:N:96:GLY:O	14:N:98:GLU:HG3	2.04	0.58
30:0:1067:A:H5'	41:0:5212:HOH:O	2.04	0.58
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.86	0.58
2:B:177:HIS:O	2:B:181:ILE:HG13	2.03	0.58
9:I:129:SER:O	9:I:130:LEU:HD23	2.03	0.58
22:V:50:ARG:HD3	41:V:2826:HOH:O	2.03	0.58
12:L:140:VAL:HB	41:L:9020:HOH:O	2.03	0.58
30:0:1527:A:H1'	30:0:1528:A:C8	2.38	0.58
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.86	0.58
13:M:159:VAL:HG12	38:M:8818:CL:CL	2.41	0.58
3:C:2:GLN:HB3	41:C:8589:HOH:O	2.02	0.58
30:0:1180:U:H1'	41:0:4130:HOH:O	2.04	0.58
5:E:84:MET:SD	5:E:168:ILE:HD13	2.43	0.58
30:0:459:A:H5''	41:0:2968:HOH:O	2.03	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2667:G:H1'	30:0:2914:A:N3	2.19	0.58
12:L:59:GLU:HA	12:L:104:ASP:OD2	2.04	0.58
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.03	0.58
15:O:31:GLU:O	15:O:35:LYS:HG3	2.04	0.58
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.69	0.58
2:B:3:PRO:HG2	41:0:9686:HOH:O	2.02	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.86	0.58
4:D:52:THR:HG21	30:0:2346:C:O2'	2.03	0.58
4:D:99:ASP:HB3	4:D:103:ASN:H	1.69	0.58
4:D:18:ILE:HG12	4:D:134:LEU:HD23	1.84	0.58
30:0:221:G:H2'	30:0:222:A:C8	2.39	0.58
30:0:264:G:H1'	30:0:265:U:H5	1.69	0.58
14:N:67:ALA:HA	14:N:71:TRP:CB	2.34	0.58
2:B:16:ARG:HB3	2:B:217:ARG:NH2	2.19	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.04	0.58
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
27:1:45:ARG:HB3	41:1:988:HOH:O	2.02	0.58
30:0:2608:C:H2'	41:0:4456:HOH:O	2.04	0.58
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.86	0.58
30:0:150:G:H1'	41:0:4496:HOH:O	2.04	0.58
30:0:157:G:H3'	41:0:4827:HOH:O	2.03	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.03	0.58
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.19	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.04	0.58
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.86	0.58
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.58
13:M:71:SER:HB2	13:M:92:THR:HG22	1.86	0.58
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.58
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.04	0.58
8:H:165:ARG:HD3	41:H:9040:HOH:O	2.03	0.58
1:A:107:ASN:OD1	1:A:120:ARG:HD2	2.04	0.58
30:0:1615:A:H5'	41:0:5049:HOH:O	2.04	0.58
11:K:77:ARG:C	11:K:78:LYS:CA	2.72	0.58
23:W:130:HIS:O	23:W:136:GLY:HA3	2.04	0.58
30:0:23:G:H1'	30:0:520:A:N6	2.19	0.58
4:D:40:ILE:HG13	4:D:41:LEU:N	2.19	0.58
30:0:31:C:H2'	41:0:9479:HOH:O	2.03	0.58
23:W:90:TYR:CD1	23:W:90:TYR:N	2.71	0.58
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.68	0.57
6:F:83:LEU:HD11	6:F:96:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.19	0.57
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.86	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.38	0.57
7:G:23:ILE:HG22	7:G:27:ILE:HD11	1.85	0.57
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.37	0.57
3:C:20:ASP:O	3:C:23:GLU:HB2	2.03	0.57
30:0:2312:G:H2'	30:0:2313:C:H5'	1.85	0.57
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.69	0.57
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.04	0.57
24:X:20:GLU:CD	24:X:21:PRO:HD2	2.24	0.57
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.57
28:2:20:ARG:HG2	41:2:5444:HOH:O	2.04	0.57
3:C:184:ARG:NH2	30:0:450:C:OP1	2.37	0.57
29:3:15:ASN:O	30:0:2408:A:H4'	2.05	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.57
6:F:4:VAL:HG13	6:F:76:PHE:CD1	2.38	0.57
23:W:55:GLY:HA3	23:W:146:ILE:HG13	1.86	0.57
21:U:52:THR:CG2	21:U:54:THR:HB	2.34	0.57
23:W:110:GLN:HA	23:W:110:GLN:NE2	2.20	0.57
30:0:2896:A:H5"	41:0:6932:HOH:O	2.04	0.57
30:0:136:C:H2'	30:0:137:U:O4'	2.04	0.57
30:0:757:C:H2'	30:0:758:A:C8	2.39	0.57
10:J:107:ASN:ND2	10:J:109:TYR:H	2.02	0.57
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.04	0.57
3:C:168:ARG:NH2	3:C:190:ALA:O	2.37	0.57
10:J:52:GLN:HG3	10:J:53:ILE:H	1.67	0.57
30:0:380:A:H2'	41:0:9039:HOH:O	2.03	0.57
2:B:86:ALA:HA	41:B:9050:HOH:O	2.05	0.57
23:W:154:ARG:NH1	30:0:588:G:O6	2.37	0.57
2:B:85:ARG:NH1	41:B:9110:HOH:O	2.37	0.57
23:W:35:VAL:HG22	23:W:36:PRO:O	2.05	0.57
16:P:77:ALA:O	16:P:78:GLY:CA	2.52	0.57
4:D:25:MET:CE	4:D:41:LEU:HG	2.30	0.57
11:K:74:VAL:HG13	11:K:113:ILE:CG2	2.29	0.57
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.70	0.57
12:L:92:ASP:OD1	12:L:94:ARG:HB2	2.04	0.57
33:6:76:8AN:N3	41:6:80:HOH:O	2.32	0.57
30:0:1097:A:H2'	30:0:1098:A:C8	2.39	0.57
30:0:1249:U:H2'	30:0:1250:C:H6	1.68	0.57
26:Z:73:ARG:HG2	26:Z:75:GLY:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.38	0.57
23:W:108:ARG:HG3	23:W:114:PRO:HG3	1.85	0.57
30:0:619:U:H3'	41:0:4175:HOH:O	2.05	0.57
14:N:23:ARG:NH1	14:N:27:LEU:HD11	2.18	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.85	0.57
1:A:105:VAL:HG12	1:A:106:CYS:N	2.20	0.57
2:B:42:ALA:HB2	2:B:162:MET:CE	2.35	0.57
2:B:77:PRO:C	2:B:78:PRO:HG3	2.25	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
13:M:92:THR:HB	30:0:401:C:O2'	2.05	0.57
30:0:2032:U:H2'	30:0:2033:G:H5''	1.87	0.57
30:0:1946:C:H2'	30:0:1971:G:C8	2.40	0.57
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.87	0.57
23:W:64:THR:O	23:W:68:THR:HG22	2.05	0.57
14:N:176:ARG:HG2	14:N:180:LEU:HD13	1.86	0.57
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.87	0.57
30:0:1165:G:O2'	30:0:1174:A:H4'	2.05	0.57
2:B:87:TYR:OH	2:B:163:GLU:OE2	2.16	0.57
1:A:117:LYS:HA	41:A:9015:HOH:O	2.05	0.57
6:F:13:GLU:OE1	6:F:77:VAL:HG13	2.04	0.57
9:I:69:PRO:HA	30:0:1164:U:OP1	2.05	0.57
30:0:447:A:O2'	30:0:448:G:H5'	2.04	0.57
29:3:36:ILE:HG23	29:3:37:ASP:N	2.19	0.57
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.19	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.20	0.57
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.57
30:0:941:G:O2'	30:0:942:U:H5'	2.04	0.57
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.05	0.57
23:W:60:GLU:O	23:W:63:GLU:HB2	2.05	0.57
30:0:1624:A:H4'	30:0:1626:A:H5''	1.86	0.57
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.33	0.56
23:W:122:ARG:HH12	23:W:154:ARG:N	2.03	0.56
15:O:14:LEU:CG	15:O:102:ILE:HD11	2.35	0.56
30:0:1342:C:O2'	30:0:1343:C:H5'	2.05	0.56
30:0:2011:A:H5'	30:0:2013:G:H1'	1.85	0.56
3:C:181:ALA:HA	41:T:2331:HOH:O	2.04	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.56
30:0:1482:A:O2'	30:0:1483:C:H5'	2.04	0.56
30:0:699:C:H2'	30:0:744:G:O4'	2.05	0.56
23:W:115:THR:HG22	23:W:116:LEU:N	2.20	0.56
30:0:710:G:O2'	30:0:711:G:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:C8	30:0:1119:G:H5''	2.37	0.56
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.86	0.56
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.58	0.56
27:1:15:THR:HG1	30:0:777:U:H5	1.53	0.56
30:0:1364:G:H1'	41:0:5657:HOH:O	2.05	0.56
7:G:63:ARG:O	7:G:67:LEU:HG	2.04	0.56
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.05	0.56
2:B:162:MET:HB2	2:B:310:ARG:NH1	2.21	0.56
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.41	0.56
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.87	0.56
30:0:255:A:H2'	30:0:256:C:C6	2.41	0.56
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.05	0.56
19:S:57:THR:HG22	19:S:58:MET:N	2.21	0.56
15:O:77:ALA:HA	15:O:96:VAL:O	2.05	0.56
30:0:1419:U:H2'	30:0:1685:A:C2	2.39	0.56
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.88	0.56
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.33	0.56
4:D:167:GLU:OE2	4:D:173:GLU:HB3	2.05	0.56
29:3:77:ALA:C	29:3:78:HIS:CA	2.74	0.56
23:W:5:VAL:HG11	23:W:153:MET:CE	2.35	0.56
30:0:499:G:O2'	30:0:500:G:H5'	2.05	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.56
16:P:91:LYS:O	16:P:95:GLU:HG3	2.05	0.56
16:P:83:LYS:HG2	30:0:793:A:H5''	1.88	0.56
13:M:82:ARG:O	13:M:84:LYS:N	2.38	0.56
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.87	0.56
30:0:1730:G:C5'	30:0:1731:C:C6	2.89	0.56
14:N:23:ARG:NH2	31:9:7:G:H4'	2.21	0.56
8:H:23:ILE:HG22	8:H:123:ILE:HD11	1.88	0.56
30:0:334:G:H2'	30:0:335:U:O4'	2.05	0.56
16:P:82:GLY:O	30:0:1761:U:H4'	2.04	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.88	0.56
12:L:55:GLN:CA	12:L:58:GLN:HE21	2.17	0.56
23:W:13:MET:HE1	23:W:18:GLN:HA	1.88	0.56
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.88	0.56
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.05	0.56
30:0:69:A:H5'	30:0:69:A:C8	2.40	0.56
30:0:706:G:N2	30:0:707:C:H41	2.04	0.56
30:0:1346:U:H2'	30:0:1347:U:C6	2.41	0.56
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.05	0.56
18:R:40:ALA:O	18:R:43:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:ARG:HD2	3:C:229:PRO:O	2.05	0.56
13:M:60:VAL:HG22	13:M:134:ILE:HD12	1.87	0.56
30:0:119:A:H2'	30:0:120:A:C5'	2.36	0.56
18:R:99:ALA:HB1	18:R:109:MET:HE3	1.87	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.86	0.56
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.88	0.56
2:B:206:THR:CG2	30:0:2716:G:H5''	2.30	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.36	0.56
25:Y:208:LYS:HZ3	30:0:1343:C:H1'	1.71	0.56
30:0:137:U:OP1	30:0:259:G:O2'	2.24	0.56
13:M:58:GLN:NE2	30:0:259:G:H21	2.03	0.56
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.41	0.56
3:C:149:LYS:NZ	30:0:327:A:OP1	2.38	0.56
31:9:54:A:O2'	31:9:55:U:H5'	2.06	0.56
30:0:622:G:O2'	30:0:623:U:H5'	2.05	0.56
2:B:144:THR:HB	41:B:9099:HOH:O	2.03	0.56
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.56
2:B:62:ARG:HA	2:B:65:MET:HE2	1.87	0.56
12:L:108:VAL:HB	12:L:125:PHE:CD2	2.41	0.56
12:L:91:VAL:CG1	12:L:120:LEU:HD23	2.36	0.56
30:0:2353:A:H4'	30:0:2354:A:O5'	2.05	0.56
10:J:93:ARG:O	10:J:96:GLU:HB2	2.06	0.56
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.69	0.56
10:J:25:GLN:NE2	10:J:116:LEU:HB3	2.20	0.56
1:A:204:GLY:N	30:0:2634:G:OP2	2.38	0.56
30:0:637:C:H2'	30:0:638:C:C6	2.41	0.56
20:T:81:LYS:HG3	20:T:87:VAL:HG13	1.88	0.56
1:A:32:VAL:HG12	1:A:34:ASP:H	1.70	0.55
25:Y:187:VAL:CG1	25:Y:205:ILE:HA	2.36	0.55
30:0:612:U:H2'	30:0:613:C:C6	2.41	0.55
17:Q:16:ASN:HB2	41:0:7765:HOH:O	2.06	0.55
10:J:19:MET:CE	10:J:132:LEU:HD11	2.36	0.55
18:R:77:ALA:C	18:R:78:GLY:CA	2.75	0.55
12:L:120:LEU:HD12	12:L:133:VAL:HG21	1.87	0.55
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.21	0.55
8:H:34:HIS:HD2	8:H:90:LEU:O	1.88	0.55
30:0:2439:C:H5'	41:0:6330:HOH:O	2.06	0.55
19:S:11:THR:O	19:S:14:ALA:HB3	2.06	0.55
30:0:2507:G:H2'	30:0:2510:C:H42	1.71	0.55
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:12:TRP:O	13:M:15:PRO:HD3	2.06	0.55
12:L:13:HIS:HB3	41:L:9060:HOH:O	2.05	0.55
16:P:36:THR:O	16:P:40:VAL:HG23	2.05	0.55
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.07	0.55
7:G:63:ARG:N	41:G:2569:HOH:O	2.39	0.55
24:X:74:ALA:CA	24:X:85:VAL:HG13	2.37	0.55
29:3:70:ARG:HB3	41:3:9062:HOH:O	2.06	0.55
1:A:211:LYS:O	30:0:1943:C:H4'	2.06	0.55
11:K:87:ARG:NH2	30:0:2720:C:O2	2.39	0.55
5:E:36:PRO:HD3	10:J:127:ILE:HG13	1.89	0.55
29:3:22:VAL:HG11	29:3:67:LEU:HD13	1.88	0.55
4:D:60:GLU:O	4:D:60:GLU:HG3	2.07	0.55
5:E:7:ILE:HD11	5:E:11:VAL:O	2.07	0.55
8:H:30:LYS:N	8:H:62:HIS:HD2	1.96	0.55
10:J:12:VAL:HG21	10:J:116:LEU:HD11	1.88	0.55
23:W:91:ASP:HB2	41:W:5425:HOH:O	2.06	0.55
21:U:20:MET:HE2	21:U:28:THR:HG21	1.88	0.55
1:A:43:VAL:HG21	1:A:59:GLU:HG3	1.87	0.55
30:0:553:G:H5'	41:0:4389:HOH:O	2.06	0.55
2:B:254:GLN:HG2	2:B:255:GLY:N	2.21	0.55
8:H:69:ARG:HD3	41:H:9037:HOH:O	2.05	0.55
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.55
25:Y:174:VAL:HG13	25:Y:177:LYS:HD2	1.88	0.55
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.36	0.55
4:D:60:GLU:O	4:D:61:PHE:C	2.45	0.55
2:B:274:GLU:HA	2:B:292:GLY:O	2.06	0.55
14:N:74:PRO:HG2	14:N:159:TYR:CE1	2.42	0.55
3:C:207:LEU:HB2	3:C:210:ALA:HB2	1.87	0.55
13:M:178:LYS:HB2	41:0:7686:HOH:O	2.06	0.55
6:F:65:GLU:HB3	41:F:5163:HOH:O	2.06	0.55
30:0:624:U:H3'	41:0:5060:HOH:O	2.07	0.55
4:D:25:MET:SD	4:D:40:ILE:HD11	2.47	0.55
13:M:12:TRP:CD2	13:M:45:ARG:HD2	2.41	0.55
30:0:292:G:H1'	30:0:360:A:H61	1.72	0.55
8:H:96:GLN:NE2	8:H:129:ARG:NH2	2.55	0.55
27:1:1:THR:O	30:0:1836:A:H1'	2.07	0.55
18:R:113:HIS:HB3	18:R:146:ILE:HD12	1.89	0.55
23:W:4:LEU:HD22	23:W:52:VAL:HB	1.88	0.55
30:0:2828:G:H8	30:0:2828:G:O5'	1.90	0.55
2:B:98:THR:HG21	2:B:127:GLN:OE1	2.06	0.55
16:P:11:ALA:HB1	16:P:16:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:HIS:HB2	4:D:72:LYS:HA	1.88	0.55
6:F:19:ALA:O	6:F:22:VAL:HG22	2.07	0.55
30:0:2562:G:H4'	41:0:5081:HOH:O	2.07	0.55
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.55
41:C:8562:HOH:O	15:O:3:THR:HG21	2.06	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
29:3:11:CYS:HB2	29:3:20:HIS:NE2	2.21	0.55
3:C:246:ARG:HD2	41:C:8576:HOH:O	2.07	0.55
24:X:23:HIS:NE2	24:X:24:LYS:HD2	2.21	0.55
30:0:2032:U:H2'	30:0:2033:G:C5'	2.37	0.55
30:0:2115:U:H2'	30:0:2116:U:C6	2.41	0.55
13:M:146:ASP:O	13:M:147:LEU:HD23	2.06	0.55
16:P:74:GLN:HG2	30:0:1786:C:OP1	2.06	0.55
14:N:21:HIS:HB2	41:N:8831:HOH:O	2.07	0.55
5:E:77:THR:O	5:E:78:GLU:CA	2.55	0.55
1:A:2:ARG:HD3	1:A:198:ASP:OD1	2.06	0.55
30:0:1260:G:H3'	30:0:1261:A:N7	2.21	0.55
1:A:66:ARG:CB	1:A:66:ARG:NH1	2.69	0.55
30:0:2401:A:H2'	30:0:2402:A:C8	2.42	0.55
22:V:20:LEU:HD22	22:V:60:GLN:HE22	1.71	0.55
2:B:36:PRO:HA	2:B:168:GLY:CA	2.25	0.55
1:A:32:VAL:HG12	1:A:34:ASP:N	2.22	0.55
1:A:189:VAL:HA	30:0:1845:A:OP1	2.07	0.55
1:A:82:VAL:HA	1:A:93:THR:O	2.07	0.55
1:A:69:LEU:HD21	1:A:120:ARG:HB3	1.88	0.55
6:F:4:VAL:HG13	6:F:76:PHE:CE1	2.42	0.55
8:H:23:ILE:CG2	8:H:123:ILE:HD11	2.37	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.42	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
4:D:172:VAL:HG12	4:D:173:GLU:N	2.13	0.55
3:C:227:GLY:O	3:C:229:PRO:HD3	2.07	0.55
25:Y:149:GLN:HE22	30:0:1293:U:H4'	1.72	0.55
30:0:1529:G:H5'	41:0:9193:HOH:O	2.05	0.55
18:R:120:GLY:HA3	41:R:8961:HOH:O	2.07	0.55
30:0:841:A:H5''	41:0:7724:HOH:O	2.07	0.55
30:0:307:G:H3'	30:0:342:C:OP2	2.07	0.55
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.88	0.55
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.55
14:N:37:ARG:NE	41:N:8833:HOH:O	2.39	0.54
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.07	0.54
18:R:82:GLU:O	18:R:86:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.87	0.54
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.36	0.54
10:J:80:LYS:HE2	10:J:98:PHE:CZ	2.43	0.54
23:W:4:LEU:HD22	23:W:52:VAL:HG11	1.89	0.54
30:0:945:U:H2'	30:0:946:C:C6	2.42	0.54
13:M:84:LYS:HE2	41:0:5258:HOH:O	2.08	0.54
30:0:905:C:H3'	41:0:6033:HOH:O	2.06	0.54
30:0:107:U:H2'	30:0:108:U:H5'	1.89	0.54
30:0:2502:C:C2'	30:0:2503:A:H5'	2.37	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
12:L:14:GLY:O	30:0:1295:G:H5''	2.06	0.54
1:A:95:PRO:HA	1:A:153:ARG:HA	1.90	0.54
30:0:1730:G:C5'	30:0:1731:C:H6	2.20	0.54
30:0:2072:G:C6	30:0:2533:C:H1'	2.43	0.54
22:V:39:ALA:N	22:V:40:PRO:CD	2.70	0.54
3:C:165:ASP:O	3:C:168:ARG:HB3	2.06	0.54
30:0:1198:U:H2'	30:0:1200:A:OP2	2.07	0.54
15:O:63:LYS:HG3	15:O:80:ASP:O	2.07	0.54
2:B:80:ARG:HB2	2:B:145:HIS:CE1	2.42	0.54
30:0:2783:A:H3'	41:0:6077:HOH:O	2.08	0.54
5:E:81:GLU:O	5:E:172:PRO:HD3	2.07	0.54
13:M:60:VAL:C	13:M:61:ILE:HD12	2.27	0.54
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.23	0.54
20:T:48:VAL:HG21	20:T:96:VAL:CG1	2.37	0.54
9:I:70:THR:HG21	41:I:5331:HOH:O	2.08	0.54
22:V:5:VAL:HG23	41:V:2271:HOH:O	2.07	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.90	0.54
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.72	0.54
30:0:1632:A:H2'	30:0:1633:C:H5'	1.90	0.54
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.54
30:0:666:A:H2'	30:0:667:C:O4'	2.08	0.54
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.38	0.54
3:C:206:ASN:HB2	30:0:329:A:OP2	2.07	0.54
19:S:15:MET:O	19:S:18:MET:HB3	2.07	0.54
3:C:80:VAL:HA	41:C:8554:HOH:O	2.08	0.54
30:0:1447:U:H3'	30:0:1506:U:O2	2.07	0.54
24:X:71:ARG:HD3	41:X:7542:HOH:O	2.07	0.54
3:C:235:PHE:CE2	3:C:243:VAL:HG21	2.41	0.54
31:9:30:C:H42	31:9:50:G:H1	1.55	0.54
28:2:48:ASP:O	28:2:49:GLU:HB2	2.08	0.54
30:0:589:U:H2'	30:0:590:A:C8	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1647:G:O2'	30:0:1648:G:H5'	2.08	0.54
4:D:36:ASN:HA	41:D:7500:HOH:O	2.07	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
30:0:1839:A:H5'	30:0:2643:G:H4'	1.89	0.54
30:0:631:A:C6	30:0:2074:A:H5'	2.43	0.54
15:O:99:GLU:HG3	41:O:6044:HOH:O	2.07	0.54
2:B:2:GLN:NE2	30:0:2545:U:OP2	2.41	0.54
30:0:1189:A:H1'	30:0:1209:C:H1'	1.90	0.54
8:H:59:GLN:HE21	8:H:129:ARG:HG2	1.73	0.54
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.22	0.54
3:C:58:ALA:HA	3:C:73:GLN:NE2	2.22	0.54
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
3:C:77:ALA:C	3:C:78:ARG:CA	2.76	0.54
30:0:2042:U:H2'	30:0:2043:U:C6	2.42	0.54
30:0:1298:U:H2'	30:0:1299:G:C8	2.42	0.54
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.54
26:Z:54:GLU:HG2	26:Z:57:MET:HE2	1.90	0.54
18:R:98:ASN:HD22	18:R:98:ASN:N	2.06	0.54
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.88	0.54
30:0:2281:C:C2'	30:0:2282:U:H5'	2.37	0.54
25:Y:136:LYS:HB3	25:Y:139:VAL:HG23	1.90	0.54
14:N:37:ARG:HH12	31:9:6:C:C5'	2.00	0.54
18:R:39:THR:HB	18:R:42:GLU:CD	2.27	0.54
30:0:1666:C:H2'	30:0:1667:A:C5'	2.37	0.54
30:0:2502:C:N3	30:0:2518:C:N4	2.55	0.54
23:W:27:HIS:CD2	30:0:1288:U:H4'	2.43	0.54
30:0:407:A:H2'	30:0:408:A:C8	2.43	0.54
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
20:T:28:SER:CA	20:T:97:ARG:HD3	2.35	0.54
18:R:132:ARG:HH21	30:0:2055:A:H4'	1.69	0.54
30:0:187:A:H3'	30:0:188:C:H6	1.73	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.07	0.54
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.87	0.54
9:I:127:CYS:C	9:I:129:SER:N	2.62	0.54
30:0:1834:C:H2'	30:0:1840:A:H62	1.72	0.54
10:J:77:GLY:C	10:J:78:ILE:CA	2.77	0.54
29:3:84:ARG:HB3	41:3:9041:HOH:O	2.08	0.54
27:1:46:ARG:HA	41:0:3919:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.07	0.54
31:9:78:G:N3	31:9:78:G:H1'	2.22	0.54
30:0:877:G:H1'	41:0:3080:HOH:O	2.07	0.53
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.09	0.53
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.08	0.53
30:0:2332:A:H3'	30:0:2333:G:H8	1.73	0.53
30:0:2526:C:O2'	30:0:2527:U:H5'	2.09	0.53
9:I:88:GLN:HA	9:I:91:PHE:HE2	1.73	0.53
30:0:2824:C:O3'	30:0:2825:C:H6	1.91	0.53
19:S:34:LYS:HG2	19:S:54:THR:HG23	1.89	0.53
8:H:66:GLU:HA	41:H:9037:HOH:O	2.07	0.53
2:B:244:PRO:HB3	30:0:1234:U:N3	2.23	0.53
13:M:84:LYS:HB2	30:0:170:U:OP1	2.08	0.53
25:Y:138:ARG:NH1	30:0:638:C:OP2	2.38	0.53
30:0:812:A:H2'	30:0:813:C:C6	2.43	0.53
30:0:1940:C:H4'	41:0:9153:HOH:O	2.07	0.53
8:H:174:LEU:HD11	30:0:1220:U:H4'	1.90	0.53
1:A:173:GLY:O	1:A:176:HIS:HB3	2.07	0.53
23:W:137:GLN:HG3	23:W:137:GLN:O	2.08	0.53
18:R:9:ASP:O	18:R:13:THR:HG22	2.08	0.53
2:B:53:LEU:HD21	2:B:270:ILE:HG23	1.91	0.53
30:0:138:U:H5''	30:0:139:C:OP2	2.08	0.53
23:W:65:VAL:HA	23:W:68:THR:HG22	1.90	0.53
30:0:705:C:H3'	30:0:706:G:H8	1.73	0.53
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.72	0.53
5:E:81:GLU:HG2	5:E:134:SER:CB	2.33	0.53
23:W:115:THR:HB	41:W:6871:HOH:O	2.09	0.53
30:0:690:G:H4'	30:0:741:C:O2	2.09	0.53
30:0:1947:G:H2'	30:0:1948:G:H8	1.71	0.53
3:C:139:VAL:HG12	41:C:8645:HOH:O	2.08	0.53
2:B:14:GLY:HA2	2:B:15:PRO:C	2.28	0.53
30:0:1118:A:C3'	30:0:1118:A:C8	2.91	0.53
30:0:1160:G:H5'	30:0:1161:A:C4'	2.38	0.53
1:A:212:PRO:HA	30:0:1943:C:O4'	2.08	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.89	0.53
6:F:20:LEU:HB2	6:F:49:PHE:CZ	2.43	0.53
23:W:39:ASP:HB2	41:W:3580:HOH:O	2.09	0.53
30:0:2802:C:H2'	30:0:2803:C:C6	2.44	0.53
30:0:708:A:H2'	30:0:709:G:O4'	2.08	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
30:0:2761:A:H2'	41:0:6484:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:89:ASN:HB3	16:P:92:GLU:HB2	1.91	0.53
3:C:1:MET:HG2	3:C:2:GLN:HE21	1.74	0.53
23:W:55:GLY:CA	23:W:146:ILE:HG13	2.38	0.53
14:N:80:SER:HB2	41:N:8835:HOH:O	2.07	0.53
3:C:233:THR:CG2	3:C:234:VAL:H	2.16	0.53
6:F:58:GLU:OE2	13:M:27:ARG:NH2	2.40	0.53
30:0:2420:G:H4'	41:0:4965:HOH:O	2.09	0.53
1:A:194:MET:SD	30:0:875:A:C2	3.02	0.53
30:0:78:G:N1	30:0:78:G:N2	2.56	0.53
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.56	0.53
30:0:2748:G:H4'	30:0:2749:U:C5'	2.39	0.53
30:0:2239:C:H2'	30:0:2240:U:H6	1.74	0.53
26:Z:54:GLU:HB2	41:Z:8712:HOH:O	2.09	0.53
13:M:91:ILE:HD13	41:0:4059:HOH:O	2.08	0.53
30:0:354:A:H2'	30:0:355:C:C6	2.43	0.53
2:B:36:PRO:HB3	2:B:174:ARG:HB3	1.90	0.53
19:S:10:VAL:HG11	22:V:36:ALA:CB	2.36	0.53
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.91	0.53
1:A:38:ILE:O	1:A:38:ILE:HG22	2.08	0.53
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.24	0.53
1:A:179:MET:HG2	1:A:186:TRP:CB	2.38	0.53
15:O:59:VAL:HG23	15:O:111:VAL:HG21	1.91	0.53
30:0:855:U:H4'	30:0:856:G:O4'	2.08	0.53
23:W:151:GLU:O	23:W:154:ARG:HB2	2.08	0.53
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.39	0.53
30:0:2698:G:H2'	30:0:2699:A:C8	2.44	0.53
11:K:76:GLN:HA	11:K:93:ASN:HA	1.90	0.53
20:T:105:ASP:OD2	20:T:107:LYS:HB2	2.08	0.53
19:S:23:LYS:HE2	41:0:5526:HOH:O	2.09	0.53
8:H:168:VAL:HG13	41:H:9015:HOH:O	2.08	0.53
14:N:37:ARG:NH1	31:9:6:C:OP1	2.42	0.53
1:A:211:LYS:NZ	1:A:223:ARG:HH21	2.07	0.53
1:A:190:ARG:HD2	30:0:1884:G:O6	2.09	0.53
1:A:207:GLN:O	1:A:208:HIS:HB3	2.07	0.53
30:0:78:G:N3	30:0:78:G:N9	2.57	0.53
30:0:820:G:O2'	30:0:856:G:H4'	2.09	0.53
13:M:107:ARG:NH1	13:M:107:ARG:HG3	2.23	0.53
23:W:39:ASP:OD1	23:W:42:ARG:NH2	2.42	0.53
2:B:8:LYS:HB3	2:B:218:TRP:O	2.08	0.53
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.38	0.53
2:B:56:ASP:HB3	2:B:322:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:839:C:H1'	41:0:6899:HOH:O	2.07	0.53
41:N:8841:HOH:O	17:Q:19:ARG:HD2	2.09	0.53
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.91	0.53
3:C:142:ASP:OD1	3:C:236:THR:HG23	2.08	0.53
15:O:3:THR:CB	30:0:656:G:H5'	2.34	0.53
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.91	0.53
10:J:131:THR:HG22	10:J:133:GLY:N	2.24	0.53
30:0:1165:G:H4'	30:0:1174:A:O2'	2.08	0.53
30:0:858:U:H2'	30:0:859:C:C6	2.43	0.53
2:B:171:VAL:HG23	2:B:172:SER:N	2.24	0.53
41:P:6012:HOH:O	30:0:1548:U:H4'	2.07	0.53
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.90	0.53
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.23	0.53
30:0:482:G:H4'	30:0:508:A:N1	2.23	0.53
23:W:117:ARG:HB3	23:W:117:ARG:HH11	1.74	0.53
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.09	0.53
4:D:172:VAL:CG1	4:D:173:GLU:H	2.15	0.53
16:P:103:THR:HA	16:P:106:ARG:HH12	1.68	0.53
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.53
1:A:34:ASP:C	1:A:36:ASP:H	2.12	0.53
1:A:199:HIS:CD2	1:A:201:PHE:HB2	2.44	0.53
2:B:5:ARG:HD2	2:B:8:LYS:HE2	1.91	0.53
12:L:54:PRO:HG2	12:L:57:VAL:HG21	1.89	0.53
19:S:33:SER:OG	19:S:36:GLU:HG3	2.09	0.53
30:0:2562:G:H1'	41:0:6532:HOH:O	2.09	0.53
13:M:67:VAL:HG11	13:M:97:ILE:HG23	1.91	0.53
18:R:15:LYS:HE3	41:R:8986:HOH:O	2.09	0.53
30:0:2274:A:O2'	30:0:2275:G:H5'	2.09	0.53
1:A:37:VAL:HG23	41:A:9074:HOH:O	2.09	0.53
30:0:1160:G:HO2'	30:0:1190:G:H8	1.57	0.52
5:E:84:MET:CG	5:E:168:ILE:HD13	2.39	0.52
30:0:558:C:O2'	30:0:559:U:H5''	2.09	0.52
8:H:14:LYS:HB3	41:H:9007:HOH:O	2.09	0.52
30:0:1218:U:H2'	30:0:1219:U:H6	1.73	0.52
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.52
14:N:27:LEU:HD22	14:N:50:LEU:HD22	1.91	0.52
29:3:80:ARG:O	30:0:2457:U:H4'	2.10	0.52
30:0:2880:A:H2'	30:0:2881:C:H5'	1.91	0.52
30:0:1445:G:N2	30:0:1678:A:H1'	2.23	0.52
2:B:122:ASP:O	2:B:126:GLU:HB2	2.09	0.52
16:P:55:LYS:HG2	16:P:56:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:THR:HG23	6:F:99:THR:O	2.09	0.52
24:X:45:GLU:HG3	41:X:6178:HOH:O	2.09	0.52
25:Y:193:LEU:CD1	25:Y:221:ALA:HB2	2.39	0.52
30:0:2786:G:H2'	41:0:7991:HOH:O	2.10	0.52
13:M:115:LEU:HD13	13:M:116:ASN:HB2	1.91	0.52
20:T:30:ASP:O	20:T:33:GLU:HB3	2.10	0.52
3:C:236:THR:HA	41:C:8648:HOH:O	2.07	0.52
9:I:98:ASP:OD1	9:I:101:LYS:HD2	2.09	0.52
8:H:33:GLN:H	8:H:69:ARG:NH1	2.07	0.52
30:0:948:G:O2'	30:0:949:U:H5'	2.08	0.52
25:Y:208:LYS:HZ1	30:0:1343:C:C2'	2.22	0.52
30:0:2584:G:H8	41:0:5461:HOH:O	1.91	0.52
5:E:106:ASN:ND2	5:E:109:GLY:HA2	2.25	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.08	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.44	0.52
10:J:130:VAL:HG12	10:J:131:THR:H	1.72	0.52
2:B:171:VAL:HG23	2:B:172:SER:H	1.74	0.52
30:0:1902:G:H2'	30:0:1903:U:O4'	2.10	0.52
30:0:1496:A:H2'	30:0:1497:G:O4'	2.09	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
3:C:18:LEU:HD12	3:C:19:PRO:HD2	1.91	0.52
13:M:77:HIS:C	13:M:78:LYS:CA	2.78	0.52
11:K:96:VAL:HG21	11:K:109:LEU:HD22	1.92	0.52
30:0:2505:G:C2'	30:0:2506:A:H5'	2.39	0.52
5:E:14:GLU:O	5:E:15:GLN:HB2	2.09	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.92	0.52
18:R:114:VAL:HB	18:R:145:LEU:CD1	2.36	0.52
4:D:136:ARG:NH1	4:D:156:ARG:O	2.41	0.52
30:0:2634:G:O2'	30:0:2635:A:H5'	2.09	0.52
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.52
19:S:57:THR:HG22	19:S:59:ASP:H	1.73	0.52
10:J:14:ALA:O	10:J:17:CYS:HB2	2.10	0.52
30:0:195:C:H2'	30:0:196:G:H5'	1.92	0.52
30:0:583:C:H2'	30:0:584:U:H6	1.75	0.52
30:0:2432:C:O2'	30:0:2433:A:H5'	2.10	0.52
3:C:123:LEU:O	3:C:126:ASP:N	2.42	0.52
4:D:21:VAL:HG23	4:D:80:ALA:HB1	1.91	0.52
1:A:96:LEU:CD2	1:A:128:LEU:HD22	2.39	0.52
25:Y:107:PRO:HD3	25:Y:182:PHE:CD1	2.44	0.52
13:M:139:PRO:HA	13:M:142:GLN:HB2	1.92	0.52
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2768:A:O2'	30:0:2769:C:H5'	2.10	0.52
4:D:99:ASP:OD2	4:D:101:THR:HB	2.08	0.52
2:B:145:HIS:HD2	2:B:146:THR:O	1.92	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.52
30:0:462:A:N6	30:0:477:A:C2	2.77	0.52
30:0:578:C:H2'	30:0:579:G:O4'	2.10	0.52
20:T:66:ASP:OD1	20:T:69:LYS:N	2.34	0.52
2:B:336:GLN:O	30:0:2862:G:H4'	2.10	0.52
30:0:1244:U:H4'	30:0:1246:A:O4'	2.10	0.52
24:X:74:ALA:HA	24:X:85:VAL:HG13	1.92	0.52
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.90	0.52
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.10	0.52
30:0:1183:C:H5	30:0:1192:A:OP1	1.91	0.52
1:A:217:ARG:NH1	1:A:217:ARG:CG	2.70	0.52
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.90	0.52
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.45	0.52
30:0:25:A:O2'	30:0:640:G:H5'	2.10	0.52
30:0:830:G:H5''	41:0:9420:HOH:O	2.09	0.52
8:H:91:ARG:O	30:0:1003:U:H4'	2.10	0.52
30:0:1314:U:H2'	41:0:6711:HOH:O	2.08	0.52
30:0:1783:A:O2'	30:0:1784:U:H5'	2.08	0.52
10:J:46:ILE:HA	41:0:3802:HOH:O	2.09	0.52
30:0:2649:A:H2'	41:0:6965:HOH:O	2.08	0.52
2:B:36:PRO:HB3	2:B:174:ARG:CB	2.40	0.52
30:0:35:U:O2'	30:0:36:C:H5'	2.09	0.52
30:0:336:G:H2'	41:0:4601:HOH:O	2.08	0.52
13:M:158:ARG:HA	13:M:163:LEU:HD12	1.90	0.52
19:S:57:THR:CG2	19:S:58:MET:N	2.73	0.52
1:A:176:HIS:CD2	30:0:857:A:H4'	2.45	0.52
20:T:66:ASP:OD1	20:T:68:ASP:N	2.42	0.52
30:0:1809:G:N2	30:0:1811:A:H3'	2.24	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.56	0.52
30:0:1117:A:H2'	41:0:5754:HOH:O	2.09	0.52
9:I:123:VAL:C	9:I:125:GLY:H	2.13	0.52
1:A:14:SER:HB2	41:A:9016:HOH:O	2.09	0.52
3:C:93:LYS:O	3:C:98:ARG:NH2	2.42	0.52
3:C:124:VAL:HG12	3:C:131:PHE:HE2	1.74	0.52
24:X:66:THR:CG2	24:X:67:PRO:HD2	2.40	0.52
30:0:37:A:H2'	30:0:38:G:C8	2.45	0.52
15:O:32:ARG:HB2	41:O:4656:HOH:O	2.10	0.52
30:0:625:U:H5'	41:0:4081:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:38:THR:CG2	23:W:39:ASP:N	2.73	0.52
30:0:204:A:C2'	30:0:205:U:H5'	2.39	0.52
30:0:1406:A:H4'	30:0:1407:A:C5'	2.39	0.52
14:N:33:ARG:HH21	14:N:48:VAL:HG11	1.74	0.52
14:N:23:ARG:NH1	41:N:8868:HOH:O	2.42	0.52
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.91	0.52
14:N:115:VAL:HG13	41:9:9103:HOH:O	2.10	0.52
2:B:258:GLY:H	2:B:260:HIS:CE1	2.28	0.52
23:W:120:PRO:HG2	30:0:1095:U:O2	2.10	0.52
15:O:44:ASN:HB2	38:O:8808:CL:CL	2.47	0.52
30:0:627:G:H1'	41:0:5293:HOH:O	2.08	0.52
41:K:4183:HOH:O	30:0:2712:G:H5'	2.10	0.52
30:0:2765:C:H2'	30:0:2766:A:C8	2.45	0.52
30:0:78:G:N3	30:0:78:G:N1	2.58	0.52
17:Q:15:LYS:NZ	41:Q:5620:HOH:O	2.43	0.52
30:0:951:A:O2'	30:0:952:G:H5'	2.10	0.52
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.91	0.52
9:I:108:HIS:N	9:I:109:PRO:CD	2.72	0.52
30:0:2314:G:H2'	30:0:2315:C:H5'	1.92	0.52
30:0:2253:G:O2'	30:0:2254:G:H5'	2.09	0.52
3:C:175:LYS:NZ	3:C:184:ARG:HB3	2.25	0.52
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.39	0.52
31:9:78:G:N1	31:9:78:G:N3	2.58	0.52
3:C:124:VAL:HG12	3:C:131:PHE:CE2	2.45	0.52
12:L:11:ARG:NH1	30:0:903:U:OP2	2.41	0.52
30:0:1574:C:H6	30:0:1574:C:O5'	1.92	0.52
30:0:396:U:O2'	30:0:418:C:H4'	2.09	0.52
30:0:1748:U:H4'	41:0:9318:HOH:O	2.10	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.09	0.52
18:R:96:VAL:O	18:R:99:ALA:HB3	2.09	0.52
27:1:28:HIS:ND1	27:1:31:LYS:HE2	2.25	0.52
30:0:2426:G:H1'	41:0:6925:HOH:O	2.09	0.52
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.10	0.52
3:C:33:LYS:HE2	41:C:8564:HOH:O	2.09	0.52
21:U:49:LEU:HG	41:U:3805:HOH:O	2.10	0.52
7:G:22:ALA:O	7:G:25:GLU:HB3	2.10	0.52
2:B:28:SER:HB3	30:0:2807:U:OP1	2.11	0.51
20:T:43:ASN:O	20:T:45:GLY:N	2.41	0.51
25:Y:150:LEU:HB2	41:0:6295:HOH:O	2.09	0.51
22:V:27:LEU:HA	22:V:49:LEU:HD13	1.92	0.51
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:157:PRO:HA	41:N:8823:HOH:O	2.09	0.51
2:B:41:PHE:CE1	2:B:79:MET:HG3	2.44	0.51
7:G:64:ASN:N	7:G:64:ASN:HD22	2.07	0.51
1:A:132:ASP:HB3	1:A:135:VAL:H	1.75	0.51
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.11	0.51
24:X:87:ALA:O	24:X:88:GLU:HB3	2.10	0.51
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.81	0.51
30:0:432:G:H2'	30:0:433:C:H6	1.75	0.51
7:G:27:ILE:HD12	7:G:70:ALA:HB1	1.92	0.51
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.92	0.51
15:O:32:ARG:NE	15:O:35:LYS:HD3	2.18	0.51
6:F:58:GLU:HA	6:F:61:MET:HE1	1.91	0.51
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.93	0.51
30:0:2247:C:H2'	30:0:2248:C:C6	2.43	0.51
10:J:90:LYS:HE2	30:0:2083:A:N6	2.26	0.51
1:A:16:PHE:HB3	41:A:9032:HOH:O	2.09	0.51
2:B:145:HIS:CD2	2:B:159:PRO:HB3	2.45	0.51
12:L:79:ASP:HB3	41:L:9021:HOH:O	2.10	0.51
30:0:105:G:O2'	30:0:106:A:H5'	2.10	0.51
1:A:77:GLY:C	1:A:78:ASP:CA	2.79	0.51
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.40	0.51
13:M:133:LEU:O	13:M:134:ILE:HD13	2.10	0.51
2:B:243:ASN:HA	2:B:244:PRO:C	2.29	0.51
29:3:84:ARG:HD3	41:3:9041:HOH:O	2.11	0.51
24:X:87:ALA:O	24:X:88:GLU:CB	2.57	0.51
30:0:1190:G:H4'	30:0:1207:A:N1	2.24	0.51
4:D:75:LEU:HD13	4:D:79:MET:O	2.10	0.51
25:Y:148:GLY:HA3	30:0:622:G:P	2.51	0.51
30:0:2765:C:H2'	30:0:2766:A:H8	1.75	0.51
16:P:139:ARG:NH1	16:P:139:ARG:HG3	2.21	0.51
16:P:125:LYS:HB3	16:P:130:GLU:HG3	1.92	0.51
1:A:96:LEU:HD22	1:A:128:LEU:HD22	1.93	0.51
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.51
23:W:142:ASP:O	23:W:145:GLY:N	2.43	0.51
3:C:140:VAL:HB	41:C:8648:HOH:O	2.10	0.51
30:0:1161:A:H1'	41:0:4752:HOH:O	2.11	0.51
7:G:23:ILE:HG22	7:G:27:ILE:CD1	2.39	0.51
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.10	0.51
25:Y:177:LYS:HE2	25:Y:183:GLU:OE2	2.09	0.51
9:I:96:SER:OG	9:I:99:GLN:HG3	2.10	0.51
22:V:64:GLY:O	22:V:65:ASP:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.10	0.51
16:P:37:ARG:NH2	30:0:1502:A:OP1	2.43	0.51
2:B:145:HIS:HD2	2:B:159:PRO:HB3	1.76	0.51
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.25	0.51
12:L:18:HIS:HB3	41:L:8973:HOH:O	2.09	0.51
30:0:2850:C:H1'	41:0:9168:HOH:O	2.10	0.51
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.92	0.51
30:0:1746:A:H5''	41:0:6929:HOH:O	2.10	0.51
30:0:1471:A:H2'	30:0:1472:C:C6	2.45	0.51
30:0:1790:C:H2'	30:0:1791:U:H6	1.75	0.51
30:0:146:U:O2'	30:0:147:G:H5'	2.11	0.51
11:K:101:ASN:O	11:K:102:GLU:HB2	2.10	0.51
20:T:40:VAL:HG23	20:T:119:ALA:OXT	2.10	0.51
2:B:316:ARG:HG3	2:B:316:ARG:O	2.11	0.51
20:T:24:ARG:HH11	20:T:24:ARG:HG2	1.75	0.51
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.93	0.51
30:0:1705:C:O2	30:0:2735:U:H5''	2.11	0.51
16:P:14:LEU:O	16:P:16:VAL:HG23	2.10	0.51
15:O:97:SER:H	15:O:100:GLN:NE2	2.08	0.51
25:Y:203:VAL:CG1	25:Y:228:VAL:HG22	2.41	0.51
9:I:91:PHE:HA	9:I:131:GLY:HA3	1.93	0.51
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.51
25:Y:112:GLU:CD	25:Y:115:ARG:HH12	2.13	0.51
31:9:96:C:H2'	31:9:97:U:C6	2.46	0.51
29:3:31:THR:O	30:0:1923:G:H4'	2.11	0.51
23:W:77:ALA:HB3	41:W:5763:HOH:O	2.11	0.51
30:0:1700:C:OP2	41:0:6868:HOH:O	2.19	0.51
30:0:1303:C:O2	30:0:1353:C:H1'	2.09	0.51
3:C:65:ARG:HG3	3:C:67:GLN:HB2	1.93	0.51
4:D:40:ILE:HA	4:D:43:GLU:OE1	2.11	0.51
1:A:109:GLU:HG2	1:A:116:GLY:N	2.20	0.51
20:T:43:ASN:HD22	20:T:108:ARG:CZ	2.24	0.51
30:0:2566:A:H61	30:0:2699:A:H61	1.59	0.51
23:W:117:ARG:CB	23:W:117:ARG:HH11	2.23	0.51
12:L:73:VAL:HG23	12:L:74:THR:H	1.75	0.51
21:U:35:LYS:HE2	21:U:51:TRP:CH2	2.46	0.51
5:E:159:VAL:O	5:E:163:GLN:HG2	2.11	0.51
30:0:1979:G:H2'	41:0:3192:HOH:O	2.10	0.51
1:A:66:ARG:CB	1:A:66:ARG:HH11	2.21	0.51
30:0:1835:U:C5	30:0:1840:A:N7	2.71	0.51
31:9:3:A:H2	31:9:21:G:N3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.51
3:C:175:LYS:HZ3	3:C:184:ARG:HB3	1.76	0.51
30:0:2502:C:H2'	30:0:2503:A:H5'	1.92	0.51
31:9:97:U:H3'	41:9:9104:HOH:O	2.11	0.51
4:D:154:LYS:HD2	4:D:154:LYS:H	1.75	0.51
8:H:87:LYS:HB2	8:H:87:LYS:NZ	2.26	0.51
9:I:134:ILE:HG22	9:I:135:GLU:N	2.26	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
2:B:11:LEU:HD21	2:B:250:THR:HG22	1.93	0.51
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.46	0.51
14:N:11:ARG:NH1	31:9:8:G:O6	2.43	0.51
31:9:92:G:H2'	31:9:93:A:H8	1.75	0.51
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.41	0.51
30:0:2735:U:H2'	30:0:2736:U:H6	1.76	0.51
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.41	0.51
20:T:107:LYS:O	20:T:111:ARG:HB2	2.09	0.51
23:W:142:ASP:HB3	41:W:2729:HOH:O	2.11	0.51
4:D:10:PHE:CE1	4:D:11:HIS:HB3	2.46	0.51
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.93	0.51
2:B:216:LYS:HA	41:0:5933:HOH:O	2.11	0.51
30:0:1477:C:H5'	30:0:1868:G:C5'	2.40	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:2911:C:H3'	41:0:6395:HOH:O	2.11	0.51
8:H:20:ARG:HD3	8:H:26:ILE:HD12	1.92	0.51
17:Q:1:PRO:HA	30:0:2299:G:O6	2.11	0.51
3:C:236:THR:HB	3:C:239:ALA:HB2	1.93	0.50
25:Y:189:ASN:HD22	25:Y:191:ASP:N	2.10	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.62	0.50
20:T:49:GLU:OE2	20:T:51:LEU:HD21	2.11	0.50
12:L:80:ASP:HB2	12:L:90:ARG:O	2.11	0.50
14:N:86:LEU:HD21	14:N:180:LEU:CD1	2.41	0.50
8:H:49:GLN:OE1	8:H:169:GLU:HG2	2.11	0.50
30:0:566:A:H2'	30:0:567:U:H5'	1.91	0.50
23:W:122:ARG:CZ	23:W:154:ARG:HB3	2.40	0.50
29:3:84:ARG:HD2	30:0:2427:C:OP2	2.10	0.50
5:E:35:TYR:HA	10:J:127:ILE:CD1	2.41	0.50
30:0:2251:G:H2'	30:0:2252:A:H8	1.76	0.50
30:0:354:A:H2'	30:0:355:C:H6	1.76	0.50
23:W:117:ARG:CB	23:W:117:ARG:NH1	2.74	0.50
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.46	0.50
4:D:135:VAL:HG22	4:D:136:ARG:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:ASN:OD1	30:0:80:A:H3'	2.11	0.50
30:0:314:G:N2	30:0:316:A:H3'	2.26	0.50
2:B:214:PRO:HB2	2:B:220:VAL:HG21	1.93	0.50
30:0:2819:C:H2'	30:0:2820:A:C8	2.46	0.50
5:E:36:PRO:HD3	10:J:127:ILE:CG1	2.42	0.50
30:0:213:G:H22	30:0:225:G:H2'	1.76	0.50
30:0:1595:G:O2'	30:0:1596:U:H5'	2.11	0.50
2:B:125:GLU:O	2:B:129:ARG:HG3	2.11	0.50
30:0:561:G:O2'	30:0:562:A:H5'	2.11	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.92	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.50
2:B:279:THR:HG22	2:B:280:VAL:N	2.26	0.50
6:F:46:GLU:OE2	6:F:100:ASP:HA	2.10	0.50
3:C:168:ARG:NH1	30:0:1310:U:OP2	2.44	0.50
25:Y:112:GLU:OE1	25:Y:115:ARG:NH1	2.44	0.50
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.47	0.50
10:J:71:TYR:CD1	10:J:72:PRO:HD2	2.46	0.50
25:Y:102:LEU:HG	41:Y:8887:HOH:O	2.11	0.50
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.50
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.75	0.50
14:N:1:ALA:HB2	31:9:14:G:O2'	2.11	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.69	0.50
31:9:106:U:O2'	31:9:107:C:H5'	2.11	0.50
16:P:134:VAL:O	16:P:138:GLU:HG3	2.11	0.50
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.92	0.50
25:Y:170:SER:HG	25:Y:175:ARG:HG3	1.76	0.50
29:3:38:ARG:NH1	30:0:396:U:OP2	2.43	0.50
30:0:2324:G:N2	30:0:2377:U:H1'	2.26	0.50
1:A:146:LYS:NZ	30:0:1855:G:O3'	2.44	0.50
23:W:73:LEU:HD22	23:W:111:GLY:HA2	1.94	0.50
9:I:97:VAL:O	9:I:101:LYS:HG3	2.12	0.50
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.93	0.50
22:V:39:ALA:O	22:V:41:GLU:N	2.43	0.50
8:H:49:GLN:O	8:H:169:GLU:HB3	2.11	0.50
14:N:183:ASP:O	14:N:184:ILE:O	2.28	0.50
12:L:13:HIS:ND1	38:L:8814:CL:CL	2.77	0.50
3:C:7:ASP:O	3:C:9:ASP:N	2.44	0.50
24:X:10:VAL:HG12	24:X:11:THR:N	2.26	0.50
5:E:83:GLY:O	5:E:169:THR:N	2.35	0.50
14:N:78:MET:HB2	14:N:146:HIS:HE1	1.76	0.50
30:0:506:G:N1	30:0:509:A:OP2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.50
20:T:52:ARG:HB2	20:T:95:ASN:HB3	1.94	0.50
4:D:170:TYR:O	4:D:171:ASP:CB	2.59	0.50
23:W:7:LEU:HD12	23:W:53:ALA:HB2	1.93	0.50
20:T:16:LEU:HB2	30:0:100:C:C4'	2.41	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
1:A:69:LEU:HD11	1:A:159:VAL:HG13	1.94	0.50
30:0:1309:U:H2'	30:0:1310:U:O4'	2.12	0.50
30:0:553:G:H2'	30:0:554:G:H5'	1.94	0.50
30:0:823:U:H3'	41:0:5310:HOH:O	2.12	0.50
30:0:371:U:H2'	30:0:372:A:H8	1.76	0.50
30:0:1649:G:O2'	30:0:1650:C:H5'	2.11	0.50
30:0:1301:C:O2'	30:0:1331:G:H4'	2.11	0.50
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.50
3:C:27:ARG:NH2	30:0:657:G:OP1	2.44	0.50
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.94	0.50
30:0:303:C:H2'	30:0:304:G:O4'	2.12	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
20:T:20:HIS:O	20:T:23:VAL:HG23	2.11	0.50
29:3:22:VAL:CG1	29:3:67:LEU:HD13	2.42	0.50
30:0:1980:U:H5'	30:0:2626:C:H1'	1.93	0.50
19:S:56:ASN:O	28:2:8:LYS:NZ	2.45	0.50
19:S:77:VAL:C	19:S:78:ALA:CA	2.80	0.50
30:0:1659:A:H2'	30:0:1660:G:O4'	2.11	0.50
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
9:I:86:GLU:HB2	9:I:90:ASP:OD2	2.12	0.50
11:K:64:MET:O	11:K:67:GLN:HB2	2.12	0.50
30:0:1805:G:O2'	30:0:1806:G:H5'	2.12	0.50
22:V:1:THR:C	22:V:3:LEU:N	2.65	0.50
5:E:40:VAL:HB	41:E:2857:HOH:O	2.11	0.50
30:0:1992:U:H2'	30:0:1994:A:OP2	2.12	0.50
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.76	0.50
30:0:1200:A:H3'	41:0:6592:HOH:O	2.11	0.50
8:H:41:LYS:O	8:H:87:LYS:HE2	2.11	0.50
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.50
22:V:6:GLN:HB2	41:0:7782:HOH:O	2.11	0.50
30:0:1590:A:H1'	30:0:1606:A:C2	2.47	0.50
2:B:197:GLY:HA3	2:B:323:LEU:HA	1.93	0.50
5:E:1:PRO:HG2	5:E:59:MET:SD	2.52	0.50
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:189:ASN:HD22	25:Y:191:ASP:H	1.59	0.50
5:E:22:VAL:O	5:E:28:SER:HA	2.11	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.50
30:0:2836:G:O2'	30:0:2838:A:N7	2.34	0.50
3:C:5:ILE:HG22	3:C:6:TYR:N	2.27	0.50
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.11	0.50
30:0:1503:U:C2'	30:0:1504:A:H5'	2.42	0.50
3:C:124:VAL:HA	3:C:230:GLY:O	2.11	0.50
30:0:445:U:O2'	30:0:446:G:H5'	2.12	0.50
12:L:10:SER:O	12:L:11:ARG:HB3	2.12	0.50
30:0:1641:A:H2'	30:0:1642:A:H5'	1.93	0.50
15:O:43:VAL:CG1	15:O:47:ARG:HD2	2.42	0.50
29:3:40:ARG:HD2	41:3:9047:HOH:O	2.12	0.50
30:0:1985:U:C5	30:0:1996:U:C2	3.00	0.50
12:L:4:LYS:HE2	30:0:645:U:OP2	2.12	0.50
30:0:162:C:H2'	30:0:163:U:H5'	1.94	0.50
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.42	0.50
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.30	0.49
29:3:68:LYS:HE2	30:0:2436:U:C5'	2.40	0.49
1:A:26:ASP:O	1:A:28:GLU:N	2.45	0.49
30:0:875:A:H5'	30:0:876:A:N7	2.27	0.49
21:U:56:ARG:O	21:U:56:ARG:CD	2.60	0.49
17:Q:16:ASN:ND2	17:Q:45:PRO:HB2	2.27	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.42	0.49
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.49
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.45	0.49
30:0:2114:C:O2'	30:0:2115:U:H5'	2.11	0.49
12:L:89:PHE:CD1	12:L:89:PHE:N	2.80	0.49
23:W:29:VAL:O	23:W:30:ASN:HB2	2.10	0.49
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.46	0.49
30:0:412:C:H2'	30:0:413:G:O4'	2.11	0.49
18:R:44:VAL:O	18:R:48:GLU:HG3	2.12	0.49
30:0:2001:G:O2'	30:0:2002:C:H5'	2.12	0.49
18:R:9:ASP:OD1	18:R:11:ASP:HB2	2.12	0.49
5:E:31:ARG:NH1	41:E:5919:HOH:O	2.46	0.49
30:0:1878:G:H1'	41:0:6953:HOH:O	2.11	0.49
30:0:2839:C:H2'	30:0:2840:A:H5''	1.95	0.49
31:9:98:C:H2'	31:9:99:U:C6	2.44	0.49
30:0:2314:G:O2'	30:0:2315:C:H5'	2.11	0.49
30:0:2252:A:H2'	30:0:2253:G:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1773:G:H4'	41:0:4407:HOH:O	2.12	0.49
30:0:1270:U:H2'	30:0:1271:A:C8	2.46	0.49
20:T:53:GLY:HA3	41:0:7613:HOH:O	2.12	0.49
2:B:1:PRO:HG3	30:0:2591:C:OP1	2.11	0.49
3:C:195:VAL:HA	3:C:213:ALA:O	2.12	0.49
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.45	0.49
30:0:1714:C:O2'	30:0:1715:C:H5'	2.12	0.49
4:D:57:THR:HG23	4:D:63:ILE:CA	2.32	0.49
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.40	0.49
41:Z:8722:HOH:O	30:0:1886:A:H5'	2.11	0.49
9:I:87:PRO:HD3	41:0:4130:HOH:O	2.12	0.49
1:A:65:ARG:C	1:A:66:ARG:HG3	2.32	0.49
30:0:283:U:H5''	30:0:284:C:OP2	2.12	0.49
20:T:1:SER:HB2	30:0:447:A:P	2.53	0.49
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.49
30:0:1165:G:H1'	30:0:1174:A:H1'	1.95	0.49
30:0:1201:C:H2'	30:0:1202:A:H5'	1.94	0.49
6:F:38:LYS:HA	6:F:41:GLU:OE1	2.12	0.49
14:N:154:LEU:O	14:N:155:GLU:HB3	2.12	0.49
3:C:202:THR:HG22	30:0:328:U:O4'	2.12	0.49
26:Z:105:ARG:O	26:Z:106:SER:C	2.50	0.49
22:V:12:THR:HG22	22:V:15:GLU:CD	2.31	0.49
13:M:133:LEU:N	13:M:133:LEU:HD12	2.26	0.49
14:N:15:GLU:O	14:N:16:ALA:HB3	2.13	0.49
12:L:108:VAL:HB	12:L:125:PHE:HD2	1.77	0.49
11:K:77:ARG:O	11:K:78:LYS:CA	2.60	0.49
31:9:78:G:N2	31:9:102:G:H2'	2.27	0.49
26:Z:77:GLY:O	26:Z:78:ILE:CA	2.61	0.49
4:D:151:ILE:CG2	4:D:155:HIS:HB3	2.43	0.49
25:Y:212:ARG:HD2	41:Y:8907:HOH:O	2.12	0.49
41:X:4132:HOH:O	30:0:2895:C:H4'	2.12	0.49
14:N:64:SER:C	14:N:66:LEU:H	2.15	0.49
4:D:77:ASP:C	4:D:78:GLU:CA	2.81	0.49
29:3:55:VAL:HB	29:3:56:PRO:HD2	1.94	0.49
19:S:40:ALA:O	19:S:44:GLN:HB2	2.12	0.49
20:T:27:LEU:HB2	20:T:32:ARG:CG	2.42	0.49
14:N:176:ARG:O	14:N:180:LEU:HD13	2.12	0.49
30:0:2296:C:H4'	30:0:2362:A:H2	1.78	0.49
30:0:568:G:C6	30:0:588:G:H1'	2.48	0.49
30:0:945:U:H2'	30:0:946:C:H6	1.78	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:TYR:CE1	5:E:92:PRO:HA	2.47	0.49
30:0:695:C:H2'	30:0:696:C:H6	1.77	0.49
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.77	0.49
2:B:277:GLU:N	2:B:278:PRO:HD2	2.27	0.49
30:0:764:C:H2'	30:0:765:G:O4'	2.13	0.49
30:0:772:G:H2'	30:0:773:A:O4'	2.12	0.49
14:N:141:ARG:HH12	31:9:35:C:H2'	1.77	0.49
16:P:64:GLU:HG2	41:P:2495:HOH:O	2.13	0.49
1:A:169:PHE:O	1:A:171:LYS:N	2.43	0.49
30:0:2289:G:H21	30:0:2291:A:H2	1.57	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
20:T:26:THR:CG2	20:T:97:ARG:HG3	2.42	0.49
2:B:161:VAL:HG12	2:B:162:MET:N	2.28	0.49
30:0:285:A:H2'	30:0:286:U:O4'	2.12	0.49
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.49
13:M:57:LYS:HZ3	13:M:144:ASP:HB2	1.78	0.49
20:T:77:VAL:C	20:T:78:THR:CA	2.81	0.49
31:9:18:U:H2'	31:9:19:G:C8	2.44	0.49
9:I:96:SER:HB3	9:I:99:GLN:NE2	2.27	0.49
13:M:58:GLN:HG3	41:M:8907:HOH:O	2.12	0.49
15:O:26:TRP:CE3	15:O:26:TRP:HA	2.48	0.49
15:O:77:ALA:C	15:O:78:ALA:CA	2.81	0.49
30:0:816:G:H5'	30:0:1598:A:H4'	1.95	0.49
16:P:6:GLN:HG2	16:P:31:ILE:HG22	1.93	0.49
15:O:38:ARG:NH1	41:O:7674:HOH:O	2.45	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
30:0:300:U:O2'	30:0:301:C:H5'	2.12	0.49
23:W:62:LEU:HD21	23:W:100:LEU:HD12	1.94	0.49
1:A:165:THR:HG22	41:A:9096:HOH:O	2.11	0.49
30:0:98:A:C2'	30:0:99:A:H5'	2.42	0.49
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.13	0.49
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.43	0.49
18:R:46:TYR:O	18:R:50:VAL:HG23	2.13	0.49
11:K:87:ARG:HD2	41:K:4066:HOH:O	2.12	0.49
31:9:29:C:H2'	31:9:30:C:C5'	2.38	0.49
2:B:279:THR:HG23	2:B:290:VAL:H	1.77	0.49
30:0:2909:G:O2'	30:0:2910:A:H5'	2.13	0.49
24:X:25:ARG:HD2	41:X:5356:HOH:O	2.13	0.49
13:M:40:ILE:HD11	13:M:62:VAL:HG12	1.94	0.49
9:I:118:ASN:HA	9:I:121:LYS:HD2	1.95	0.49
30:0:2566:A:H2	30:0:2695:C:O2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2583:A:H3'	41:0:5461:HOH:O	2.13	0.49
30:0:1314:U:H5''	30:0:1316:G:O4'	2.12	0.49
19:S:5:ILE:HD12	19:S:44:GLN:HG3	1.93	0.49
30:0:98:A:H2'	30:0:99:A:H5'	1.95	0.49
30:0:1230:A:OP1	30:0:1230:A:H8	1.95	0.49
29:3:16:GLU:HB2	41:0:6515:HOH:O	2.12	0.49
2:B:29:TRP:CZ3	2:B:164:THR:HG23	2.48	0.49
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.12	0.49
11:K:9:THR:O	11:K:10:GLN:C	2.51	0.49
30:0:2718:C:H6	30:0:2718:C:H5'	1.78	0.49
13:M:144:ASP:O	13:M:148:SER:HB3	2.12	0.49
30:0:2426:G:H5''	30:0:2427:C:O4'	2.11	0.49
30:0:565:A:OP2	30:0:592:G:N1	2.42	0.49
15:O:26:TRP:HA	15:O:26:TRP:HE3	1.78	0.49
19:S:56:ASN:HD22	30:0:1676:G:P	2.34	0.49
26:Z:54:GLU:HA	26:Z:57:MET:HB3	1.93	0.49
4:D:80:ALA:O	4:D:83:PHE:HB3	2.13	0.49
30:0:1367:A:H2'	30:0:1368:U:O4'	2.12	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.13	0.49
10:J:67:ASN:OD1	30:0:2082:G:H1'	2.12	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.49
14:N:140:GLN:O	14:N:143:ARG:HB2	2.13	0.49
30:0:1666:C:C2'	30:0:1667:A:C5'	2.91	0.49
30:0:658:C:O2'	30:0:662:U:OP1	2.25	0.49
2:B:52:VAL:C	2:B:53:LEU:HD12	2.33	0.49
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.48	0.49
23:W:129:LYS:HE2	30:0:1098:A:O3'	2.12	0.49
28:2:20:ARG:HG3	28:2:21:VAL:N	2.28	0.49
30:0:222:A:H2'	30:0:223:G:O4'	2.12	0.49
30:0:690:G:H1'	30:0:731:U:H1'	1.95	0.49
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.48	0.49
3:C:131:PHE:CD2	3:C:232:LEU:HD22	2.47	0.49
23:W:34:LEU:HD13	23:W:100:LEU:HD13	1.94	0.49
30:0:737:A:H2'	30:0:738:G:O4'	2.12	0.49
3:C:188:ARG:NH2	41:C:8523:HOH:O	2.44	0.49
24:X:63:ARG:HG2	24:X:63:ARG:O	2.13	0.49
30:0:1393:A:H2'	30:0:1394:C:C6	2.48	0.49
29:3:51:LYS:HB2	41:0:5348:HOH:O	2.12	0.49
41:A:9044:HOH:O	30:0:871:G:H4'	2.12	0.49
1:A:211:LYS:HB2	41:A:9098:HOH:O	2.13	0.49
20:T:101:LEU:HD22	20:T:108:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:42:ARG:HA	23:W:45:VAL:HG22	1.95	0.49
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.49
28:2:43:ARG:HH21	30:0:1685:A:H4'	1.78	0.49
30:0:2642:G:H2'	30:0:2643:G:O4'	2.13	0.49
12:L:4:LYS:HD2	41:0:5885:HOH:O	2.13	0.49
30:0:1774:G:H1'	41:0:5405:HOH:O	2.13	0.49
2:B:128:ILE:O	2:B:131:ALA:HB3	2.12	0.49
30:0:71:G:H8	41:0:4782:HOH:O	1.96	0.49
30:0:883:U:C5	30:0:888:U:H5'	2.48	0.49
3:C:87:ARG:NH2	30:0:894:A:C2	2.80	0.49
17:Q:77:ASP:C	17:Q:78:GLY:CA	2.82	0.49
30:0:17:G:H2'	30:0:18:C:C6	2.48	0.49
10:J:52:GLN:NE2	30:0:1119:G:C2'	2.63	0.48
30:0:2073:G:H2'	41:0:4699:HOH:O	2.13	0.48
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.43	0.48
30:0:2387:U:O2	30:0:2402:A:C2	2.66	0.48
30:0:1175:G:H1'	30:0:1193:A:H2'	1.94	0.48
6:F:100:ASP:O	6:F:101:ALA:O	2.31	0.48
14:N:155:GLU:O	14:N:156:GLU:HG3	2.13	0.48
4:D:52:THR:CG2	30:0:2346:C:H4'	2.43	0.48
5:E:137:ASP:O	5:E:141:VAL:HG23	2.13	0.48
23:W:117:ARG:HB2	23:W:117:ARG:NH1	2.28	0.48
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.48
30:0:1139:U:H2'	30:0:1140:C:C6	2.48	0.48
20:T:44:ALA:HA	20:T:62:VAL:HG12	1.95	0.48
30:0:2473:U:O3'	30:0:2474:A:H3'	2.13	0.48
14:N:37:ARG:HH11	14:N:37:ARG:HG3	1.78	0.48
31:9:28:U:H2'	31:9:29:C:C6	2.48	0.48
16:P:41:ARG:O	16:P:44:VAL:HB	2.13	0.48
2:B:280:VAL:HG13	2:B:333:GLU:O	2.14	0.48
12:L:6:ARG:NH2	41:L:9012:HOH:O	2.45	0.48
4:D:59:GLY:O	4:D:61:PHE:N	2.46	0.48
30:0:2312:G:C2'	30:0:2313:C:H5'	2.43	0.48
26:Z:54:GLU:HG2	26:Z:57:MET:CE	2.43	0.48
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.48	0.48
2:B:285:VAL:O	2:B:286:ASN:HB2	2.13	0.48
30:0:2688:U:H2'	30:0:2689:A:H8	1.79	0.48
30:0:1121:G:H4'	41:0:6381:HOH:O	2.13	0.48
7:G:14:GLU:HB3	41:G:4173:HOH:O	2.13	0.48
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.13	0.48
14:N:143:ARG:HA	14:N:172:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1666:C:C2'	30:0:1667:A:H5''	2.42	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.12	0.48
2:B:316:ARG:HB2	30:0:2768:A:C8	2.48	0.48
15:O:102:ILE:HB	41:O:7481:HOH:O	2.13	0.48
8:H:23:ILE:HG22	8:H:123:ILE:CD1	2.43	0.48
41:J:2219:HOH:O	30:0:1103:C:H5''	2.13	0.48
27:1:50:TRP:O	30:0:890:C:O2'	2.28	0.48
28:2:28:LYS:O	30:0:87:C:H2'	2.13	0.48
30:0:1505:U:H4'	41:0:6027:HOH:O	2.12	0.48
21:U:52:THR:HG22	21:U:54:THR:HB	1.95	0.48
30:0:380:A:O4'	30:0:382:U:H1'	2.13	0.48
1:A:179:MET:C	1:A:181:ALA:H	2.17	0.48
30:0:2607:U:H4'	41:0:3343:HOH:O	2.12	0.48
41:B:9059:HOH:O	30:0:2819:C:H5'	2.13	0.48
30:0:2780:C:H2'	30:0:2781:U:C6	2.49	0.48
16:P:77:ALA:C	16:P:78:GLY:CA	2.81	0.48
28:2:42:TRP:CZ3	28:2:43:ARG:HB2	2.48	0.48
2:B:45:LYS:HG2	2:B:305:ASP:HA	1.94	0.48
3:C:37:ALA:O	3:C:38:ALA:C	2.51	0.48
14:N:100:ALA:HB3	14:N:129:ILE:HG12	1.95	0.48
8:H:122:LYS:O	8:H:124:VAL:HG13	2.13	0.48
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.48
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.43	0.48
11:K:98:VAL:CG1	11:K:99:ASP:N	2.76	0.48
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.77	0.48
8:H:24:THR:O	8:H:123:ILE:HD12	2.13	0.48
1:A:4:ILE:HG22	1:A:198:ASP:O	2.14	0.48
25:Y:193:LEU:HD13	25:Y:221:ALA:HB2	1.95	0.48
9:I:81:GLU:N	9:I:81:GLU:OE1	2.46	0.48
25:Y:108:ASP:OD1	25:Y:108:ASP:N	2.47	0.48
30:0:1475:G:N3	30:0:1866:A:H2	2.11	0.48
30:0:1405:U:H2'	41:0:7653:HOH:O	2.14	0.48
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.48
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.96	0.48
4:D:23:VAL:O	4:D:23:VAL:HG23	2.13	0.48
4:D:45:THR:HB	4:D:75:LEU:HD11	1.96	0.48
30:0:368:C:C2'	30:0:369:G:H5'	2.44	0.48
29:3:64:LYS:HA	29:3:84:ARG:HA	1.94	0.48
20:T:21:LYS:HA	20:T:24:ARG:CG	2.42	0.48
30:0:694:A:H2'	30:0:695:C:H5'	1.95	0.48
22:V:27:LEU:O	22:V:30:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:887:G:H2'	30:0:888:U:C6	2.48	0.48
30:0:2755:G:H1'	41:0:5540:HOH:O	2.12	0.48
4:D:50:VAL:O	4:D:71:ALA:HA	2.13	0.48
30:0:1409:G:H5'	41:0:4602:HOH:O	2.13	0.48
10:J:61:VAL:HA	41:0:3397:HOH:O	2.13	0.48
30:0:1876:C:H4'	30:0:1877:G:OP2	2.14	0.48
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.48	0.48
12:L:150:GLN:HB3	41:L:9035:HOH:O	2.14	0.48
5:E:81:GLU:OE2	5:E:132:THR:OG1	2.31	0.48
2:B:16:ARG:NH1	41:B:9091:HOH:O	2.45	0.48
20:T:20:HIS:HB3	20:T:41:ARG:HD2	1.95	0.48
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.13	0.48
30:0:333:G:O2'	30:0:334:G:H5'	2.13	0.48
25:Y:182:PHE:HD2	25:Y:200:THR:O	1.95	0.48
30:0:1394:C:H3'	30:0:1433:G:H22	1.78	0.48
5:E:162:PHE:CD1	5:E:162:PHE:N	2.81	0.48
12:L:97:VAL:HB	12:L:100:ALA:HB2	1.96	0.48
30:0:2351:C:H2'	30:0:2352:G:O4'	2.14	0.48
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.96	0.48
18:R:100:ASP:C	18:R:102:GLN:H	2.16	0.48
30:0:1189:A:H1'	30:0:1209:C:C1'	2.43	0.48
28:2:46:ASP:OD1	28:2:47:THR:O	2.32	0.48
30:0:111:C:C2'	30:0:112:G:H5'	2.44	0.48
30:0:746:A:H4'	30:0:747:G:H5'	1.95	0.48
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.78	0.48
12:L:77:ALA:C	12:L:79:ASP:H	2.17	0.48
30:0:1353:C:H5"	41:0:7423:HOH:O	2.12	0.48
13:M:46:LEU:HD22	13:M:50:ARG:HD2	1.96	0.48
22:V:42:ASN:O	22:V:44:GLY:N	2.47	0.48
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.48
9:I:127:CYS:O	9:I:129:SER:N	2.47	0.48
1:A:57:ALA:HB1	1:A:65:ARG:HE	1.78	0.48
25:Y:117:LEU:CD1	25:Y:174:VAL:HG11	2.40	0.48
13:M:95:LYS:CE	30:0:157:G:H4'	2.44	0.48
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.44	0.48
20:T:81:LYS:HE3	30:0:486:A:O5'	2.13	0.48
26:Z:51:ALA:HA	41:Z:8712:HOH:O	2.13	0.48
30:0:696:C:O2'	30:0:731:U:OP1	2.30	0.48
30:0:1819:G:H2'	30:0:1820:G:H5'	1.96	0.48
13:M:5:TYR:CE2	13:M:50:ARG:HD3	2.49	0.48
30:0:670:G:H2'	30:0:671:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1490:G:H4'	30:0:1533:A:OP1	2.14	0.48
17:Q:77:ASP:O	17:Q:78:GLY:C	2.51	0.48
21:U:37:GLU:HB3	41:U:408:HOH:O	2.12	0.48
28:2:5:LYS:O	28:2:9:LYS:HG3	2.14	0.48
17:Q:86:VAL:HG11	17:Q:91:LEU:HD21	1.94	0.48
2:B:294:TYR:CD1	2:B:294:TYR:C	2.87	0.48
30:0:419:A:H1'	30:0:1921:A:C2	2.49	0.48
23:W:128:VAL:O	23:W:138:LEU:HD11	2.14	0.48
30:0:349:U:O2'	30:0:350:G:H5'	2.14	0.48
21:U:11:THR:CG2	21:U:53:ASP:HB2	2.42	0.48
22:V:50:ARG:HH12	30:0:56:G:C5'	2.26	0.48
20:T:9:LYS:CE	20:T:13:ARG:NH1	2.76	0.48
16:P:104:LYS:HE2	16:P:138:GLU:HG2	1.95	0.48
11:K:66:ARG:NH2	30:0:1994:A:P	2.87	0.48
14:N:151:ASP:O	14:N:154:LEU:HD13	2.13	0.48
30:0:2253:G:H2'	30:0:2254:G:H8	1.78	0.48
26:Z:73:ARG:HB2	26:Z:79:TRP:CZ3	2.49	0.48
31:9:78:G:N3	31:9:78:G:N2	2.62	0.48
30:0:1819:G:C2'	30:0:1820:G:H5'	2.43	0.48
30:0:1457:U:O2'	30:0:1458:A:H5'	2.13	0.48
30:0:2045:G:H5''	41:0:9032:HOH:O	2.14	0.48
3:C:107:ARG:NH2	30:0:678:G:OP2	2.46	0.48
13:M:150:ILE:HA	13:M:155:GLN:HG3	1.95	0.48
2:B:264:GLU:HG3	41:B:9010:HOH:O	2.13	0.48
11:K:49:LEU:HD22	11:K:80:ILE:HD13	1.96	0.48
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.20	0.47
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.37	0.47
9:I:87:PRO:HG3	30:0:1181:A:H1'	1.96	0.47
14:N:82:TYR:HE1	14:N:120:GLU:HG2	1.77	0.47
30:0:559:U:C6	30:0:559:U:H5'	2.48	0.47
12:L:53:ARG:NH2	12:L:57:VAL:CG1	2.76	0.47
15:O:26:TRP:N	41:O:3062:HOH:O	2.47	0.47
30:0:1346:U:H2'	30:0:1347:U:H6	1.79	0.47
2:B:123:ALA:O	2:B:126:GLU:HB3	2.14	0.47
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.72	0.47
30:0:1057:A:H1'	30:0:2492:U:O2'	2.14	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.96	0.47
30:0:1159:G:H1	30:0:1208:C:H42	1.62	0.47
11:K:8:VAL:HG12	11:K:9:THR:N	2.29	0.47
21:U:11:THR:HG22	21:U:53:ASP:CG	2.34	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.54	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:567:U:O5'	30:0:567:U:H6	1.96	0.47
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.47
30:0:100:C:H2'	30:0:101:C:H6	1.80	0.47
30:0:1248:A:H2'	30:0:1249:U:C6	2.49	0.47
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.44	0.47
30:0:1278:A:H2'	30:0:1280:A:C8	2.49	0.47
2:B:132:HIS:CE1	2:B:171:VAL:HG21	2.50	0.47
26:Z:54:GLU:HA	26:Z:57:MET:HE2	1.95	0.47
18:R:98:ASN:ND2	18:R:98:ASN:N	2.62	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
30:0:1948:G:H2'	30:0:1949:G:C8	2.49	0.47
23:W:117:ARG:HB3	30:0:1263:C:OP1	2.14	0.47
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.47
30:0:364:U:H2'	30:0:365:G:O4'	2.14	0.47
8:H:52:LEU:HD13	8:H:153:PHE:HB3	1.96	0.47
18:R:136:TRP:CE2	30:0:2053:G:H4'	2.50	0.47
30:0:1033:C:H2'	30:0:1034:G:H5'	1.96	0.47
5:E:103:VAL:HG12	5:E:104:ILE:N	2.29	0.47
8:H:32:ALA:C	8:H:33:GLN:HG3	2.34	0.47
30:0:1067:A:H3'	41:0:5158:HOH:O	2.14	0.47
30:0:1383:U:O2'	30:0:1384:C:H5'	2.14	0.47
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.96	0.47
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.47
30:0:425:U:O2'	30:0:426:G:H5'	2.14	0.47
3:C:53:GLY:O	3:C:79:ARG:HA	2.14	0.47
9:I:129:SER:HB3	30:0:1192:A:N6	2.29	0.47
30:0:876:A:H2'	30:0:876:A:N3	2.29	0.47
30:0:2578:G:C8	30:0:2578:G:H5'	2.40	0.47
18:R:82:GLU:CG	18:R:83:LYS:N	2.77	0.47
27:1:4:GLY:O	27:1:8:GLN:HG2	2.14	0.47
11:K:115:ARG:HG3	11:K:116:GLU:N	2.29	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
5:E:60:SER:OG	30:0:2784:A:H1'	2.15	0.47
30:0:1819:G:H2'	30:0:1820:G:H4'	1.96	0.47
30:0:1816:C:H2'	30:0:1817:U:O4'	2.15	0.47
30:0:514:G:H3'	30:0:514:G:OP1	2.15	0.47
8:H:77:ILE:C	8:H:78:LYS:CA	2.83	0.47
1:A:80:LEU:HD22	1:A:91:GLY:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:VAL:HG21	8:H:173:GLU:HG2	1.96	0.47
30:0:1079:A:N3	30:0:2078:U:H1'	2.30	0.47
24:X:72:VAL:HG23	24:X:86:GLU:O	2.15	0.47
6:F:56:PRO:HG3	13:M:44:THR:HA	1.95	0.47
18:R:106:GLY:O	18:R:109:MET:HB2	2.14	0.47
1:A:58:VAL:O	1:A:65:ARG:HA	2.15	0.47
8:H:96:GLN:HE21	8:H:129:ARG:HH21	1.62	0.47
30:0:78:G:N1	30:0:78:G:N7	2.62	0.47
30:0:1973:A:C8	30:0:1973:A:H5'	2.42	0.47
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.29	0.47
30:0:2520:G:O2'	30:0:2521:A:H5'	2.14	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.95	0.47
30:0:1736:A:H5'	41:0:5472:HOH:O	2.14	0.47
9:I:118:ASN:HA	9:I:121:LYS:CD	2.44	0.47
30:0:1259:A:N1	30:0:1261:A:H1'	2.29	0.47
4:D:21:VAL:CG2	4:D:80:ALA:HB1	2.45	0.47
2:B:17:LYS:O	2:B:260:HIS:HD2	1.97	0.47
7:G:65:THR:HG23	41:0:6310:HOH:O	2.15	0.47
41:N:8812:HOH:O	31:9:36:C:H4'	2.13	0.47
30:0:323:C:O2'	30:0:324:G:H5'	2.14	0.47
30:0:1051:C:H2'	30:0:1052:G:O4'	2.15	0.47
30:0:344:C:H2'	30:0:345:G:O4'	2.13	0.47
6:F:117:GLU:C	6:F:119:ARG:H	2.17	0.47
1:A:212:PRO:HB2	41:A:9041:HOH:O	2.14	0.47
30:0:544:G:H2'	30:0:545:G:H5''	1.97	0.47
23:W:110:GLN:HA	23:W:110:GLN:HE21	1.78	0.47
30:0:1180:U:H2'	30:0:1181:A:C8	2.50	0.47
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.43	0.47
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.47
30:0:1976:G:O2'	30:0:1977:U:C5'	2.63	0.47
30:0:264:G:H1'	30:0:265:U:C5	2.49	0.47
30:0:695:C:H2'	30:0:696:C:C6	2.50	0.47
23:W:142:ASP:O	23:W:143:THR:C	2.53	0.47
27:1:13:THR:HG22	27:1:14:THR:N	2.30	0.47
30:0:270:U:H5''	41:0:5432:HOH:O	2.14	0.47
6:F:21:GLU:O	6:F:24:ARG:CG	2.63	0.47
13:M:137:ASN:ND2	30:0:145:A:H4'	2.29	0.47
2:B:248:ARG:NH2	41:B:8995:HOH:O	2.47	0.47
21:U:52:THR:HG21	21:U:54:THR:HB	1.96	0.47
30:0:1730:G:H5'	30:0:1731:C:H5	1.75	0.47
17:Q:27:GLN:NE2	31:9:8:G:H4'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:LEU:HG	14:N:28:LYS:HE3	1.97	0.47
30:0:1972:U:H2'	30:0:1973:A:C5'	2.44	0.47
13:M:57:LYS:NZ	13:M:144:ASP:HB2	2.30	0.47
2:B:214:PRO:C	2:B:220:VAL:HG22	2.35	0.47
1:A:83:GLY:O	1:A:94:LEU:HB3	2.14	0.47
3:C:34:ALA:CB	3:C:220:THR:HG21	2.44	0.47
14:N:152:GLU:C	14:N:154:LEU:N	2.67	0.47
30:0:1309:U:O2'	30:0:1310:U:H5'	2.13	0.47
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
18:R:98:ASN:ND2	18:R:98:ASN:H	2.12	0.47
31:9:78:G:N1	31:9:78:G:N7	2.62	0.47
30:0:352:A:H2'	30:0:353:G:C8	2.50	0.47
8:H:39:LYS:HA	8:H:87:LYS:HZ1	1.78	0.47
30:0:1333:U:H2'	30:0:1334:C:H6	1.79	0.47
30:0:636:G:H5'	30:0:2059:U:OP2	2.14	0.47
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.72	0.47
8:H:85:ASP:OD2	8:H:142:ASN:ND2	2.37	0.47
10:J:39:VAL:HG13	10:J:106:GLY:O	2.14	0.47
13:M:149:TRP:C	13:M:151:CYS:H	2.18	0.47
30:0:970:U:H6	30:0:970:U:O5'	1.98	0.47
31:9:100:G:H3'	41:9:9133:HOH:O	2.14	0.47
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.47
4:D:166:ILE:O	4:D:169:THR:N	2.48	0.47
1:A:26:ASP:O	1:A:26:ASP:CG	2.52	0.47
14:N:49:THR:HB	14:N:58:LEU:HD13	1.97	0.47
30:0:187:A:H3'	30:0:188:C:C6	2.50	0.47
30:0:1309:U:C2'	30:0:1310:U:H5'	2.45	0.47
30:0:2517:A:C2'	30:0:2518:C:H5'	2.44	0.47
13:M:69:LYS:HG2	13:M:127:LYS:HE3	1.95	0.47
30:0:1809:G:H2'	30:0:1811:A:OP2	2.15	0.47
30:0:366:U:H2'	30:0:367:G:O4'	2.15	0.47
6:F:79:GLN:HB2	6:F:82:ASP:OD2	2.14	0.47
11:K:28:GLU:HB3	11:K:59:LYS:HB2	1.95	0.47
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.15	0.47
30:0:1519:U:H2'	30:0:1520:G:C8	2.50	0.47
15:O:35:LYS:O	15:O:40:HIS:NE2	2.47	0.47
14:N:86:LEU:HA	14:N:121:GLY:O	2.14	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG1	2.45	0.47
30:0:1203:G:O2'	30:0:1204:C:H5'	2.15	0.47
30:0:185:G:C4'	30:0:186:A:H4'	2.45	0.47
4:D:60:GLU:O	4:D:62:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:GLU:OE2	11:K:44:HIS:HB2	2.14	0.47
30:0:1745:G:H22	30:0:2033:G:H5'	1.80	0.47
30:0:1682:A:H2'	41:0:3704:HOH:O	2.15	0.47
1:A:6:GLY:HA3	41:0:5481:HOH:O	2.15	0.47
30:0:2515:C:H2'	30:0:2516:G:O4'	2.14	0.47
16:P:69:ARG:HA	16:P:73:HIS:O	2.14	0.47
2:B:36:PRO:CG	2:B:169:GLY:H	2.16	0.47
4:D:40:ILE:HG13	4:D:41:LEU:H	1.79	0.47
24:X:7:GLU:HG3	24:X:74:ALA:O	2.15	0.47
29:3:77:ALA:O	29:3:78:HIS:CA	2.63	0.47
30:0:1665:G:H2'	30:0:1666:C:O4'	2.14	0.47
30:0:308:U:H5'	30:0:309:C:OP1	2.14	0.47
14:N:164:ASP:OD2	14:N:167:ASP:HA	2.15	0.47
30:0:400:C:H2'	30:0:401:C:C6	2.51	0.47
30:0:1347:U:H2'	30:0:1348:A:C8	2.50	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
30:0:1503:U:H2'	30:0:1504:A:H5'	1.96	0.47
19:S:44:GLN:HB3	19:S:45:TYR:CD1	2.50	0.47
30:0:2499:U:O2'	30:0:2500:C:H5'	2.14	0.47
3:C:173:LYS:HB3	3:C:187:ARG:HG3	1.96	0.47
2:B:147:VAL:O	2:B:147:VAL:HG12	2.15	0.47
23:W:106:THR:OG1	23:W:109:GLU:HG3	2.14	0.47
13:M:170:ASN:HB2	41:M:8837:HOH:O	2.15	0.47
3:C:238:SER:O	3:C:241:ALA:HB3	2.14	0.46
25:Y:100:ARG:HD2	25:Y:218:GLU:OE1	2.15	0.46
13:M:68:ARG:HG2	13:M:73:ARG:CZ	2.45	0.46
30:0:1909:A:H2'	30:0:1910:A:C8	2.50	0.46
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.46
8:H:12:ILE:HD12	8:H:57:THR:CG2	2.45	0.46
14:N:108:SER:HA	14:N:109:PRO:HD3	1.79	0.46
31:9:11:A:O2'	31:9:12:C:H3'	2.15	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.03	0.46
15:O:112:ARG:HD2	41:0:3570:HOH:O	2.15	0.46
30:0:512:G:H1'	41:0:7627:HOH:O	2.15	0.46
30:0:2554:U:H1'	41:0:6968:HOH:O	2.15	0.46
30:0:615:G:H2'	30:0:616:U:C6	2.50	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:2102:G:H5''	30:0:2538:A:C2	2.51	0.46
6:F:15:ASP:O	6:F:18:GLU:HB2	2.16	0.46
12:L:24:ALA:CB	12:L:30:ARG:HG3	2.46	0.46
15:O:25:VAL:CG1	30:0:710:G:H5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:136:ALA:HB3	41:L:9038:HOH:O	2.15	0.46
25:Y:204:ARG:HH22	30:0:553:G:P	2.37	0.46
3:C:67:GLN:O	30:0:1359:U:C4	2.68	0.46
30:0:1131:G:C6	30:0:1230:A:C4	3.03	0.46
30:0:1361:C:H2'	30:0:1362:U:H6	1.80	0.46
30:0:824:G:N2	41:0:6935:HOH:O	2.48	0.46
12:L:134:GLU:HA	12:L:138:GLY:O	2.15	0.46
10:J:36:VAL:CG1	10:J:37:ALA:N	2.78	0.46
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.46
30:0:2568:A:H2'	30:0:2569:A:O4'	2.14	0.46
3:C:48:SER:OG	3:C:91:PRO:HB2	2.16	0.46
30:0:1077:G:H2'	30:0:1080:C:H42	1.79	0.46
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.46
4:D:167:GLU:C	4:D:169:THR:H	2.19	0.46
3:C:51:TYR:HA	3:C:54:LEU:HD12	1.97	0.46
30:0:1931:A:C2'	30:0:1932:G:H5'	2.44	0.46
16:P:91:LYS:NZ	30:0:816:G:OP1	2.39	0.46
30:0:107:U:C2'	30:0:108:U:H5'	2.45	0.46
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.80	0.46
29:3:42:ARG:HH11	29:3:42:ARG:HG3	1.79	0.46
30:0:1477:C:H5'	30:0:1868:G:H5'	1.97	0.46
30:0:920:C:H2'	30:0:2109:U:C2	2.51	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.48	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.03	0.46
2:B:148:PRO:HG2	2:B:158:LYS:O	2.15	0.46
11:K:21:ALA:HB1	11:K:110:LYS:O	2.14	0.46
30:0:2651:C:H2'	30:0:2652:U:O4'	2.15	0.46
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.97	0.46
1:A:109:GLU:HG2	1:A:114:ASP:OD1	2.15	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.15	0.46
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.16	0.46
30:0:292:G:H1'	30:0:360:A:N6	2.29	0.46
30:0:2296:C:H4'	30:0:2362:A:C2	2.51	0.46
31:9:3:A:H2'	41:9:9043:HOH:O	2.15	0.46
29:3:36:ILE:CG2	29:3:37:ASP:N	2.79	0.46
8:H:149:VAL:HG22	41:H:9034:HOH:O	2.13	0.46
8:H:87:LYS:HB2	8:H:87:LYS:HZ2	1.81	0.46
11:K:62:PRO:HA	11:K:65:ARG:NH2	2.31	0.46
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.30	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.14	0.46
2:B:251:VAL:HG23	2:B:253:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.46
18:R:135:ALA:O	30:0:2054:A:H4'	2.16	0.46
23:W:10:GLU:O	23:W:13:MET:HB3	2.16	0.46
14:N:29:SER:HB3	30:0:2415:A:O2'	2.16	0.46
3:C:176:ALA:HB2	30:0:1343:C:C5	2.50	0.46
4:D:18:ILE:HG12	4:D:134:LEU:CD2	2.45	0.46
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.15	0.46
13:M:52:GLN:HG2	13:M:116:ASN:CG	2.36	0.46
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.97	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.64	0.46
1:A:42:VAL:O	1:A:76:VAL:HG13	2.14	0.46
30:0:1410:G:H3'	41:0:6433:HOH:O	2.15	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
3:C:90:HIS:HB2	41:C:8544:HOH:O	2.14	0.46
30:0:2453:G:H5'	41:0:5549:HOH:O	2.15	0.46
3:C:241:ALA:O	3:C:244:ALA:HB3	2.14	0.46
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.41	0.46
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.46
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.97	0.46
16:P:134:VAL:O	16:P:137:LEU:HB3	2.16	0.46
30:0:2838:A:H2'	30:0:2839:C:C6	2.51	0.46
1:A:27:LEU:HD11	1:A:51:ARG:HE	1.79	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:1971:G:H5''	41:0:7875:HOH:O	2.14	0.46
30:0:699:C:H6	30:0:744:G:O4'	1.98	0.46
5:E:7:ILE:HD11	5:E:11:VAL:C	2.36	0.46
15:O:44:ASN:CG	15:O:67:SER:HB3	2.36	0.46
30:0:1791:U:H2'	30:0:1792:C:C6	2.51	0.46
3:C:178:GLN:O	3:C:179:GLY:C	2.54	0.46
30:0:1001:U:O2'	30:0:1002:G:H5'	2.15	0.46
30:0:574:G:H2'	30:0:575:A:O4'	2.16	0.46
4:D:39:ASP:HB2	41:D:5583:HOH:O	2.15	0.46
1:A:75:GLY:HA2	26:Z:88:PHE:HA	1.98	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.96	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.32	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:791:A:H2'	30:0:792:G:O4'	2.16	0.46
13:M:45:ARG:HB2	13:M:118:TYR:CE1	2.51	0.46
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.31	0.46
30:0:558:C:H2'	30:0:559:U:H5'	1.97	0.46
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:566:A:C2'	30:0:567:U:H5'	2.46	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.51	0.46
22:V:49:LEU:O	22:V:53:ILE:HG13	2.15	0.46
30:0:2842:G:C2'	30:0:2843:A:H5'	2.45	0.46
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.98	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
13:M:98:GLN:HB2	13:M:129:HIS:CD2	2.51	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
11:K:81:ARG:HG3	11:K:85:GLY:O	2.15	0.46
9:I:82:THR:CG2	30:0:1168:C:H5''	2.45	0.46
2:B:284:PHE:HB2	2:B:287:TYR:HB3	1.96	0.46
18:R:119:VAL:HG23	18:R:142:ASP:HB2	1.98	0.46
30:0:612:U:H2'	30:0:613:C:H6	1.80	0.46
30:0:1202:A:H2'	30:0:1203:G:O4'	2.16	0.46
19:S:49:VAL:HG13	19:S:66:VAL:HG13	1.96	0.46
30:0:1098:A:H2'	30:0:1099:G:O4'	2.15	0.46
2:B:238:ASN:ND2	2:B:240:GLY:H	2.11	0.46
2:B:109:LEU:HD22	2:B:145:HIS:CE1	2.51	0.46
31:9:39:U:H1'	31:9:44:A:H61	1.81	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
30:0:535:G:C5	30:0:2063:U:C4	3.04	0.46
16:P:107:GLU:C	16:P:109:ARG:H	2.19	0.46
30:0:1135:G:H5'	41:0:6761:HOH:O	2.16	0.46
30:0:111:C:O2'	30:0:112:G:H5'	2.16	0.46
14:N:164:ASP:OD1	14:N:167:ASP:OD1	2.34	0.46
17:Q:25:PRO:HB3	41:9:9006:HOH:O	2.15	0.46
6:F:49:PHE:HB2	6:F:96:ALA:HB3	1.98	0.46
31:9:74:G:C6	31:9:75:G:N7	2.84	0.46
19:S:68:LEU:HB3	19:S:72:ASP:HB2	1.97	0.46
13:M:40:ILE:HD11	13:M:130:GLU:HG2	1.97	0.46
30:0:1260:G:H3'	30:0:1261:A:C8	2.51	0.46
3:C:139:VAL:HG13	3:C:240:LEU:HD12	1.98	0.46
10:J:45:VAL:HG23	10:J:129:PHE:HD1	1.81	0.46
11:K:64:MET:HA	11:K:67:GLN:HE21	1.80	0.46
2:B:305:ASP:O	2:B:306:LYS:CB	2.63	0.46
20:T:38:ARG:HH21	30:0:306:A:P	2.38	0.46
30:0:956:G:H5'	31:9:81:C:H4'	1.98	0.46
11:K:23:ASN:HD21	11:K:107:THR:HB	1.80	0.46
30:0:1304:U:H2'	30:0:1305:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2371:G:H5'	41:0:5865:HOH:O	2.14	0.46
15:O:19:ARG:HH11	30:0:1276:U:H3'	1.81	0.46
30:0:1206:U:C6	30:0:1206:U:H5'	2.42	0.46
18:R:39:THR:O	18:R:40:ALA:C	2.55	0.46
2:B:76:THR:O	2:B:77:PRO:C	2.53	0.46
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.30	0.46
8:H:49:GLN:NE2	8:H:140:TYR:CE2	2.84	0.46
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.80	0.46
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.80	0.46
14:N:26:LEU:HD21	14:N:103:ASP:HA	1.97	0.46
30:0:2748:G:H4'	30:0:2749:U:H5'	1.98	0.46
30:0:25:A:H2'	30:0:26:U:H5'	1.98	0.46
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.31	0.46
30:0:2760:C:H5"	41:0:6171:HOH:O	2.16	0.46
5:E:158:ASP:OD1	5:E:160:ARG:HB2	2.15	0.46
22:V:23:LEU:O	22:V:24:LYS:C	2.54	0.46
8:H:86:TYR:C	8:H:86:TYR:CD1	2.90	0.46
2:B:337:GLY:N	41:B:9013:HOH:O	2.49	0.46
30:0:1607:A:H2'	30:0:1608:G:O4'	2.16	0.46
30:0:1209:C:O2'	30:0:1210:G:H5'	2.15	0.45
16:P:115:SER:N	16:P:118:GLN:HE21	1.89	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
18:R:8:ALA:HB1	18:R:13:THR:CG2	2.35	0.45
28:2:45:ASN:HB3	28:2:46:ASP:H	1.58	0.45
6:F:8:VAL:HG13	6:F:12:LEU:HD13	1.98	0.45
1:A:135:VAL:HG13	1:A:135:VAL:O	2.16	0.45
16:P:104:LYS:HG2	16:P:137:LEU:HD23	1.98	0.45
41:N:8846:HOH:O	31:9:7:G:H5'	2.16	0.45
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.17	0.45
30:0:37:A:C2	30:0:446:G:C2	3.04	0.45
31:9:39:U:HO2'	31:9:42:C:H5	1.57	0.45
30:0:1393:A:N1	30:0:1725:C:O2'	2.43	0.45
15:O:19:ARG:NH1	30:0:1276:U:H3'	2.30	0.45
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.45
30:0:2269:C:H2'	30:0:2270:G:O4'	2.15	0.45
30:0:1739:G:H1'	30:0:2726:U:O4	2.16	0.45
22:V:1:THR:O	22:V:3:LEU:N	2.50	0.45
3:C:2:GLN:HB2	41:C:8534:HOH:O	2.16	0.45
30:0:2507:G:H2'	30:0:2510:C:N4	2.31	0.45
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:544:G:C2'	30:0:545:G:H5''	2.45	0.45
30:0:820:G:H5'	30:0:821:U:C5'	2.47	0.45
25:Y:174:VAL:HA	25:Y:177:LYS:HE3	1.97	0.45
20:T:23:VAL:O	20:T:42:VAL:HG23	2.16	0.45
25:Y:106:THR:CG2	25:Y:107:PRO:HD2	2.46	0.45
30:0:425:U:H4'	41:0:7746:HOH:O	2.16	0.45
20:T:29:ALA:HA	41:T:7653:HOH:O	2.16	0.45
30:0:2087:C:C2	30:0:2658:G:C2	3.04	0.45
4:D:27:ILE:HD11	4:D:37:ALA:HB2	1.98	0.45
1:A:105:VAL:HG13	1:A:155:THR:O	2.16	0.45
3:C:193:LEU:HD23	3:C:233:THR:HG23	1.99	0.45
30:0:1183:C:H41	30:0:1192:A:P	2.39	0.45
4:D:149:ARG:HH12	14:N:15:GLU:HA	1.79	0.45
30:0:2004:U:O2	30:0:2004:U:C2'	2.64	0.45
33:6:76:8AN:H2	41:6:82:HOH:O	2.15	0.45
11:K:115:ARG:O	11:K:118:ALA:HB3	2.16	0.45
23:W:31:HIS:HB3	23:W:115:THR:HG21	1.98	0.45
30:0:710:G:C2'	30:0:711:G:H5'	2.47	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.45
23:W:117:ARG:HH22	30:0:1264:U:P	2.39	0.45
30:0:584:U:H3'	41:0:6928:HOH:O	2.17	0.45
25:Y:112:GLU:CD	25:Y:115:ARG:NH1	2.69	0.45
22:V:44:GLY:HA3	30:0:92:G:H4'	1.98	0.45
30:0:1361:C:H2'	30:0:1362:U:C6	2.51	0.45
30:0:1588:G:H1'	30:0:1607:A:H61	1.81	0.45
30:0:644:G:H1'	41:0:7230:HOH:O	2.16	0.45
30:0:1864:C:H2'	30:0:1865:A:O4'	2.16	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.97	0.45
30:0:1619:G:H2'	30:0:1620:C:O4'	2.15	0.45
18:R:64:SER:OG	30:0:1369:A:H5''	2.16	0.45
30:0:2560:C:H4'	41:0:7451:HOH:O	2.17	0.45
7:G:23:ILE:CD1	7:G:67:LEU:HD23	2.42	0.45
20:T:52:ARG:HD2	30:0:317:A:H5''	1.97	0.45
2:B:279:THR:HA	2:B:284:PHE:HE1	1.81	0.45
23:W:52:VAL:CG2	23:W:53:ALA:N	2.49	0.45
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.45
11:K:125:ALA:O	11:K:127:ALA:N	2.50	0.45
2:B:88:GLU:HB3	2:B:97:LEU:HD12	1.99	0.45
3:C:101:ASP:HA	41:C:8646:HOH:O	2.16	0.45
12:L:125:PHE:CE1	12:L:140:VAL:HG22	2.52	0.45
20:T:41:ARG:NH1	20:T:42:VAL:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:16:VAL:HG12	16:P:17:GLY:N	2.31	0.45
1:A:48:ASP:OD2	1:A:51:ARG:HG3	2.17	0.45
9:I:91:PHE:CD2	9:I:131:GLY:HA2	2.50	0.45
24:X:87:ALA:O	24:X:88:GLU:HG2	2.16	0.45
30:0:2842:G:H2'	30:0:2843:A:C5'	2.46	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
13:M:8:ILE:O	13:M:11:ALA:HB3	2.17	0.45
30:0:2894:C:O2'	30:0:2895:C:H5'	2.16	0.45
18:R:100:ASP:C	18:R:102:GLN:N	2.68	0.45
16:P:73:HIS:HE1	30:0:1789:G:O6	2.00	0.45
31:9:12:C:H4'	31:9:69:U:O2	2.17	0.45
30:0:652:G:C2	30:0:653:U:H1'	2.51	0.45
30:0:27:U:H2'	30:0:28:G:O4'	2.17	0.45
30:0:2846:C:H2'	30:0:2847:G:H8	1.80	0.45
6:F:67:ALA:HB1	6:F:72:VAL:O	2.16	0.45
20:T:82:THR:HA	41:0:4859:HOH:O	2.15	0.45
8:H:141:CYS:HB2	41:H:8997:HOH:O	2.15	0.45
11:K:132:VAL:HG11	21:U:22:VAL:HG22	1.98	0.45
30:0:1181:A:H2'	30:0:1182:C:C5'	2.47	0.45
2:B:140:LEU:HD13	2:B:175:LEU:HA	1.98	0.45
30:0:1165:G:H21	30:0:1173:A:H5''	1.82	0.45
30:0:604:G:H2'	41:0:9543:HOH:O	2.16	0.45
1:A:23:TYR:CD1	1:A:50:ALA:HB2	2.51	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.82	0.45
14:N:73:ALA:HB1	14:N:74:PRO:HD2	1.97	0.45
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.16	0.45
30:0:731:U:H2'	30:0:732:C:C6	2.52	0.45
30:0:1810:C:H2'	30:0:1811:A:O4'	2.17	0.45
14:N:72:GLU:HB3	14:N:163:PHE:CE1	2.52	0.45
30:0:1394:C:H3'	30:0:1433:G:N2	2.32	0.45
6:F:21:GLU:O	6:F:24:ARG:HG2	2.17	0.45
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.98	0.45
30:0:1889:C:H2'	30:0:1890:U:O4'	2.17	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
14:N:77:ASN:C	14:N:78:MET:CA	2.84	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
5:E:20:ILE:O	5:E:30:THR:HG23	2.16	0.45
11:K:101:ASN:O	11:K:102:GLU:CB	2.63	0.45
30:0:2419:U:H5''	30:0:2420:G:H5'	1.97	0.45
19:S:73:ASP:HB3	19:S:76:GLU:OE1	2.17	0.45
1:A:199:HIS:N	41:A:9110:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1833:U:O2'	30:0:1834:C:H5'	2.16	0.45
7:G:64:ASN:OD1	30:0:1211:G:H5''	2.16	0.45
31:9:13:A:H3'	31:9:14:G:H5'	1.99	0.45
20:T:43:ASN:ND2	20:T:108:ARG:CZ	2.79	0.45
30:0:168:C:H5'	30:0:2277:U:OP1	2.16	0.45
27:1:15:THR:O	27:1:29:THR:N	2.46	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
2:B:185:GLY:HA2	41:B:9109:HOH:O	2.15	0.45
30:0:1484:G:H2'	41:0:3021:HOH:O	2.17	0.45
30:0:116:G:H2'	30:0:117:A:C8	2.52	0.45
3:C:76:ARG:HB3	3:C:78:ARG:NH1	2.32	0.45
30:0:1831:U:O4	30:0:1845:A:H2	1.99	0.45
15:O:59:VAL:HG23	15:O:111:VAL:CG2	2.46	0.45
20:T:17:HIS:HB3	30:0:100:C:O2	2.17	0.45
12:L:66:VAL:CG2	12:L:67:ARG:N	2.78	0.45
14:N:151:ASP:OD1	14:N:154:LEU:HD13	2.17	0.45
13:M:69:LYS:O	30:0:2263:G:H4'	2.17	0.45
30:0:2081:A:H2'	30:0:2082:G:O4'	2.17	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.17	0.45
30:0:343:C:O2'	30:0:344:C:H5'	2.16	0.45
14:N:102:LEU:HG	14:N:104:ILE:HG23	1.98	0.45
30:0:1741:U:H5''	41:0:3669:HOH:O	2.17	0.45
22:V:43:PRO:O	22:V:46:ILE:HG22	2.16	0.45
17:Q:14:LEU:HB3	41:Q:3971:HOH:O	2.16	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.16	0.45
1:A:211:LYS:HZ2	1:A:223:ARG:HH21	1.64	0.45
3:C:193:LEU:HA	3:C:211:ASP:O	2.17	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.17	0.45
23:W:122:ARG:NH2	41:0:6133:HOH:O	2.50	0.45
31:9:1:U:H5'	31:9:121:C:O2	2.16	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.80	0.45
2:B:141:ARG:CG	2:B:165:ARG:HA	2.47	0.45
17:Q:62:THR:O	17:Q:64:GLU:HG2	2.16	0.45
30:0:750:A:H2'	30:0:751:U:C6	2.51	0.45
12:L:130:ARG:HA	41:L:9020:HOH:O	2.17	0.45
29:3:65:THR:HG23	29:3:67:LEU:HG	1.99	0.45
30:0:2011:A:H5'	30:0:2013:G:C1'	2.46	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
30:0:12:U:C2'	30:0:13:G:H5'	2.47	0.45
20:T:27:LEU:HB2	20:T:32:ARG:HG3	1.99	0.45
8:H:9:TYR:HE2	8:H:99:ARG:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:HIS:HD1	2:B:188:HIS:H	1.64	0.45
30:0:325:U:H2'	30:0:326:G:H8	1.79	0.45
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.45
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.45
3:C:219:ASN:O	3:C:223:LEU:HB2	2.16	0.45
23:W:80:ASP:H	23:W:83:TRP:HB3	1.82	0.45
2:B:74:ILE:HG13	41:B:9078:HOH:O	2.16	0.45
13:M:30:GLU:O	13:M:34:GLU:HG3	2.16	0.45
30:0:2443:C:H3'	41:0:4363:HOH:O	2.17	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.45
10:J:36:VAL:HG12	10:J:37:ALA:N	2.32	0.45
30:0:2135:A:O4'	30:0:2243:C:N4	2.50	0.45
15:O:49:GLU:OE1	15:O:70:LEU:HD12	2.16	0.45
30:0:2887:G:H2'	30:0:2888:U:C6	2.52	0.45
18:R:27:HIS:O	18:R:31:ILE:HG13	2.17	0.45
26:Z:37:ARG:HD3	41:Z:8713:HOH:O	2.16	0.45
3:C:236:THR:O	3:C:237:GLU:C	2.55	0.45
29:3:73:GLU:C	29:3:75:GLY:N	2.69	0.45
2:B:113:LEU:HD21	2:B:161:VAL:HG21	1.97	0.45
2:B:297:VAL:HB	41:B:9078:HOH:O	2.17	0.45
30:0:290:C:O2'	30:0:291:C:H5'	2.16	0.45
30:0:2361:A:H2'	30:0:2362:A:C8	2.51	0.45
30:0:191:A:C4	30:0:237:G:N7	2.85	0.45
16:P:138:GLU:O	16:P:139:ARG:C	2.54	0.45
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.45
17:Q:95:GLU:HA	30:0:949:U:C4'	2.46	0.45
24:X:20:GLU:CG	24:X:21:PRO:HD2	2.45	0.45
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.49	0.45
30:0:1985:U:C2	30:0:1996:U:O4'	2.70	0.45
2:B:294:TYR:HE2	41:B:9128:HOH:O	1.99	0.45
2:B:66:GLU:OE1	2:B:328:ARG:HD2	2.17	0.45
23:W:25:ASN:OD1	30:0:1025:C:H5''	2.17	0.45
30:0:2088:C:H1'	30:0:2841:A:C2	2.52	0.45
14:N:22:GLN:HB3	41:N:8873:HOH:O	2.17	0.45
4:D:141:VAL:HG13	4:D:144:ARG:NH2	2.32	0.45
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.87	0.44
13:M:80:GLY:C	13:M:81:ARG:HD2	2.37	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.25	0.44
13:M:72:ALA:HB1	13:M:93:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:73:A:H61	31:9:108:C:N4	2.13	0.44
1:A:94:LEU:N	1:A:94:LEU:HD23	2.31	0.44
30:0:1165:G:O2'	30:0:1174:A:C4'	2.65	0.44
30:0:1477:C:H4'	30:0:1868:G:OP1	2.17	0.44
30:0:2335:C:H2'	30:0:2336:G:H8	1.82	0.44
30:0:1031:G:O3'	30:0:1032:A:H8	2.00	0.44
30:0:2435:U:H1'	41:0:6273:HOH:O	2.17	0.44
5:E:9:GLU:HG2	41:E:7544:HOH:O	2.17	0.44
30:0:1291:A:H2	41:0:6136:HOH:O	2.00	0.44
30:0:297:U:H1'	41:0:4807:HOH:O	2.16	0.44
18:R:62:HIS:HB3	30:0:1370:G:O5'	2.16	0.44
8:H:67:ALA:HB1	8:H:159:LYS:HD3	1.98	0.44
14:N:37:ARG:HH21	14:N:105:GLY:CA	2.30	0.44
27:1:42:SER:HB3	30:0:1473:U:O4'	2.17	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.57	0.44
29:3:24:LYS:HE3	29:3:90:PHE:CE1	2.52	0.44
12:L:54:PRO:HG2	12:L:57:VAL:CG2	2.47	0.44
17:Q:61:GLY:HA3	17:Q:74:ASP:O	2.17	0.44
11:K:44:HIS:O	11:K:45:PRO:C	2.56	0.44
23:W:126:ASP:O	23:W:136:GLY:HA2	2.16	0.44
30:0:23:G:C6	30:0:24:G:N1	2.85	0.44
23:W:115:THR:HG23	41:W:5420:HOH:O	2.17	0.44
26:Z:77:GLY:C	26:Z:78:ILE:CA	2.86	0.44
23:W:56:GLU:O	23:W:143:THR:HG23	2.17	0.44
30:0:2394:A:H4'	41:0:9457:HOH:O	2.16	0.44
2:B:195:ARG:HG3	2:B:196:ALA:N	2.31	0.44
30:0:2869:G:H2'	30:0:2870:C:C6	2.52	0.44
25:Y:95:THR:O	25:Y:95:THR:HG22	2.16	0.44
25:Y:95:THR:N	25:Y:236:VAL:O	2.51	0.44
27:1:54:ALA:HB2	30:0:892:G:H5"	1.98	0.44
15:O:62:GLY:O	15:O:79:VAL:HG23	2.18	0.44
23:W:9:GLY:N	30:0:1086:A:OP1	2.50	0.44
3:C:145:GLU:CD	3:C:196:THR:HB	2.38	0.44
2:B:261:GLN:HG2	30:0:2808:U:OP1	2.17	0.44
30:0:1187:U:HO2'	30:0:1188:A:H8	1.65	0.44
24:X:41:PHE:HD2	24:X:76:ARG:HB2	1.81	0.44
30:0:2592:G:H2'	30:0:2593:C:C6	2.52	0.44
10:J:70:PHE:HE1	30:0:2676:C:C4'	2.19	0.44
18:R:39:THR:CG2	18:R:42:GLU:HG3	2.48	0.44
30:0:877:G:C2	30:0:885:G:O4'	2.70	0.44
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:34:C:H2'	30:0:35:U:C6	2.52	0.44
30:0:1298:U:H2'	30:0:1299:G:H8	1.81	0.44
30:0:254:C:H2'	30:0:255:A:O4'	2.18	0.44
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.44
2:B:274:GLU:HG3	2:B:292:GLY:C	2.38	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
19:S:67:ARG:HD3	41:0:5526:HOH:O	2.16	0.44
12:L:73:VAL:HG23	12:L:74:THR:N	2.31	0.44
10:J:57:TYR:O	10:J:61:VAL:HG23	2.18	0.44
13:M:98:GLN:HB2	13:M:129:HIS:NE2	2.32	0.44
2:B:209:LYS:HE2	41:B:9040:HOH:O	2.15	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.47	0.44
30:0:2323:G:H5'	41:0:7829:HOH:O	2.17	0.44
30:0:1021:G:O2'	30:0:1022:A:H5'	2.18	0.44
25:Y:186:ARG:HD2	41:0:5056:HOH:O	2.17	0.44
30:0:1617:C:C5	30:0:1643:C:H4'	2.53	0.44
5:E:73:PHE:O	5:E:76:VAL:HG22	2.18	0.44
30:0:1803:C:H2'	30:0:1804:A:C8	2.52	0.44
30:0:542:A:H1'	41:0:5534:HOH:O	2.16	0.44
3:C:77:ALA:O	3:C:78:ARG:CA	2.65	0.44
2:B:79:MET:HE3	2:B:144:THR:CG2	2.47	0.44
2:B:41:PHE:HB3	2:B:190:MET:CE	2.42	0.44
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
13:M:28:GLN:HA	13:M:31:TRP:HB2	1.98	0.44
15:O:65:LEU:HD13	30:0:746:A:N6	2.33	0.44
23:W:12:ASN:HA	30:0:1067:A:O2'	2.17	0.44
23:W:65:VAL:HA	23:W:68:THR:CG2	2.47	0.44
30:0:941:G:C5	30:0:942:U:C4	3.06	0.44
13:M:122:GLN:HB2	13:M:126:GLN:O	2.18	0.44
2:B:22:GLU:HA	2:B:205:VAL:HG21	1.98	0.44
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.82	0.44
11:K:65:ARG:C	11:K:67:GLN:H	2.19	0.44
30:0:166:A:H2'	30:0:2109:U:H5	1.83	0.44
30:0:2846:C:H4'	41:0:5931:HOH:O	2.16	0.44
30:0:1558:C:O2	30:0:1563:G:N2	2.45	0.44
12:L:98:GLU:O	12:L:99:GLU:HB2	2.16	0.44
12:L:36:ASP:HB2	41:0:5147:HOH:O	2.18	0.44
30:0:1238:C:H5'	30:0:1239:G:OP2	2.17	0.44
26:Z:34:SER:OG	30:0:797:A:H4'	2.18	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HA	30:0:1943:C:C4'	2.48	0.44
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.44
24:X:49:ARG:NH1	30:0:1385:G:O3'	2.51	0.44
18:R:88:PHE:O	18:R:91:LEU:HB3	2.17	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.63	0.44
29:3:24:LYS:HE3	29:3:90:PHE:HE1	1.83	0.44
30:0:255:A:C5	30:0:256:C:C4	3.05	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.44	0.44
20:T:92:ASP:OD2	30:0:335:U:H4'	2.18	0.44
9:I:91:PHE:HA	9:I:131:GLY:CA	2.47	0.44
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.32	0.44
2:B:84:LEU:HB2	2:B:182:VAL:HG21	2.00	0.44
30:0:1913:C:H2'	30:0:1914:C:C6	2.52	0.44
30:0:376:C:O5'	30:0:376:C:H6	2.00	0.44
19:S:20:PHE:CD2	19:S:20:PHE:N	2.85	0.44
17:Q:56:PHE:HE2	38:Q:8811:CL:CL	2.38	0.44
30:0:2285:G:H1	33:6:74:C:H42	1.65	0.44
10:J:41:ALA:HB2	10:J:103:VAL:CG1	2.47	0.44
6:F:31:LYS:HD2	41:0:5661:HOH:O	2.17	0.44
13:M:179:GLY:O	30:0:399:C:H5'	2.18	0.44
13:M:188:ARG:HD3	30:0:155:C:OP2	2.18	0.44
9:I:98:ASP:C	9:I:100:VAL:H	2.21	0.44
1:A:192:VAL:HG12	41:A:9070:HOH:O	2.18	0.44
30:0:1878:G:O2'	30:0:1879:U:H6	2.01	0.44
31:9:107:C:H2'	31:9:108:C:H6	1.82	0.44
23:W:4:LEU:CD2	23:W:52:VAL:HB	2.47	0.44
30:0:2889:U:H4'	30:0:2890:A:H5'	1.98	0.44
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.28	0.44
5:E:35:TYR:HB2	5:E:61:THR:HG21	2.00	0.44
30:0:2415:A:C2'	30:0:2416:G:H5'	2.47	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
15:O:96:VAL:HG13	15:O:100:GLN:CD	2.37	0.44
30:0:462:A:N6	30:0:477:A:H2	2.15	0.44
30:0:1457:U:H5	41:0:9660:HOH:O	2.00	0.44
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.44
30:0:362:G:O2'	30:0:363:C:H5'	2.18	0.44
30:0:1644:C:O2'	30:0:1645:U:H5'	2.18	0.44
15:O:87:THR:O	15:O:88:LYS:C	2.55	0.44
30:0:522:U:O2'	30:0:1366:C:H5'	2.17	0.44
14:N:35:VAL:HG11	31:9:6:C:H4'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HG21	1:A:100:PRO:HG3	1.99	0.44
4:D:104:PHE:CE2	4:D:166:ILE:HD13	2.53	0.44
20:T:48:VAL:HG22	20:T:97:ARG:C	2.37	0.44
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.18	0.44
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.51	0.44
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.44
23:W:122:ARG:NH2	41:W:5817:HOH:O	2.44	0.44
30:0:1174:A:C5	30:0:1201:C:H4'	2.52	0.44
9:I:124:VAL:O	9:I:124:VAL:HG12	2.18	0.44
8:H:54:VAL:HG12	8:H:56:GLU:O	2.17	0.44
29:3:10:TYR:CD1	30:0:2408:A:H1'	2.52	0.44
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.44
25:Y:102:LEU:O	25:Y:227:ARG:HG3	2.18	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.52	0.44
13:M:46:LEU:HD11	30:0:263:U:O3'	2.17	0.44
25:Y:212:ARG:HB3	41:Y:8835:HOH:O	2.18	0.44
30:0:970:U:H2'	41:0:7156:HOH:O	2.16	0.44
3:C:177:GLY:HA2	41:0:3551:HOH:O	2.17	0.44
30:0:1826:C:O2'	30:0:1827:G:H5'	2.17	0.44
1:A:157:GLY:HA2	26:Z:103:VAL:CG1	2.48	0.44
13:M:74:LYS:HG3	41:M:8878:HOH:O	2.18	0.44
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.44
9:I:71:ALA:O	9:I:75:LYS:HE3	2.17	0.44
30:0:844:A:C6	30:0:882:A:C6	3.06	0.44
9:I:97:VAL:CG1	9:I:101:LYS:HE3	2.28	0.44
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.44
4:D:45:THR:OG1	4:D:46:GLY:N	2.48	0.44
3:C:225:PRO:CD	3:C:231:ARG:HD2	2.48	0.44
1:A:190:ARG:NE	41:A:9070:HOH:O	2.51	0.44
7:G:64:ASN:ND2	7:G:64:ASN:N	2.65	0.44
30:0:236:A:H8	30:0:236:A:OP1	2.00	0.44
17:Q:16:ASN:HD21	17:Q:45:PRO:CD	2.29	0.44
2:B:141:ARG:CB	2:B:165:ARG:HA	2.47	0.44
30:0:2634:G:H5'	41:0:3070:HOH:O	2.16	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
30:0:834:G:H4'	30:0:835:U:OP2	2.18	0.44
4:D:99:ASP:CB	4:D:103:ASN:HB2	2.48	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.01	0.44
14:N:21:HIS:CD2	30:0:2369:A:H5''	2.53	0.44
5:E:90:HIS:CD2	30:0:2694:A:H5''	2.53	0.44
2:B:109:LEU:HA	2:B:159:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:HA	1:A:158:VAL:O	2.18	0.44
30:0:70:A:H4'	41:0:4782:HOH:O	2.17	0.44
30:0:349:U:H2'	30:0:350:G:O4'	2.17	0.44
8:H:77:ILE:O	8:H:78:LYS:C	2.55	0.44
2:B:251:VAL:HG22	41:0:5183:HOH:O	2.18	0.44
30:0:2344:G:N3	30:0:2344:G:H2'	2.32	0.44
30:0:1586:G:O2'	30:0:1587:U:H5'	2.17	0.44
30:0:1534:C:O2'	30:0:1656:A:OP1	2.24	0.44
19:S:21:GLN:NE2	30:0:1508:C:H5'	2.32	0.44
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.90	0.44
13:M:36:ALA:O	13:M:65:VAL:HG13	2.18	0.44
5:E:105:GLU:HG2	5:E:113:PRO:HB3	2.00	0.44
22:V:1:THR:C	22:V:3:LEU:H	2.20	0.44
14:N:79:PRO:HG3	14:N:143:ARG:C	2.38	0.44
31:9:56:A:C3'	31:9:57:A:H5''	2.48	0.44
13:M:9:ARG:NH2	30:0:378:A:OP1	2.42	0.44
30:0:1845:A:O2'	30:0:1846:U:H5'	2.17	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HB3	2.00	0.44
28:2:48:ASP:O	28:2:49:GLU:CB	2.65	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
22:V:5:VAL:CG1	22:V:9:ARG:NH1	2.80	0.44
13:M:163:LEU:O	13:M:168:ARG:NH1	2.51	0.44
2:B:132:HIS:CE1	2:B:171:VAL:CG2	3.01	0.44
2:B:17:LYS:O	2:B:260:HIS:CD2	2.71	0.44
1:A:171:LYS:NZ	41:A:8996:HOH:O	2.51	0.44
12:L:149:ARG:O	12:L:150:GLN:HB2	2.17	0.44
16:P:107:GLU:O	16:P:109:ARG:N	2.50	0.44
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.18	0.44
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.18	0.44
30:0:491:C:H2'	30:0:492:C:C6	2.53	0.44
30:0:2379:G:N3	30:0:2418:G:H2'	2.33	0.44
7:G:63:ARG:HG2	30:0:1210:G:OP1	2.18	0.43
14:N:79:PRO:HG3	14:N:144:GLY:CA	2.47	0.43
21:U:45:GLU:O	21:U:46:ALA:C	2.56	0.43
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.50	0.43
28:2:14:LEU:HD13	28:2:47:THR:CG2	2.48	0.43
5:E:119:HIS:HB2	5:E:144:THR:OG1	2.17	0.43
2:B:74:ILE:CD1	2:B:309:VAL:HG21	2.39	0.43
1:A:194:MET:CE	1:A:199:HIS:HB2	2.48	0.43
30:0:1267:C:O2'	30:0:1268:C:H5'	2.18	0.43
8:H:19:ARG:HG2	41:H:8976:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2907:C:H2'	30:0:2908:A:O4'	2.17	0.43
14:N:5:ARG:HB2	41:0:7582:HOH:O	2.18	0.43
30:0:1776:A:C8	30:0:1778:A:O4'	2.71	0.43
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.43
12:L:66:VAL:HG23	12:L:67:ARG:H	1.80	0.43
30:0:2106:C:H2'	30:0:2107:U:C6	2.53	0.43
3:C:51:TYR:HE1	27:1:55:GLY:O	2.00	0.43
4:D:103:ASN:OD1	4:D:133:ASN:ND2	2.51	0.43
30:0:23:G:H1'	30:0:520:A:H61	1.83	0.43
10:J:11:ILE:HD13	10:J:109:TYR:CD1	2.52	0.43
30:0:619:U:H2'	30:0:629:A:O4'	2.18	0.43
30:0:2031:C:H2'	30:0:2032:U:C6	2.53	0.43
3:C:181:ALA:HB2	30:0:30:U:OP2	2.18	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.17	0.43
30:0:1902:G:N2	30:0:1936:C:C2	2.86	0.43
12:L:18:HIS:HB2	30:0:903:U:O4	2.18	0.43
15:O:47:ARG:NH1	15:O:47:ARG:HG3	2.32	0.43
30:0:2059:U:H2'	30:0:2060:A:C8	2.53	0.43
30:0:2616:G:N3	30:0:2616:G:H2'	2.33	0.43
27:1:5:THR:N	27:1:6:PRO:HD2	2.32	0.43
30:0:1096:U:H5''	30:0:1258:G:O6	2.17	0.43
12:L:5:LYS:HE3	30:0:1354:G:O6	2.17	0.43
4:D:146:LYS:NZ	14:N:38:LYS:HE2	2.33	0.43
23:W:21:LEU:HD22	23:W:26:ILE:HD13	2.01	0.43
31:9:5:G:O2'	31:9:6:C:H5'	2.18	0.43
1:A:11:ARG:HH12	1:A:13:THR:CG2	2.31	0.43
11:K:96:VAL:CG2	11:K:109:LEU:HD22	2.48	0.43
30:0:2361:A:H8	30:0:2361:A:H5'	1.83	0.43
8:H:36:MET:HB3	8:H:73:ASN:HD21	1.83	0.43
30:0:2402:A:H1'	41:0:4055:HOH:O	2.17	0.43
3:C:7:ASP:OD1	3:C:11:ASN:O	2.36	0.43
30:0:2346:C:H6	30:0:2346:C:O5'	2.02	0.43
30:0:637:C:H2'	30:0:638:C:H6	1.83	0.43
30:0:697:G:H4'	30:0:730:G:O3'	2.19	0.43
1:A:128:LEU:HG	41:A:9054:HOH:O	2.18	0.43
30:0:2019:A:H5'	41:0:5405:HOH:O	2.17	0.43
6:F:119:ARG:HD3	6:F:119:ARG:OXT	2.18	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.17	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.18	0.43
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.53	0.43
30:0:702:G:O2'	30:0:703:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:GLN:NE2	31:9:5:G:N3	2.65	0.43
30:0:1667:A:H2'	30:0:1668:U:C6	2.52	0.43
12:L:35:ARG:NE	12:L:46:LEU:CD2	2.81	0.43
2:B:51:VAL:HG13	2:B:53:LEU:CD1	2.49	0.43
14:N:82:TYR:CD2	14:N:82:TYR:C	2.92	0.43
30:0:1878:G:O2'	30:0:1879:U:C6	2.65	0.43
30:0:603:A:H5''	30:0:604:G:OP1	2.18	0.43
12:L:56:LYS:CE	30:0:2443:C:H1'	2.48	0.43
14:N:155:GLU:O	14:N:156:GLU:CG	2.66	0.43
15:O:25:VAL:HG23	15:O:26:TRP:N	2.33	0.43
27:1:36:SER:O	27:1:46:ARG:HD3	2.17	0.43
30:0:2332:A:H3'	30:0:2333:G:C8	2.51	0.43
13:M:5:TYR:O	13:M:8:ILE:N	2.51	0.43
30:0:1914:C:H2'	30:0:1915:U:H6	1.82	0.43
30:0:923:A:H2'	41:0:6521:HOH:O	2.17	0.43
20:T:47:THR:HB	20:T:100:ASP:HB3	2.00	0.43
30:0:1768:C:H2'	30:0:1769:C:O4'	2.18	0.43
31:9:70:U:H2'	31:9:71:C:O4'	2.19	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	2.01	0.43
30:0:1119:G:N2	30:0:1246:A:N1	2.66	0.43
13:M:24:GLN:HE21	13:M:27:ARG:HD2	1.83	0.43
3:C:7:ASP:C	3:C:9:ASP:H	2.21	0.43
1:A:43:VAL:HG21	1:A:59:GLU:CG	2.48	0.43
29:3:42:ARG:HD2	41:3:9003:HOH:O	2.17	0.43
7:G:21:ASP:O	7:G:22:ALA:C	2.56	0.43
25:Y:150:LEU:HB3	41:Y:8857:HOH:O	2.17	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2120:U:H2'	30:0:2121:G:O4'	2.18	0.43
30:0:2345:A:N6	41:0:6637:HOH:O	2.49	0.43
18:R:65:GLY:HA3	41:R:9001:HOH:O	2.18	0.43
29:3:69:TYR:O	29:3:77:ALA:HA	2.17	0.43
30:0:657:G:H2'	30:0:658:C:C6	2.54	0.43
23:W:110:GLN:NE2	23:W:110:GLN:CA	2.81	0.43
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.18	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
18:R:114:VAL:HA	18:R:144:GLU:O	2.18	0.43
2:B:77:PRO:O	2:B:78:PRO:CA	2.67	0.43
10:J:131:THR:CG2	10:J:133:GLY:H	2.31	0.43
30:0:292:G:H8	30:0:292:G:O5'	2.01	0.43
2:B:27:ASN:ND2	2:B:27:ASN:C	2.71	0.43
30:0:2852:A:H4'	30:0:2853:U:H5	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:235:C:O2'	30:0:236:A:H2'	2.18	0.43
25:Y:100:ARG:HE	25:Y:234:VAL:HG21	1.84	0.43
23:W:38:THR:HG22	23:W:39:ASP:H	1.81	0.43
3:C:174:ILE:HD11	30:0:338:C:H4'	2.00	0.43
9:I:96:SER:H	9:I:99:GLN:CD	2.21	0.43
30:0:463:A:H3'	41:0:7246:HOH:O	2.19	0.43
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.48	0.43
12:L:30:ARG:HD3	30:0:164:G:H4'	2.00	0.43
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.81	0.43
31:9:95:C:O2'	31:9:96:C:H5'	2.19	0.43
30:0:1359:U:O5'	30:0:1360:C:H5''	2.17	0.43
31:9:39:U:H3'	31:9:40:C:H5''	2.00	0.43
2:B:277:GLU:N	2:B:278:PRO:CD	2.81	0.43
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.43
30:0:960:G:N3	30:0:960:G:H3'	2.33	0.43
30:0:1006:A:N1	30:0:2311:A:H1'	2.34	0.43
1:A:213:LYS:CE	30:0:1942:A:H5''	2.48	0.43
28:2:35:ARG:N	41:2:2691:HOH:O	2.50	0.43
9:I:98:ASP:HA	9:I:101:LYS:HD2	2.01	0.43
9:I:111:LEU:HD22	9:I:122:GLU:OE1	2.18	0.43
7:G:12:ILE:HG22	7:G:17:GLN:HE21	1.81	0.43
22:V:19:GLU:HG3	22:V:56:ILE:HD11	2.01	0.43
30:0:1171:A:N6	30:0:1172:G:C2	2.87	0.43
27:1:15:THR:O	27:1:28:HIS:HA	2.18	0.43
5:E:93:MET:CE	5:E:165:GLY:H	2.32	0.43
30:0:29:C:O2'	30:0:30:U:H5'	2.19	0.43
12:L:18:HIS:CD2	30:0:902:G:N7	2.87	0.43
30:0:1359:U:O4	30:0:2101:A:H5''	2.19	0.43
13:M:50:ARG:HH11	13:M:50:ARG:HG2	1.84	0.43
4:D:107:GLY:O	30:0:2338:G:O3'	2.37	0.43
12:L:72:ASN:O	12:L:76:LEU:HG	2.19	0.43
18:R:125:ARG:HG2	41:R:8948:HOH:O	2.18	0.43
21:U:38:ASN:O	21:U:42:LEU:HG	2.18	0.43
24:X:70:ILE:O	24:X:70:ILE:HG23	2.18	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
3:C:236:THR:HB	3:C:239:ALA:CB	2.48	0.43
24:X:85:VAL:HG12	24:X:86:GLU:N	2.34	0.43
30:0:1167:G:H1	30:0:1179:C:H42	1.67	0.43
15:O:106:PRO:HG2	15:O:107:GLU:OE2	2.18	0.43
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.18	0.43
12:L:144:ASP:O	12:L:147:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:854:G:H5''	30:0:855:U:OP1	2.18	0.43
30:0:1299:G:N2	41:0:5541:HOH:O	2.52	0.43
30:0:1766:U:H2'	30:0:1776:A:N6	2.34	0.43
33:6:75:C:H5''	33:6:76:8AN:O1P	2.18	0.43
2:B:87:TYR:CE2	2:B:96:PRO:HG3	2.54	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
5:E:93:MET:HE3	5:E:93:MET:HB2	1.81	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.17	0.43
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.82	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.84	0.43
3:C:240:LEU:O	3:C:240:LEU:HD23	2.18	0.43
6:F:99:THR:HA	41:F:3461:HOH:O	2.18	0.43
9:I:119:ALA:O	9:I:123:VAL:HG23	2.18	0.43
10:J:88:PRO:O	10:J:94:GLY:HA3	2.18	0.43
2:B:29:TRP:CH2	2:B:164:THR:HA	2.53	0.43
30:0:936:C:H42	30:0:1034:G:H1	1.66	0.43
30:0:1077:G:H2'	30:0:1080:C:N4	2.34	0.43
15:O:15:LYS:HD3	15:O:19:ARG:NH2	2.34	0.43
14:N:41:LYS:HD3	41:9:9061:HOH:O	2.18	0.43
30:0:581:G:O2'	30:0:582:U:H5'	2.18	0.43
26:Z:97:THR:O	26:Z:98:PRO:C	2.56	0.43
4:D:140:ARG:NH1	31:9:45:A:OP1	2.50	0.43
7:G:71:LEU:O	7:G:73:ASP:N	2.52	0.43
5:E:2:ARG:HH21	5:E:48:VAL:HG21	1.82	0.43
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.43
2:B:51:VAL:HG22	2:B:327:VAL:HG13	2.00	0.43
20:T:101:LEU:HD13	20:T:112:LEU:HD11	2.01	0.43
10:J:74:ARG:CG	10:J:74:ARG:HH11	2.31	0.43
31:9:73:A:N6	31:9:108:C:H42	2.15	0.43
22:V:45:ARG:C	22:V:47:LYS:N	2.72	0.43
20:T:21:LYS:HA	20:T:24:ARG:CD	2.49	0.43
30:0:790:A:H1'	30:0:1710:A:C2'	2.49	0.43
6:F:1:PRO:HB2	41:M:8924:HOH:O	2.17	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.19	0.43
14:N:72:GLU:HG2	14:N:163:PHE:HD1	1.84	0.43
27:1:48:TYR:CZ	30:0:773:A:H4'	2.54	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.18	0.43
30:0:2752:C:O2'	30:0:2753:G:H5'	2.19	0.43
2:B:103:ASP:HB2	41:B:9064:HOH:O	2.17	0.43
30:0:234:A:H4'	30:0:437:A:O4'	2.19	0.43
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2005:G:N2	30:0:2008:U:H1'	2.34	0.43
30:0:1473:U:O2'	30:0:1474:C:H5''	2.18	0.43
9:I:112:LEU:HG	41:I:6070:HOH:O	2.19	0.43
14:N:11:ARG:HG2	14:N:15:GLU:OE2	2.18	0.43
30:0:2073:G:N1	30:0:2607:U:C6	2.86	0.43
2:B:87:TYR:O	2:B:138:GLY:N	2.42	0.43
30:0:710:G:N2	30:0:719:C:C2	2.87	0.43
25:Y:184:GLU:HG2	25:Y:229:LEU:HD11	2.01	0.43
6:F:22:VAL:HG23	6:F:104:ALA:HB2	2.00	0.43
2:B:145:HIS:CD2	2:B:146:THR:O	2.72	0.43
30:0:1503:U:H2'	30:0:1504:A:O4'	2.18	0.43
30:0:812:A:H2'	30:0:813:C:H6	1.83	0.43
10:J:123:ARG:NH1	10:J:129:PHE:HZ	2.16	0.43
22:V:27:LEU:CA	22:V:49:LEU:HD13	2.48	0.43
30:0:1476:A:O2'	30:0:1477:C:H5'	2.18	0.43
27:1:53:LYS:O	27:1:54:ALA:C	2.57	0.43
30:0:1616:A:H5''	30:0:1617:C:OP1	2.18	0.43
4:D:48:MET:HE2	4:D:48:MET:HB3	1.89	0.43
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.19	0.43
24:X:85:VAL:HG12	24:X:86:GLU:H	1.83	0.43
18:R:46:TYR:CD2	18:R:47:LEU:HD23	2.50	0.43
20:T:48:VAL:HG22	20:T:96:VAL:HG13	2.00	0.43
4:D:156:ARG:HH11	4:D:156:ARG:HG3	1.84	0.43
10:J:130:VAL:CG1	10:J:131:THR:N	2.82	0.43
14:N:24:LEU:CD1	17:Q:26:PRO:HB3	2.49	0.43
30:0:1217:G:O2'	30:0:1218:U:H5'	2.19	0.43
16:P:20:ARG:HD2	30:0:1718:G:OP2	2.19	0.43
30:0:462:A:H2'	41:0:5741:HOH:O	2.19	0.43
1:A:171:LYS:HG3	1:A:174:ASN:ND2	2.33	0.43
1:A:231:LYS:O	1:A:232:ARG:HB3	2.19	0.43
30:0:228:C:C2'	30:0:229:G:H5'	2.49	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.43
25:Y:216:ARG:O	25:Y:219:GLU:HG2	2.19	0.43
16:P:50:GLN:HG2	41:P:6904:HOH:O	2.19	0.43
14:N:37:ARG:HA	14:N:37:ARG:HD3	1.90	0.42
30:0:542:A:H2'	30:0:543:G:O4'	2.19	0.42
12:L:145:LEU:O	12:L:145:LEU:HD23	2.19	0.42
30:0:1972:U:H2'	30:0:1973:A:H5'	2.01	0.42
31:9:107:C:H2'	31:9:108:C:C6	2.54	0.42
33:6:75:C:H2'	41:6:80:HOH:O	2.19	0.42
3:C:149:LYS:NZ	30:0:328:U:OP1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1819:G:H2'	30:0:1820:G:C4'	2.49	0.42
30:0:431:G:O2'	30:0:432:G:H5'	2.19	0.42
8:H:87:LYS:CB	8:H:87:LYS:NZ	2.82	0.42
15:O:49:GLU:O	15:O:72:LYS:HE3	2.19	0.42
30:0:1724:U:H5''	41:0:4609:HOH:O	2.19	0.42
30:0:2029:C:H2'	30:0:2030:A:O4'	2.19	0.42
30:0:1245:C:H6	30:0:1245:C:O5'	2.01	0.42
30:0:1767:A:H3'	41:0:5918:HOH:O	2.19	0.42
8:H:83:GLU:O	8:H:84:GLY:C	2.58	0.42
30:0:2241:C:O2'	30:0:2242:U:H5'	2.19	0.42
30:0:1925:G:O2'	30:0:1926:G:H5'	2.19	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.19	0.42
10:J:20:GLY:HA3	30:0:1242:A:O3'	2.20	0.42
1:A:95:PRO:C	1:A:97:ALA:H	2.23	0.42
11:K:8:VAL:CG1	11:K:9:THR:N	2.81	0.42
2:B:280:VAL:HG11	2:B:335:ASN:OD1	2.19	0.42
10:J:93:ARG:HH11	10:J:93:ARG:CB	2.27	0.42
12:L:144:ASP:HA	12:L:147:GLU:HG3	2.01	0.42
17:Q:43:ILE:O	17:Q:45:PRO:HD3	2.20	0.42
16:P:104:LYS:HA	16:P:104:LYS:HD2	1.91	0.42
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.42
23:W:125:HIS:CD2	23:W:125:HIS:H	2.37	0.42
30:0:1632:A:C2'	30:0:1633:C:H5'	2.48	0.42
30:0:1503:U:H2'	30:0:1504:A:C5'	2.48	0.42
30:0:639:A:H2'	30:0:640:G:C8	2.54	0.42
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	2.00	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.51	0.42
23:W:66:LEU:HD23	23:W:66:LEU:HA	1.87	0.42
15:O:105:ASN:HD21	15:O:109:SER:H	1.66	0.42
30:0:67:A:H2'	41:0:5002:HOH:O	2.19	0.42
23:W:47:LYS:HE2	30:0:944:G:O3'	2.19	0.42
12:L:16:GLY:HA2	30:0:1294:A:O3'	2.19	0.42
29:3:63:LYS:NZ	30:0:2460:A:OP1	2.51	0.42
3:C:142:ASP:CG	3:C:238:SER:HG	2.23	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.53	0.42
7:G:12:ILE:HG22	7:G:12:ILE:O	2.17	0.42
31:9:14:G:C6	31:9:68:G:C2	3.07	0.42
14:N:14:ARG:NH2	31:9:13:A:N3	2.66	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.81	0.42
13:M:57:LYS:HZ2	13:M:144:ASP:CG	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:52:VAL:HG22	23:W:52:VAL:H	1.45	0.42
8:H:61:ARG:O	8:H:64:SER:N	2.43	0.42
3:C:246:ARG:NH2	30:0:677:C:H4'	2.34	0.42
27:1:8:GLN:HE22	27:1:11:LYS:HZ1	1.66	0.42
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.54	0.42
14:N:179:LEU:HD23	14:N:184:ILE:HD12	2.01	0.42
7:G:19:GLU:O	7:G:20:VAL:C	2.57	0.42
27:1:45:ARG:NH2	41:1:2086:HOH:O	2.50	0.42
13:M:163:LEU:HD21	30:0:188:C:H5''	2.00	0.42
13:M:95:LYS:HE2	30:0:157:G:H4'	2.01	0.42
30:0:1971:G:N2	30:0:2009:G:H2'	2.34	0.42
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.42
10:J:45:VAL:CG2	10:J:129:PHE:CD1	3.02	0.42
30:0:432:G:O2'	30:0:433:C:H5'	2.19	0.42
4:D:10:PHE:CD1	4:D:11:HIS:N	2.87	0.42
6:F:24:ARG:HG3	6:F:25:ASP:N	2.34	0.42
30:0:1362:U:O2'	30:0:1363:G:H5'	2.19	0.42
4:D:143:LYS:O	31:9:45:A:H4'	2.19	0.42
2:B:48:MET:O	2:B:49:THR:HG23	2.19	0.42
8:H:157:TYR:CD1	8:H:157:TYR:C	2.92	0.42
5:E:16:ASP:O	5:E:17:HIS:HB2	2.19	0.42
30:0:1566:C:H2'	30:0:1567:G:C8	2.54	0.42
30:0:2647:C:H1'	41:0:7245:HOH:O	2.19	0.42
30:0:2464:C:H5''	30:0:2465:A:OP1	2.20	0.42
12:L:101:ASP:C	12:L:103:ALA:H	2.23	0.42
6:F:109:GLU:O	6:F:113:ASP:OD2	2.37	0.42
3:C:27:ARG:HG2	3:C:29:ASP:OD1	2.19	0.42
9:I:130:LEU:HA	41:I:7210:HOH:O	2.19	0.42
2:B:162:MET:CE	2:B:310:ARG:HH11	2.31	0.42
30:0:611:U:H2'	30:0:612:U:C6	2.54	0.42
14:N:119:GLN:HG2	14:N:123:ILE:HD11	2.01	0.42
2:B:243:ASN:ND2	30:0:2607:U:OP2	2.45	0.42
1:A:135:VAL:HG21	1:A:147:ARG:NH1	2.35	0.42
10:J:77:GLY:O	10:J:78:ILE:CA	2.68	0.42
21:U:56:ARG:HD2	21:U:56:ARG:O	2.20	0.42
30:0:1058:A:H2'	30:0:1060:C:H5'	2.00	0.42
11:K:4:LEU:HD23	11:K:4:LEU:HA	1.86	0.42
30:0:564:G:H2'	30:0:592:G:C6	2.54	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
9:I:114:TYR:CD1	9:I:114:TYR:N	2.87	0.42
13:M:71:SER:CB	13:M:92:THR:HG22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HD3	41:A:9015:HOH:O	2.19	0.42
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.92	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.38	0.42
30:0:640:G:C6	30:0:641:G:N7	2.87	0.42
3:C:40:ALA:O	3:C:43:LYS:HB2	2.19	0.42
11:K:28:GLU:OE2	11:K:58:THR:HG21	2.19	0.42
15:O:18:ALA:HB2	15:O:27:GLY:N	2.34	0.42
9:I:67:VAL:HG13	9:I:68:PRO:HD2	2.00	0.42
17:Q:34:ASP:HB2	17:Q:37:GLU:HG3	2.00	0.42
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.42
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.52	0.42
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.31	0.42
18:R:119:VAL:CG1	18:R:119:VAL:O	2.67	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:559:U:H2'	30:0:560:U:O4'	2.20	0.42
30:0:1299:G:H2'	30:0:1300:G:O4'	2.20	0.42
3:C:174:ILE:HD12	30:0:338:C:H4'	1.99	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
12:L:27:ARG:HH22	12:L:30:ARG:HG2	1.81	0.42
13:M:84:LYS:HZ1	30:0:391:U:P	2.42	0.42
21:U:20:MET:CG	21:U:28:THR:HG23	2.50	0.42
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.19	0.42
8:H:77:ILE:O	8:H:78:LYS:CA	2.68	0.42
30:0:1821:A:O2'	30:0:1822:A:H5'	2.20	0.42
28:2:18:ASN:ND2	28:2:18:ASN:O	2.52	0.42
30:0:2604:A:H4'	41:0:9401:HOH:O	2.20	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
23:W:82:GLU:O	23:W:86:GLU:HG3	2.19	0.42
30:0:2470:A:H5''	41:0:4137:HOH:O	2.19	0.42
41:Y:8878:HOH:O	30:0:1355:A:H5''	2.19	0.42
11:K:74:VAL:HG21	11:K:96:VAL:HG23	2.01	0.42
14:N:40:ASN:HB2	41:9:9062:HOH:O	2.20	0.42
17:Q:27:GLN:HB2	41:9:9006:HOH:O	2.19	0.42
31:9:24:U:H3'	31:9:25:G:H5'	2.01	0.42
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.55	0.42
28:2:43:ARG:HH21	30:0:1685:A:C4'	2.32	0.42
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.42
25:Y:231:PRO:HG2	25:Y:233:TYR:CE1	2.55	0.42
30:0:370:G:O2'	30:0:371:U:H5'	2.19	0.42
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.35	0.42
30:0:2039:A:H4'	30:0:2760:C:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:193:LYS:HB3	30:0:392:U:H5''	2.01	0.42
30:0:2791:U:C4	30:0:2794:G:O6	2.73	0.42
8:H:53:ILE:HG23	8:H:133:GLY:O	2.20	0.42
3:C:68:ALA:O	3:C:70:VAL:N	2.52	0.42
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.39	0.42
13:M:78:LYS:HE2	30:0:870:G:OP1	2.19	0.42
13:M:61:ILE:N	13:M:61:ILE:CD1	2.81	0.42
2:B:52:VAL:O	2:B:53:LEU:HD12	2.19	0.42
30:0:2355:G:H5''	30:0:2356:A:OP2	2.20	0.42
25:Y:100:ARG:HE	25:Y:234:VAL:CG2	2.32	0.42
23:W:13:MET:HA	41:W:4944:HOH:O	2.20	0.42
22:V:45:ARG:HA	22:V:48:GLU:HB2	2.01	0.42
30:0:2819:C:H2'	30:0:2820:A:H8	1.84	0.42
14:N:103:ASP:OD1	14:N:103:ASP:C	2.57	0.42
2:B:238:ASN:HD21	30:0:2609:G:N2	2.17	0.42
30:0:1684:A:H5'	30:0:1692:C:OP1	2.19	0.42
5:E:88:TYR:CD1	5:E:91:PHE:O	2.71	0.42
30:0:353:G:O2'	30:0:354:A:H5'	2.19	0.42
30:0:1548:U:O2'	30:0:1798:C:O2	2.32	0.42
2:B:205:VAL:O	2:B:307:ARG:NE	2.53	0.42
20:T:30:ASP:O	20:T:33:GLU:N	2.53	0.42
2:B:7:ARG:CZ	2:B:11:LEU:HD13	2.49	0.42
16:P:109:ARG:NH1	16:P:119:TYR:CE2	2.88	0.42
3:C:21:VAL:HG22	41:C:8598:HOH:O	2.20	0.42
30:0:2673:U:C4	30:0:2674:G:C6	3.07	0.42
1:A:163:GLY:CA	1:A:166:ASP:OD2	2.68	0.42
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.42
15:O:89:ILE:HG21	15:O:95:ALA:HB2	2.01	0.42
16:P:81:LYS:HG2	41:O:3439:HOH:O	2.19	0.42
22:V:1:THR:CB	30:0:93:C:H5''	2.46	0.42
16:P:115:SER:O	16:P:117:SER:N	2.52	0.42
14:N:175:LEU:HA	14:N:175:LEU:HD12	1.86	0.42
4:D:94:ALA:HA	4:D:174:VAL:C	2.40	0.42
30:0:2506:A:H2'	30:0:2506:A:O5'	2.20	0.42
9:I:87:PRO:HB3	9:I:129:SER:O	2.19	0.42
13:M:171:ARG:HD3	30:0:156:C:C5'	2.43	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH2	2.34	0.42
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42
18:R:82:GLU:CG	18:R:83:LYS:H	2.29	0.42
31:9:72:C:H2'	31:9:73:A:H8	1.85	0.42
24:X:30:MET:HG2	30:0:1384:C:H5'	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1504:A:O2'	30:0:1506:U:OP2	2.38	0.42
29:3:42:ARG:NH1	30:0:396:U:H5'	2.35	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.50	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
29:3:1:MET:N	29:3:87:ARG:O	2.49	0.42
2:B:54:VAL:O	2:B:55:ASN:C	2.56	0.42
30:0:312:U:O5'	30:0:312:U:H6	2.02	0.42
22:V:59:ILE:HA	22:V:62:GLU:HB2	2.02	0.42
26:Z:96:GLU:OE1	26:Z:104:ARG:NH2	2.53	0.42
4:D:55:LYS:O	4:D:56:ARG:HB2	2.20	0.42
11:K:69:LEU:HD12	11:K:97:ILE:HD13	2.02	0.42
30:0:2510:C:H5'	30:0:2511:A:OP2	2.20	0.42
24:X:49:ARG:O	24:X:49:ARG:CG	2.58	0.42
30:0:1603:A:H5'	30:0:1605:G:C4'	2.49	0.42
29:3:71:CYS:O	29:3:75:GLY:HA2	2.20	0.42
1:A:34:ASP:O	1:A:36:ASP:N	2.53	0.42
14:N:165:ALA:C	14:N:167:ASP:H	2.22	0.42
10:J:75:PRO:HD3	10:J:136:SER:CB	2.50	0.42
30:0:1044:C:H5	41:0:7418:HOH:O	2.03	0.42
2:B:244:PRO:HB3	30:0:1234:U:C2	2.55	0.42
8:H:59:GLN:HE21	8:H:129:ARG:CG	2.32	0.42
18:R:82:GLU:HB2	18:R:86:LYS:HE3	2.02	0.42
30:0:1972:U:C2'	30:0:1973:A:H5''	2.50	0.42
30:0:1165:G:N2	30:0:1173:A:H5''	2.35	0.42
20:T:24:ARG:NH1	20:T:24:ARG:HG2	2.35	0.42
30:0:2106:C:H1'	30:0:2484:U:C2	2.55	0.42
11:K:66:ARG:NH2	30:0:1994:A:OP2	2.42	0.42
2:B:56:ASP:HB3	2:B:322:ARG:NH2	2.35	0.42
3:C:150:THR:OG1	30:0:327:A:H2'	2.19	0.42
12:L:18:HIS:HD2	30:0:902:G:N7	2.18	0.42
3:C:63:SER:OG	30:0:2101:A:H2'	2.20	0.42
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.54	0.42
29:3:51:LYS:C	29:3:53:SER:H	2.23	0.42
6:F:118:LEU:O	6:F:119:ARG:OXT	2.38	0.42
16:P:107:GLU:C	16:P:109:ARG:N	2.73	0.42
30:0:644:G:N3	30:0:644:G:H5'	2.34	0.42
26:Z:34:SER:HB3	41:Z:8723:HOH:O	2.18	0.42
14:N:111:PRO:HD2	31:9:37:C:H4'	2.02	0.42
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.42
30:0:912:A:H4'	41:0:6799:HOH:O	2.19	0.42
30:0:461:C:H2'	41:0:4868:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:47:ARG:HG3	41:U:4381:HOH:O	2.20	0.42
30:0:1664:A:OP1	30:0:1664:A:H8	2.03	0.42
30:0:75:U:H2'	30:0:76:G:C8	2.55	0.42
25:Y:178:HIS:CG	25:Y:179:PRO:HD2	2.55	0.42
30:0:1141:U:O2'	30:0:1142:C:H5'	2.19	0.42
14:N:44:ARG:NH2	31:9:4:G:O2'	2.52	0.42
6:F:39:SER:O	6:F:43:GLY:N	2.53	0.42
19:S:29:ASP:OD1	19:S:31:ARG:HG3	2.20	0.42
10:J:47:THR:HB	30:0:1244:U:C6	2.55	0.42
14:N:79:PRO:HA	14:N:142:THR:O	2.20	0.42
5:E:69:ILE:O	5:E:72:MET:HB2	2.19	0.42
20:T:51:LEU:O	20:T:52:ARG:HG2	2.20	0.42
4:D:138:GLY:HA2	31:9:29:C:O3'	2.20	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
23:W:4:LEU:O	23:W:32:CYS:HA	2.19	0.42
30:0:2519:C:O2'	30:0:2520:G:H5'	2.20	0.42
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.01	0.42
11:K:66:ARG:HH22	30:0:1994:A:P	2.40	0.42
9:I:117:THR:O	9:I:120:ALA:HB3	2.19	0.42
12:L:133:VAL:HA	41:L:9038:HOH:O	2.20	0.42
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.85	0.42
13:M:122:GLN:HB3	13:M:127:LYS:HG2	2.02	0.42
9:I:88:GLN:HE21	9:I:128:THR:CG2	2.33	0.42
30:0:696:C:O2'	30:0:697:G:H5'	2.20	0.42
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.01	0.42
30:0:432:G:H2'	30:0:433:C:C6	2.55	0.42
3:C:94:THR:C	3:C:96:LYS:H	2.22	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
26:Z:37:ARG:HD2	30:0:818:A:O2'	2.20	0.42
2:B:66:GLU:HG2	41:B:9125:HOH:O	2.20	0.42
8:H:157:TYR:C	8:H:157:TYR:HD1	2.24	0.42
30:0:2462:G:O4'	30:0:2464:C:C2	2.73	0.42
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.42
2:B:334:SER:HG	30:0:2861:G:HO2'	1.62	0.42
30:0:2467:A:H5'	41:0:5160:HOH:O	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
3:C:236:THR:N	3:C:239:ALA:HB3	2.28	0.41
9:I:94:ASP:O	9:I:95:LEU:HD23	2.20	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.20	0.41
15:O:21:SER:CB	15:O:106:PRO:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:271:C:N4	30:0:378:A:H2	2.06	0.41
13:M:9:ARG:HG3	41:0:4079:HOH:O	2.20	0.41
2:B:190:MET:CE	2:B:194:PHE:CD1	3.02	0.41
10:J:42:GLU:O	10:J:131:THR:HG23	2.20	0.41
30:0:289:G:O2'	30:0:290:C:H5'	2.19	0.41
2:B:175:LEU:C	2:B:175:LEU:CD2	2.88	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.20	0.41
13:M:31:TRP:CA	13:M:34:GLU:HG3	2.48	0.41
2:B:217:ARG:HB2	2:B:257:THR:HG21	2.01	0.41
14:N:182:GLY:O	14:N:183:ASP:C	2.59	0.41
18:R:29:LYS:HD3	41:0:5581:HOH:O	2.20	0.41
30:0:2896:A:C2'	30:0:2896:A:N3	2.83	0.41
1:A:56:ALA:O	1:A:68:ILE:N	2.53	0.41
2:B:274:GLU:HG3	2:B:292:GLY:HA2	2.02	0.41
3:C:81:PRO:HD3	41:C:8554:HOH:O	2.20	0.41
30:0:1153:C:N3	30:0:2786:G:O6	2.52	0.41
20:T:68:ASP:HB2	41:T:4787:HOH:O	2.20	0.41
30:0:25:A:C2'	30:0:26:U:H5'	2.50	0.41
25:Y:112:GLU:HA	25:Y:112:GLU:OE1	2.20	0.41
30:0:163:U:O3'	30:0:896:C:H4'	2.20	0.41
18:R:61:GLN:HG2	18:R:62:HIS:CD2	2.55	0.41
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.84	0.41
18:R:122:GLN:HB3	18:R:138:SER:HB2	2.01	0.41
30:0:1844:C:H6	30:0:1844:C:O5'	2.03	0.41
14:N:127:LEU:HB2	41:N:8856:HOH:O	2.19	0.41
30:0:310:U:H2'	30:0:311:C:C6	2.54	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.53	0.41
8:H:160:ILE:HD11	8:H:164:CYS:SG	2.60	0.41
16:P:133:SER:HA	41:P:1882:HOH:O	2.20	0.41
23:W:92:ASP:OD2	23:W:94:SER:HB2	2.19	0.41
31:9:77:A:N1	31:9:103:A:H5''	2.35	0.41
13:M:102:GLU:CD	13:M:164:THR:HG21	2.41	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41
14:N:116:PHE:O	14:N:119:GLN:HB3	2.20	0.41
17:Q:30:VAL:O	17:Q:31:GLU:C	2.59	0.41
30:0:2072:G:O2'	30:0:2489:G:N2	2.52	0.41
23:W:10:GLU:HG2	41:0:3876:HOH:O	2.19	0.41
3:C:7:ASP:C	3:C:9:ASP:N	2.74	0.41
4:D:101:THR:HG22	4:D:101:THR:O	2.21	0.41
13:M:157:ASP:O	13:M:158:ARG:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:99:ARG:NE	13:M:167:GLY:HA2	2.35	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.02	0.41
13:M:82:ARG:O	13:M:83:SER:C	2.59	0.41
30:0:2281:C:O2'	30:0:2282:U:H5'	2.20	0.41
30:0:432:G:H3'	41:0:8000:HOH:O	2.18	0.41
30:0:1131:G:H5'	31:9:91:C:O4'	2.21	0.41
8:H:153:PHE:HD1	8:H:166:ILE:HG23	1.84	0.41
9:I:67:VAL:CG1	9:I:68:PRO:HD2	2.50	0.41
17:Q:68:GLY:HA3	30:0:2404:G:C5'	2.50	0.41
10:J:52:GLN:HE21	30:0:1119:G:H5'	1.84	0.41
14:N:77:ASN:O	14:N:78:MET:CA	2.68	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD12	1.94	0.41
30:0:506:G:N2	30:0:509:A:H5'	2.16	0.41
4:D:23:VAL:HG22	4:D:73:VAL:HB	2.02	0.41
2:B:335:ASN:HA	41:0:4561:HOH:O	2.20	0.41
1:A:38:ILE:HD11	1:A:62:ASP:OD1	2.21	0.41
1:A:208:HIS:O	1:A:208:HIS:CG	2.74	0.41
31:9:3:A:N6	31:9:22:G:H1'	2.35	0.41
1:A:35:GLY:C	1:A:37:VAL:H	2.23	0.41
30:0:2649:A:C8	30:0:2649:A:H5'	2.55	0.41
3:C:93:LYS:HD2	30:0:646:G:O4'	2.20	0.41
30:0:1741:U:O2'	30:0:2723:G:H4'	2.20	0.41
30:0:1741:U:H5'	30:0:1742:A:OP1	2.20	0.41
30:0:2398:A:O2'	30:0:2428:G:H4'	2.20	0.41
3:C:22:PHE:HA	3:C:116:ALA:HA	2.01	0.41
30:0:11:A:N3	30:0:11:A:H2'	2.36	0.41
30:0:921:G:H4'	30:0:924:G:C6	2.55	0.41
4:D:42:GLY:N	41:D:5828:HOH:O	2.53	0.41
30:0:497:A:H2'	30:0:498:A:C5'	2.51	0.41
14:N:91:ARG:HD3	41:N:8811:HOH:O	2.20	0.41
30:0:600:G:N2	30:0:601:G:H1'	2.35	0.41
11:K:79:PRO:HG3	11:K:89:LYS:HB3	2.01	0.41
16:P:115:SER:C	16:P:117:SER:N	2.73	0.41
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.01	0.41
30:0:558:C:C2'	30:0:559:U:C5'	2.89	0.41
3:C:246:ARG:CB	3:C:246:ARG:HH11	2.32	0.41
19:S:32:ALA:HA	19:S:36:GLU:OE1	2.20	0.41
11:K:125:ALA:C	11:K:127:ALA:N	2.69	0.41
30:0:2265:U:H2'	30:0:2266:A:C8	2.56	0.41
10:J:126:ASN:HA	38:J:8801:CL:CL	2.57	0.41
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1526:A:H4'	30:0:1527:A:C5'	2.50	0.41
30:0:1416:G:H2'	30:0:1417:G:C5'	2.50	0.41
2:B:266:ASN:OD1	2:B:317:PRO:HA	2.20	0.41
30:0:553:G:C2'	30:0:554:G:H5'	2.50	0.41
30:0:2783:A:H2'	30:0:2784:A:C8	2.55	0.41
10:J:45:VAL:HG22	10:J:46:ILE:N	2.35	0.41
30:0:1588:G:C6	30:0:1589:G:C6	3.08	0.41
10:J:64:GLY:HA3	38:J:8821:CL:CL	2.57	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.55	0.41
12:L:41:HIS:CD2	30:0:926:A:O2'	2.73	0.41
30:0:2095:A:OP1	30:0:2096:A:H4'	2.20	0.41
16:P:135:ALA:HB2	41:P:4754:HOH:O	2.20	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.51	0.41
13:M:139:PRO:C	13:M:141:ILE:N	2.71	0.41
20:T:51:LEU:O	20:T:52:ARG:NH1	2.52	0.41
30:0:111:C:H2'	30:0:112:G:H5'	2.03	0.41
30:0:1212:C:H2'	30:0:1213:C:H5'	2.02	0.41
30:0:282:C:H2'	30:0:283:U:O4'	2.20	0.41
17:Q:11:ARG:HD3	41:Q:5620:HOH:O	2.20	0.41
14:N:5:ARG:HD3	41:0:7778:HOH:O	2.20	0.41
17:Q:94:GLN:HG2	17:Q:95:GLU:OE1	2.21	0.41
2:B:141:ARG:HG2	2:B:165:ARG:CA	2.49	0.41
30:0:2669:U:H2'	30:0:2670:G:C8	2.55	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.41
30:0:407:A:H5'	41:0:6858:HOH:O	2.20	0.41
3:C:98:ARG:NH1	41:C:8560:HOH:O	2.53	0.41
17:Q:47:VAL:HB	17:Q:90:HIS:CE1	2.55	0.41
30:0:2847:G:O2'	30:0:2848:G:H5'	2.20	0.41
2:B:195:ARG:HD2	2:B:324:ASP:OD1	2.20	0.41
23:W:9:GLY:H	30:0:1086:A:P	2.42	0.41
30:0:154:C:H2'	30:0:155:C:C6	2.55	0.41
30:0:390:G:H5'	41:0:3451:HOH:O	2.20	0.41
10:J:143:LYS:HG3	10:J:145:TRP:CE2	2.56	0.41
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.41
2:B:321:PRO:HG3	41:B:9072:HOH:O	2.19	0.41
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.51	0.41
27:1:26:SER:CB	27:1:36:SER:HB2	2.51	0.41
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.20	0.41
11:K:64:MET:HA	11:K:67:GLN:NE2	2.36	0.41
30:0:1033:C:H2'	30:0:1034:G:C5'	2.51	0.41
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:98:GLU:O	12:L:99:GLU:CB	2.67	0.41
30:0:581:G:H2'	30:0:582:U:H6	1.85	0.41
30:0:75:U:H2'	30:0:76:G:H8	1.86	0.41
30:0:2133:U:H4'	30:0:2134:G:C5'	2.51	0.41
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.41
30:0:2022:A:H5''	30:0:2023:G:OP2	2.21	0.41
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
4:D:29:HIS:HB2	41:D:2768:HOH:O	2.20	0.41
30:0:1513:C:H2'	30:0:1514:C:H6	1.85	0.41
30:0:1205:U:H2'	30:0:1206:U:H5'	2.00	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
11:K:113:ILE:HG22	11:K:114:ALA:H	1.86	0.41
5:E:2:ARG:NH2	5:E:48:VAL:HG21	2.36	0.41
30:0:111:C:H2'	30:0:112:G:C5'	2.50	0.41
18:R:132:ARG:HD3	41:0:3121:HOH:O	2.20	0.41
18:R:119:VAL:HG21	18:R:142:ASP:OD1	2.20	0.41
30:0:293:A:P	30:0:358:G:H22	2.44	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.19	0.41
8:H:48:VAL:O	8:H:140:TYR:HA	2.21	0.41
1:A:228:ILE:O	1:A:229:ALA:C	2.58	0.41
3:C:51:TYR:CD1	27:1:56:GLU:HB2	2.56	0.41
30:0:400:C:H2'	30:0:401:C:H6	1.86	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
30:0:1684:A:O2'	30:0:1685:A:H5''	2.20	0.41
20:T:94:SER:OG	30:0:334:G:N2	2.54	0.41
30:0:1839:A:C5'	30:0:2643:G:H4'	2.51	0.41
30:0:2332:A:H5'	30:0:2333:G:OP2	2.21	0.41
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.69	0.41
8:H:143:VAL:CG2	8:H:173:GLU:HG2	2.51	0.41
17:Q:47:VAL:O	17:Q:51:ARG:NE	2.48	0.41
14:N:69:TYR:CD1	14:N:69:TYR:N	2.89	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.55	0.41
19:S:80:ARG:HA	41:S:8538:HOH:O	2.21	0.41
30:0:1065:G:H2'	30:0:1066:U:C6	2.56	0.41
24:X:41:PHE:CZ	24:X:74:ALA:HB3	2.56	0.41
5:E:40:VAL:HA	5:E:48:VAL:O	2.21	0.41
21:U:52:THR:HB	21:U:55:ALA:H	1.85	0.41
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.41
29:3:20:HIS:CD2	29:3:71:CYS:HA	2.56	0.41
27:1:20:ARG:HH21	30:0:120:A:H5'	1.85	0.41
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:131:THR:HG22	10:J:134:GLU:N	2.28	0.41
27:1:25:LYS:CG	27:1:25:LYS:O	2.67	0.41
30:0:1170:U:O2'	30:0:1172:G:N7	2.49	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.04	0.41
24:X:23:HIS:C	24:X:24:LYS:HG3	2.41	0.41
30:0:727:G:H5'	30:0:728:C:OP2	2.21	0.41
30:0:2867:G:H2'	30:0:2868:C:C6	2.56	0.41
12:L:27:ARG:NE	41:L:8980:HOH:O	2.39	0.41
30:0:1736:A:H1'	41:0:9381:HOH:O	2.21	0.41
30:0:537:G:H4'	30:0:538:C:O5'	2.21	0.41
30:0:705:C:H3'	30:0:706:G:C8	2.55	0.41
3:C:123:LEU:HD11	41:C:8660:HOH:O	2.20	0.41
30:0:240:C:H1'	30:0:431:G:N2	2.35	0.41
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.35	0.41
29:3:47:GLY:HA2	30:0:2121:G:H4'	2.01	0.41
30:0:52:A:C2	30:0:110:C:C2	3.08	0.41
30:0:215:A:N1	30:0:393:G:H1'	2.36	0.41
4:D:128:LEU:HB2	41:D:6007:HOH:O	2.19	0.41
30:0:1522:A:H2'	30:0:1523:G:H5'	2.03	0.41
10:J:91:LYS:O	10:J:92:GLN:C	2.58	0.41
30:0:1118:A:H3'	30:0:1119:G:H5''	2.03	0.41
1:A:105:VAL:HG12	1:A:106:CYS:H	1.83	0.41
3:C:194:PHE:HA	3:C:234:VAL:CG1	2.47	0.41
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.61	0.41
13:M:20:LEU:HA	13:M:23:LEU:HB2	2.03	0.41
20:T:52:ARG:HH22	30:0:308:U:H2'	1.85	0.41
9:I:130:LEU:HB2	9:I:132:VAL:HG23	2.03	0.41
30:0:1211:G:H2'	30:0:1212:C:H6	1.85	0.41
17:Q:31:GLU:OE1	17:Q:31:GLU:HA	2.21	0.41
20:T:1:SER:H3	20:T:7:GLN:HE21	1.69	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.20	0.41
30:0:1973:A:H2'	30:0:1974:G:O4'	2.21	0.41
29:3:60:LYS:HG3	41:0:9354:HOH:O	2.21	0.41
18:R:94:ASN:ND2	30:0:500:G:O2'	2.47	0.41
30:0:1343:C:H2'	30:0:1344:G:O5'	2.21	0.41
30:0:2305:A:H4'	30:0:2392:C:C6	2.56	0.41
23:W:130:HIS:C	23:W:136:GLY:HA3	2.40	0.41
10:J:107:ASN:HD22	10:J:108:PRO:N	2.19	0.41
23:W:31:HIS:HB3	23:W:115:THR:CG2	2.51	0.41
15:O:25:VAL:HG23	15:O:26:TRP:CE3	2.56	0.41
3:C:123:LEU:O	3:C:125:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1573:A:N7	30:0:1574:C:C2	2.89	0.41
30:0:2531:U:C2'	30:0:2532:A:H5'	2.51	0.41
30:0:1358:A:N7	30:0:1360:C:C2	2.89	0.41
30:0:1421:C:H2'	30:0:1422:U:H6	1.86	0.41
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.52	0.41
6:F:59:ILE:HD13	30:0:263:U:O4'	2.20	0.41
2:B:286:ASN:O	2:B:306:LYS:HE3	2.21	0.41
30:0:2474:A:H4'	30:0:2475:C:O5'	2.21	0.41
30:0:1456:C:H2'	30:0:1457:U:C6	2.56	0.41
6:F:24:ARG:HG3	6:F:25:ASP:H	1.86	0.41
30:0:116:G:H2'	30:0:117:A:H8	1.86	0.41
23:W:23:MET:C	23:W:25:ASN:H	2.22	0.41
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.41
30:0:491:C:H2'	30:0:492:C:H6	1.86	0.41
16:P:98:ILE:HG21	30:0:1597:A:H5''	2.02	0.41
30:0:919:U:H5'	30:0:2465:A:O2'	2.21	0.41
30:0:2397:G:H2'	30:0:2398:A:C8	2.56	0.41
30:0:2096:A:H2'	30:0:2539:U:O4'	2.21	0.41
30:0:1757:U:H6	30:0:1757:U:O5'	2.03	0.41
1:A:235:ARG:NH1	41:A:9014:HOH:O	2.53	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
30:0:10:U:O4	30:0:532:A:OP2	2.39	0.41
30:0:2573:G:O2'	30:0:2574:G:H5'	2.20	0.41
30:0:2111:G:H2'	30:0:2112:A:O4'	2.21	0.41
4:D:158:ASN:HB2	4:D:161:ASP:HB2	2.02	0.41
16:P:28:GLN:HB2	41:P:6051:HOH:O	2.20	0.41
30:0:113:A:H3'	30:0:114:A:C5'	2.50	0.41
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.41
30:0:544:G:H2'	30:0:545:G:C5'	2.51	0.41
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.56	0.41
9:I:95:LEU:HG	9:I:132:VAL:CG1	2.51	0.41
18:R:84:ALA:O	18:R:88:PHE:HD1	2.04	0.41
14:N:165:ALA:HA	41:N:8823:HOH:O	2.21	0.41
16:P:59:ARG:O	16:P:62:ALA:HB3	2.20	0.41
30:0:907:A:H4'	30:0:1328:A:C2	2.56	0.41
17:Q:15:LYS:HD3	30:0:2364:A:H5''	2.02	0.41
2:B:221:GLN:HB2	41:B:9055:HOH:O	2.21	0.41
11:K:6:ALA:HB3	11:K:116:GLU:HG2	2.01	0.41
19:S:41:VAL:HG21	19:S:66:VAL:HG21	2.03	0.41
31:9:3:A:C2	31:9:21:G:N3	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:20:GLU:HG3	24:X:21:PRO:HD2	2.03	0.41
30:0:2326:C:H4'	30:0:2412:G:O4'	2.21	0.41
28:2:21:VAL:O	28:2:22:PRO:C	2.59	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:2032:U:O2'	30:0:2033:G:H5''	2.21	0.41
30:0:1220:U:O2'	30:0:1221:G:H5'	2.20	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
13:M:5:TYR:O	13:M:7:TYR:N	2.54	0.41
30:0:574:G:O2'	30:0:575:A:H5'	2.21	0.41
30:0:287:C:H2'	30:0:288:A:H8	1.86	0.41
2:B:71:VAL:HG11	2:B:296:LEU:HD22	2.02	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.21	0.41
3:C:133:ARG:HD2	41:C:8613:HOH:O	2.21	0.41
19:S:7:HIS:HA	19:S:8:PRO:HD3	1.92	0.41
13:M:54:TYR:CG	13:M:55:LYS:N	2.89	0.41
5:E:15:GLN:CG	5:E:20:ILE:HG12	2.48	0.40
3:C:78:ARG:O	3:C:79:ARG:HB3	2.21	0.40
13:M:72:ALA:CB	13:M:93:ARG:NE	2.84	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.03	0.40
20:T:43:ASN:C	20:T:45:GLY:N	2.72	0.40
30:0:2851:G:H2'	30:0:2852:A:H5'	2.00	0.40
3:C:136:VAL:HG22	3:C:137:PRO:HA	2.03	0.40
2:B:215:VAL:N	2:B:220:VAL:HG22	2.36	0.40
8:H:170:ARG:HD2	41:H:8992:HOH:O	2.21	0.40
2:B:223:ARG:NE	2:B:232:TRP:HB3	2.35	0.40
26:Z:48:ARG:O	26:Z:51:ALA:HB3	2.21	0.40
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.40
30:0:1359:U:C5	30:0:2101:A:C8	3.10	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.89	0.40
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.40
30:0:1588:G:H1'	30:0:1607:A:N6	2.37	0.40
30:0:1739:G:O2'	30:0:1740:U:H5'	2.21	0.40
30:0:1065:G:H2'	30:0:1066:U:O4'	2.21	0.40
30:0:2057:U:O5'	30:0:2057:U:H6	2.03	0.40
20:T:75:GLU:HB3	41:T:4772:HOH:O	2.21	0.40
30:0:85:C:H3'	30:0:86:A:H2'	2.03	0.40
2:B:233:ARG:HD2	41:0:9321:HOH:O	2.21	0.40
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.40
30:0:2656:G:O2'	30:0:2657:G:H5'	2.20	0.40
30:0:267:G:H2'	30:0:268:U:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:191:GLY:O	30:0:175:G:H5''	2.21	0.40
9:I:132:VAL:HG12	9:I:132:VAL:O	2.21	0.40
9:I:70:THR:O	9:I:74:ILE:HG13	2.22	0.40
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.56	0.40
30:0:1552:G:N2	30:0:1634:G:H1'	2.36	0.40
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.19	0.40
8:H:43:ALA:HB1	8:H:140:TYR:CE2	2.56	0.40
30:0:451:C:C2'	30:0:452:G:H5'	2.51	0.40
20:T:21:LYS:HA	20:T:24:ARG:HD2	2.03	0.40
30:0:632:A:OP2	30:0:2534:C:O2'	2.34	0.40
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.40
23:W:115:THR:CG2	23:W:116:LEU:N	2.84	0.40
30:0:69:A:C3'	30:0:69:A:C8	3.04	0.40
30:0:2831:C:H2'	30:0:2832:C:C5'	2.51	0.40
30:0:1041:U:H4'	30:0:1295:G:H5'	2.02	0.40
29:3:42:ARG:NH1	29:3:42:ARG:HG3	2.36	0.40
30:0:297:U:H6	30:0:297:U:O5'	2.03	0.40
30:0:233:U:H2'	30:0:234:A:O4'	2.21	0.40
30:0:1724:U:H2'	41:0:5552:HOH:O	2.21	0.40
29:3:86:GLY:HA3	30:0:2318:C:OP1	2.21	0.40
30:0:2800:A:H5'	30:0:2801:A:OP2	2.21	0.40
30:0:2563:U:H2'	30:0:2565:C:O5'	2.21	0.40
10:J:47:THR:HB	30:0:1244:U:H6	1.85	0.40
14:N:143:ARG:NH2	14:N:169:PRO:HB2	2.35	0.40
30:0:36:C:C2	30:0:447:A:C2	3.10	0.40
20:T:2:LYS:HE2	41:T:2822:HOH:O	2.21	0.40
30:0:80:A:H4'	30:0:81:G:O5'	2.22	0.40
2:B:215:VAL:HG11	2:B:234:ARG:NH2	2.36	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.20	0.40
30:0:190:G:O2'	30:0:204:A:N3	2.46	0.40
5:E:36:PRO:CD	10:J:127:ILE:HG13	2.52	0.40
30:0:1445:G:H21	30:0:1678:A:H1'	1.84	0.40
30:0:1270:U:H2'	30:0:1271:A:H8	1.87	0.40
30:0:426:G:H5''	41:0:9419:HOH:O	2.21	0.40
8:H:142:ASN:O	8:H:144:GLU:N	2.53	0.40
30:0:653:U:H3	30:0:752:G:H1	1.70	0.40
5:E:70:GLU:O	5:E:73:PHE:HB2	2.21	0.40
15:O:87:THR:O	15:O:91:GLN:HG3	2.20	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.21	0.40
2:B:70:PRO:HG3	30:0:2719:A:C2	2.57	0.40
30:0:2685:C:O2'	30:0:2686:C:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:MET:HE1	41:0:9290:HOH:O	2.20	0.40
7:G:23:ILE:O	7:G:27:ILE:HG13	2.21	0.40
29:3:6:ARG:HB3	29:3:20:HIS:O	2.21	0.40
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.11	0.40
2:B:267:LYS:HA	41:0:3465:HOH:O	2.22	0.40
4:D:170:TYR:CD1	4:D:170:TYR:N	2.89	0.40
30:0:2852:A:H4'	30:0:2853:U:C5	2.57	0.40
2:B:229:ARG:NH2	30:0:1753:C:O2	2.38	0.40
6:F:26:THR:HG21	6:F:102:GLY:O	2.20	0.40
30:0:168:C:H6	30:0:168:C:O5'	2.05	0.40
30:0:661:G:C5	30:0:686:A:C2	3.10	0.40
12:L:130:ARG:O	12:L:132:LYS:N	2.54	0.40
19:S:45:TYR:HE2	19:S:81:ILE:HG12	1.86	0.40
30:0:17:G:H2'	30:0:18:C:H6	1.85	0.40
8:H:82:GLU:O	8:H:83:GLU:HG3	2.22	0.40
15:O:4:ASN:HA	15:O:5:PRO:HD3	1.88	0.40
30:0:2325:U:O2'	30:0:2411:C:H1'	2.21	0.40
30:0:1114:A:H2'	30:0:1115:U:H6	1.86	0.40
18:R:43:ALA:O	18:R:46:TYR:HB3	2.22	0.40
2:B:51:VAL:HG23	2:B:329:TYR:O	2.21	0.40
25:Y:100:ARG:HD2	25:Y:232:THR:HB	2.03	0.40
23:W:54:PHE:CZ	23:W:140:LYS:HB2	2.57	0.40
17:Q:16:ASN:ND2	17:Q:45:PRO:CG	2.84	0.40
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.54	0.40
31:9:1:U:O3'	31:9:3:A:H5''	2.21	0.40
20:T:16:LEU:HD12	30:0:100:C:H5'	2.02	0.40
30:0:1228:C:H2'	30:0:1229:C:O4'	2.21	0.40
12:L:104:ASP:O	12:L:105:TYR:HB3	2.21	0.40
30:0:1688:G:C6	30:0:1692:C:C6	3.09	0.40
30:0:69:A:H3'	30:0:69:A:C8	2.56	0.40
1:A:2:ARG:HG3	1:A:197:VAL:HG22	2.03	0.40
26:Z:54:GLU:HA	26:Z:57:MET:CE	2.50	0.40
30:0:2824:C:H5''	30:0:2825:C:H5'	2.04	0.40
10:J:71:TYR:HA	10:J:72:PRO:HD2	1.89	0.40
29:3:40:ARG:HG3	29:3:52:PHE:CD2	2.57	0.40
14:N:41:LYS:HE3	41:9:9020:HOH:O	2.22	0.40
30:0:2604:A:H5'	41:0:6629:HOH:O	2.22	0.40
29:3:91:GLN:O	29:3:92:GLU:HB2	2.22	0.40
2:B:298:LYS:HG2	41:0:6362:HOH:O	2.21	0.40
30:0:862:U:O2'	30:0:863:G:H5'	2.21	0.40
18:R:2:ILE:HG22	30:0:21:G:H4'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2551:C:O2'	30:0:2552:C:H5'	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/240 (97%)	198 (85%)	25 (11%)	10 (4%)	3	16
2	B	333/338 (98%)	285 (86%)	41 (12%)	7 (2%)	9	37
3	C	242/246 (98%)	202 (84%)	32 (13%)	8 (3%)	5	23
4	D	132/177 (75%)	87 (66%)	35 (26%)	10 (8%)	1	5
5	E	168/178 (94%)	150 (89%)	17 (10%)	1 (1%)	30	70
6	F	115/120 (96%)	94 (82%)	15 (13%)	6 (5%)	2	12
7	G	25/348 (7%)	15 (60%)	7 (28%)	3 (12%)	0	1
8	H	154/177 (87%)	125 (81%)	23 (15%)	6 (4%)	4	19
9	I	66/162 (41%)	43 (65%)	18 (27%)	5 (8%)	1	5
10	J	138/145 (95%)	120 (87%)	15 (11%)	3 (2%)	8	35
11	K	128/132 (97%)	115 (90%)	8 (6%)	5 (4%)	4	19
12	L	139/165 (84%)	106 (76%)	27 (19%)	6 (4%)	3	16
13	M	190/196 (97%)	170 (90%)	16 (8%)	4 (2%)	9	37
14	N	182/187 (97%)	153 (84%)	19 (10%)	10 (6%)	2	11
15	O	111/116 (96%)	92 (83%)	19 (17%)	0	100	100
16	P	139/149 (93%)	129 (93%)	8 (6%)	2 (1%)	14	49
17	Q	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	3	16
18	R	146/155 (94%)	131 (90%)	12 (8%)	3 (2%)	9	37
19	S	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	115/120 (96%)	95 (83%)	17 (15%)	3 (3%)	7	30
21	U	51/67 (76%)	45 (88%)	4 (8%)	2 (4%)	4	19
22	V	63/71 (89%)	53 (84%)	9 (14%)	1 (2%)	12	45
23	W	150/154 (97%)	131 (87%)	19 (13%)	0	100	100
24	X	78/92 (85%)	68 (87%)	7 (9%)	3 (4%)	4	19
25	Y	140/240 (58%)	128 (91%)	11 (8%)	1 (1%)	26	67
26	Z	69/116 (60%)	51 (74%)	13 (19%)	5 (7%)	1	6
27	1	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	10	40
28	2	42/50 (84%)	34 (81%)	8 (19%)	0	100	100
29	3	88/92 (96%)	77 (88%)	9 (10%)	2 (2%)	8	34
All	All	3659/4471 (82%)	3087 (84%)	460 (13%)	112 (3%)	5	25

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL
1	A	208	HIS
2	B	181	ILE
4	D	16	PRO
4	D	27	ILE
4	D	171	ASP
6	F	101	ALA
9	I	113	SER
12	L	80	ASP
13	M	83	SER
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
24	X	87	ALA
26	Z	44	ARG
26	Z	105	ARG
29	3	56	PRO
1	A	205	GLY
2	B	291	ASP
3	C	69	HIS
6	F	27	GLY

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Mol	Chain	Res	Type
8	H	84	GLY
9	I	124	VAL
12	L	82	ALA
14	N	165	ALA
20	T	44	ALA
20	T	53	GLY
21	U	55	ALA
22	V	43	PRO
24	X	81	GLY
26	Z	59	GLU
1	A	24	LYS
1	A	119	ALA
3	C	8	LEU
3	C	121	ALA
4	D	28	GLY
4	D	60	GLU
4	D	61	PHE
4	D	137	PRO
4	D	147	ALA
5	E	164	ASP
6	F	100	ASP
7	G	72	ASP
8	H	71	SER
8	H	82	GLU
9	I	128	THR
10	J	15	ARG
10	J	76	ASP
11	K	65	ARG
11	K	126	SER
12	L	21	ARG
14	N	65	ASP
14	N	74	PRO
14	N	164	ASP
14	N	167	ASP
14	N	182	GLY
16	P	19	ASN
16	P	108	LEU
17	Q	23	THR
17	Q	48	PRO
19	S	4	VAL
21	U	46	ALA
24	X	70	ILE

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Mol	Chain	Res	Type
2	B	55	ASN
2	B	185	GLY
4	D	56	ARG
6	F	61	MET
6	F	64	PRO
8	H	70	LEU
8	H	143	VAL
8	H	145	ASP
12	L	50	GLY
12	L	102	ASP
13	M	6	SER
13	M	35	GLY
18	R	114	VAL
20	T	30	ASP
29	3	52	PHE
2	B	2	GLN
3	C	232	LEU
3	C	234	VAL
4	D	46	GLY
9	I	73	LEU
11	K	66	ARG
12	L	131	GLU
17	Q	31	GLU
18	R	20	GLU
26	Z	66	CYS
27	1	54	ALA
1	A	204	GLY
2	B	182	VAL
3	C	95	GLU
6	F	59	ILE
11	K	102	GLU
13	M	88	VAL
17	Q	54	PRO
18	R	32	ALA
25	Y	182	PHE
1	A	192	VAL
3	C	124	VAL
10	J	18	ILE
26	Z	67	GLY
2	B	30	PRO
1	A	88	ILE
3	C	57	PRO

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Mol	Chain	Res	Type
7	G	13	PRO
11	K	83	PRO
14	N	157	PRO
7	G	20	VAL
9	I	109	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	167 (94%)	11 (6%)	23	58
2	B	281/283 (99%)	266 (95%)	15 (5%)	28	65
3	C	192/193 (100%)	179 (93%)	13 (7%)	20	54
4	D	116/148 (78%)	111 (96%)	5 (4%)	35	73
5	E	151/156 (97%)	144 (95%)	7 (5%)	33	71
6	F	92/94 (98%)	92 (100%)	0	100	100
7	G	27/283 (10%)	26 (96%)	1 (4%)	41	77
8	H	133/145 (92%)	127 (96%)	6 (4%)	34	72
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	90
10	J	117/121 (97%)	109 (93%)	8 (7%)	20	54
11	K	105/106 (99%)	102 (97%)	3 (3%)	50	82
12	L	113/127 (89%)	108 (96%)	5 (4%)	35	72
13	M	157/160 (98%)	149 (95%)	8 (5%)	29	67
14	N	148/150 (99%)	143 (97%)	5 (3%)	44	79
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	66	89
17	Q	79/80 (99%)	77 (98%)	2 (2%)	55	85
18	R	117/122 (96%)	112 (96%)	5 (4%)	35	73
19	S	71/74 (96%)	69 (97%)	2 (3%)	51	83
20	T	104/106 (98%)	99 (95%)	5 (5%)	31	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	44/53 (83%)	42 (96%)	2 (4%)	34	72
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	27	64
24	X	65/74 (88%)	58 (89%)	7 (11%)	8	28
25	Y	120/195 (62%)	111 (92%)	9 (8%)	17	49
26	Z	59/94 (63%)	56 (95%)	3 (5%)	29	67
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	40 (95%)	2 (5%)	31	69
29	3	78/79 (99%)	76 (97%)	2 (3%)	54	84
All	All	3079/3646 (84%)	2943 (96%)	136 (4%)	35	72

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	69	LEU
1	A	120	ARG
1	A	131	HIS
1	A	153	ARG
1	A	171	LYS
1	A	179	MET
1	A	192	VAL
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	71	VAL
2	B	82	VAL
2	B	90	THR
2	B	103	ASP
2	B	132	HIS
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	254	GLN
2	B	277	GLU

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Mol	Chain	Res	Type
2	B	312	ARG
3	C	16	VAL
3	C	27	ARG
3	C	76	ARG
3	C	101	ASP
3	C	115	LEU
3	C	132	ASP
3	C	172	THR
3	C	187	ARG
3	C	188	ARG
3	C	211	ASP
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
4	D	24	HIS
4	D	50	VAL
4	D	131	THR
4	D	133	ASN
4	D	137	PRO
5	E	7	ILE
5	E	102	VAL
5	E	126	ILE
5	E	132	THR
5	E	143	GLN
5	E	155	ASN
5	E	164	ASP
7	G	73	ASP
8	H	21	GLU
8	H	51	SER
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	135	GLU
10	J	46	ILE
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
10	J	131	THR

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Mol	Chain	Res	Type
11	K	4	LEU
11	K	7	ASP
11	K	10	GLN
12	L	35	ARG
12	L	43	HIS
12	L	89	PHE
12	L	101	ASP
12	L	140	VAL
13	M	46	LEU
13	M	52	GLN
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	130	GLU
13	M	154	ASP
14	N	49	THR
14	N	103	ASP
14	N	110	THR
14	N	124	ASP
14	N	139	TRP
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	39	THR
18	R	61	GLN
18	R	70	SER
18	R	76	ASP
18	R	90	ASP
19	S	12	GLU
19	S	44	GLN
20	T	23	VAL
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
21	U	19	THR
21	U	53	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL

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Mol	Chain	Res	Type
23	W	73	LEU
23	W	88	THR
23	W	125	HIS
23	W	146	ILE
24	X	8	ARG
24	X	27	ASP
24	X	46	ASP
24	X	49	ARG
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
25	Y	204	ARG
25	Y	220	GLU
25	Y	235	GLU
26	Z	46	SER
26	Z	68	GLU
26	Z	106	SER
28	2	16	ASN
28	2	18	ASN
29	3	15	ASN
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	11	ASN
3	C	39	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	129	HIS
4	D	47	GLN
4	D	103	ASN
4	D	133	ASN
4	D	155	HIS
5	E	74	HIS
5	E	90	HIS
5	E	106	ASN
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	148	HIS
9	I	88	GLN
9	I	99	GLN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	42	ASN
12	L	18	HIS
12	L	20	ASN
12	L	41	HIS
12	L	42	ASN
12	L	43	HIS
12	L	58	GLN
13	M	24	GLN
13	M	52	GLN
13	M	58	GLN
13	M	137	ASN
14	N	21	HIS
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
14	N	153	GLN
15	O	100	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN

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Mol	Chain	Res	Type
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
17	Q	67	GLN
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	44	GLN
19	S	51	GLN
19	S	53	ASN
20	T	7	GLN
20	T	11	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	49	ASN
23	W	59	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	240 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	2 (1%)
32	5	1/3 (33%)	0	0
33	6	1/3 (33%)	0	0
All	All	2868/3051 (94%)	258 (8%)	32 (1%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G

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Mol	Chain	Res	Type
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	593	A
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	702	G
30	0	735	C
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A

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Mol	Chain	Res	Type
30	0	877	G
30	0	878	G
30	0	882	A
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	938	G
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1351	G

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Mol	Chain	Res	Type
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1873	G
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A

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Mol	Chain	Res	Type
30	0	1971	G
30	0	1973	A
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2527	U

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Mol	Chain	Res	Type
30	0	2533	C
30	0	2536	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2648	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2786	G
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G

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Mol	Chain	Res	Type
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
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 (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1474	C
30	0	1684	A
30	0	1692	C
30	0	1730	G
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2011	A
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2637	A

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Mol	Chain	Res	Type
30	0	2649	A
30	0	2681	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2852	A
31	9	55	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$
30	OMU	0	2587	30	12,22,23	0.97	2 (16%)	19,31,34	3.17	2 (10%)
30	OMG	0	2588	32,30	17,26,27	1.03	1 (5%)	21,38,41	2.65	3 (14%)
30	UR3	0	2619	30	12,22,23	0.84	1 (8%)	16,32,35	0.74	0
30	PSU	0	2621	30	13,21,22	1.69	2 (15%)	18,30,33	6.17	4 (22%)
30	1MA	0	628	30,36	14,25,26	1.01	1 (7%)	15,37,40	1.21	1 (6%)
33	8AN	6	76	33,30	15,24,25	1.02	1 (6%)	11,35,38	1.99	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	32,30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,36	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	8AN	6	76	33,30	-	0/3/25/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.05	1.47	1.52
30	0	2587	OMU	C6-C5	-2.21	1.33	1.38
30	0	2619	UR3	C6-C5	-2.18	1.33	1.38
33	6	76	8AN	C3'-N3'	-2.15	1.44	1.47
30	0	2587	OMU	C4-N3	2.18	1.37	1.33
30	0	628	1MA	C6-N6	2.71	1.34	1.29
30	0	2621	PSU	C4-N3	2.92	1.38	1.33
30	0	2588	OMG	C6-N1	3.19	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.73	114.47	128.33
30	0	2588	OMG	C5-C6-N1	-8.92	111.39	123.59
30	0	628	1MA	C2-N3-C4	-3.76	110.58	116.40
30	0	2587	OMU	C5-C4-N3	-3.38	114.44	123.12
30	0	2588	OMG	N3-C2-N1	-2.62	123.45	127.44
30	0	2621	PSU	C5-C1'-C2'	-2.16	111.68	115.52
30	0	2621	PSU	C6-N1-C2	2.87	120.09	115.47
33	6	76	8AN	C2'-C1'-N9	3.39	119.47	114.29
33	6	76	8AN	O4'-C4'-C3'	3.40	109.19	104.09
33	6	76	8AN	O2'-C2'-C3'	3.98	121.22	111.26
30	0	2588	OMG	C6-N1-C2	7.01	125.67	115.94
30	0	2587	OMU	C4-N3-C2	13.20	127.21	114.14
30	0	2621	PSU	C4-N3-C2	13.61	127.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2588	OMG	2	0
30	0	2619	UR3	1	0
33	6	76	8AN	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 305 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
34	PHE	6	77	-	10,11,12	1.26	2 (20%)	10,13,15	0.66	0
34	ACA	6	78	-	7,7,8	1.87	2 (28%)	5,6,8	1.61	1 (20%)

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
34	PHE	6	77	-	-	0/4/6/8	0/1/1/1
34	ACA	6	78	-	-	0/4/5/6	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	6	78	ACA	C3-C2	-4.17	1.36	1.52
34	6	77	PHE	CA-N	-2.05	1.41	1.47
34	6	78	ACA	C5-C6	2.23	1.62	1.51
34	6	77	PHE	CE1-CD1	2.57	1.44	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	6	78	ACA	C5-C4-C3	-2.32	102.56	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.33	4 (1%) 73 53	24, 46, 80, 105	0
2	B	337/338 (99%)	-0.53	1 (0%) 94 87	26, 49, 75, 88	0
3	C	246/246 (100%)	-0.45	0 100 100	24, 45, 69, 80	0
4	D	140/177 (79%)	1.01	31 (22%) 1 1	64, 93, 124, 135	0
5	E	172/178 (96%)	-0.16	4 (2%) 64 43	41, 62, 84, 92	0
6	F	119/120 (99%)	0.42	11 (9%) 11 6	50, 73, 100, 114	0
7	G	29/348 (8%)	0.83	2 (6%) 20 10	75, 95, 109, 113	0
8	H	160/177 (90%)	-0.12	2 (1%) 79 61	39, 58, 93, 99	0
9	I	70/162 (43%)	3.48	48 (68%) 0 0	141, 152, 166, 168	0
10	J	142/145 (97%)	-0.46	0 100 100	35, 47, 66, 86	0
11	K	132/132 (100%)	-0.67	0 100 100	28, 41, 63, 73	0
12	L	145/165 (87%)	-0.08	1 (0%) 89 76	22, 67, 105, 121	0
13	M	194/196 (98%)	-0.48	0 100 100	25, 46, 68, 82	0
14	N	186/187 (99%)	-0.11	5 (2%) 58 37	42, 63, 116, 124	0
15	O	115/116 (99%)	-0.36	0 100 100	39, 55, 67, 75	0
16	P	143/149 (95%)	-0.47	0 100 100	35, 51, 62, 68	0
17	Q	95/96 (98%)	-0.38	0 100 100	35, 49, 66, 75	0
18	R	150/155 (96%)	-0.56	0 100 100	22, 42, 62, 69	0
19	S	81/85 (95%)	-0.29	1 (1%) 81 63	44, 56, 81, 94	0
20	T	119/120 (99%)	-0.16	3 (2%) 61 39	38, 54, 84, 116	0
21	U	53/67 (79%)	-0.32	1 (1%) 70 50	38, 49, 73, 86	0
22	V	65/71 (91%)	0.93	10 (15%) 3 1	55, 78, 115, 122	0
23	W	154/154 (100%)	-0.37	1 (0%) 90 78	37, 48, 72, 86	0
24	X	82/92 (89%)	-0.19	5 (6%) 25 13	39, 55, 80, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/240 (59%)	-0.53	2 (1%) 78 59	25, 44, 64, 90	0
26	Z	73/116 (62%)	0.12	4 (5%) 29 16	48, 67, 87, 96	0
27	1	56/57 (98%)	-0.59	0 100 100	22, 32, 39, 51	0
28	2	46/50 (92%)	-0.14	2 (4%) 39 23	29, 61, 76, 89	0
29	3	92/92 (100%)	-0.25	1 (1%) 82 65	33, 58, 71, 81	0
30	0	2749/2923 (94%)	-0.50	17 (0%) 90 78	16, 45, 92, 179	0
31	9	122/122 (100%)	-0.56	2 (1%) 74 55	36, 65, 92, 148	0
32	5	2/3 (66%)	2.15	1 (50%) 0 0	100, 100, 100, 102	0
33	6	2/3 (66%)	1.75	1 (50%) 0 0	96, 96, 96, 104	0
All	All	6650/7522 (88%)	-0.32	160 (2%) 62 41	16, 50, 99, 179	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	66	GLY	16.5
22	V	40	PRO	8.9
9	I	113	SER	8.1
9	I	72	GLU	7.6
9	I	132	VAL	7.4
9	I	74	ILE	7.0
4	D	57	THR	7.0
9	I	108	HIS	6.9
9	I	70	THR	6.8
9	I	71	ALA	6.6
22	V	1	THR	6.6
9	I	103	ILE	6.3
9	I	111	LEU	6.1
4	D	63	ILE	6.0
9	I	69	PRO	5.8
9	I	98	ASP	5.7
22	V	38	GLY	5.6
9	I	100	VAL	5.5
4	D	90	LEU	5.5
9	I	112	LEU	5.4
20	T	119	ALA	5.2
9	I	97	VAL	5.1
9	I	99	GLN	5.1
26	Z	35	SER	5.1
26	Z	34	SER	5.1

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Mol	Chain	Res	Type	RSRZ
19	S	81	ILE	4.8
9	I	101	LYS	4.8
9	I	121	LYS	4.6
9	I	116	LEU	4.5
9	I	73	LEU	4.4
9	I	109	PRO	4.4
9	I	80	PHE	4.4
9	I	76	ASP	4.4
26	Z	46	SER	4.3
4	D	93	LEU	4.2
9	I	105	GLU	4.2
30	0	1172	G	4.2
4	D	106	PHE	4.2
9	I	123	VAL	4.2
28	2	49	GLU	4.2
9	I	104	ALA	4.1
7	G	23	ILE	4.1
6	F	16	ALA	3.9
30	0	1199	A	3.8
4	D	134	LEU	3.8
4	D	84	LEU	3.6
14	N	166	ALA	3.6
4	D	92	GLU	3.6
22	V	39	ALA	3.6
9	I	129	SER	3.6
9	I	119	ALA	3.5
22	V	46	ILE	3.5
4	D	41	LEU	3.5
9	I	102	GLN	3.5
4	D	40	ILE	3.5
4	D	44	ILE	3.4
26	Z	58	ASN	3.4
9	I	106	GLN	3.4
6	F	17	LEU	3.3
6	F	22	VAL	3.3
6	F	28	ALA	3.3
4	D	26	GLY	3.2
9	I	128	THR	3.2
9	I	91	PHE	3.2
9	I	94	ASP	3.2
9	I	86	GLU	3.1
14	N	160	SER	3.1

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Mol	Chain	Res	Type	RSRZ
9	I	82	THR	3.1
9	I	127	CYS	3.1
4	D	166	ILE	3.1
6	F	47	LEU	3.1
30	0	1200	A	3.0
4	D	74	THR	3.0
5	E	10	ASP	3.0
30	0	735	C	3.0
9	I	67	VAL	2.9
1	A	37	VAL	2.9
14	N	180	LEU	2.9
9	I	120	ALA	2.9
33	6	75	C	2.8
9	I	90	ASP	2.8
4	D	88	LEU	2.8
24	X	71	ARG	2.8
6	F	23	ALA	2.8
23	W	86	GLU	2.8
21	U	47	ARG	2.8
8	H	169	GLU	2.7
22	V	37	GLY	2.7
6	F	49	PHE	2.7
4	D	18	ILE	2.7
4	D	91	ALA	2.7
30	0	1198	U	2.7
9	I	131	GLY	2.7
30	0	1202	A	2.7
22	V	8	ILE	2.7
2	B	117	GLU	2.6
12	L	91	VAL	2.6
4	D	85	GLN	2.6
14	N	179	LEU	2.6
9	I	133	THR	2.6
5	E	45	ASP	2.6
8	H	174	LEU	2.6
24	X	88	GLU	2.6
32	5	76	A	2.6
4	D	104	PHE	2.6
31	9	1	U	2.5
9	I	77	GLU	2.5
4	D	61	PHE	2.5
9	I	126	THR	2.5

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Mol	Chain	Res	Type	RSRZ
30	0	1177	A	2.5
4	D	27	ILE	2.4
24	X	65	ASN	2.4
4	D	130	VAL	2.4
30	0	1165	G	2.4
4	D	170	TYR	2.4
20	T	35	TYR	2.4
30	0	1196	C	2.4
1	A	236	GLY	2.3
25	Y	236	VAL	2.3
29	3	55	VAL	2.3
4	D	77	ASP	2.3
4	D	154	LYS	2.3
6	F	20	LEU	2.3
30	0	1197	G	2.3
6	F	96	ALA	2.2
22	V	36	ALA	2.2
7	G	27	ILE	2.2
14	N	147	ILE	2.2
5	E	154	ILE	2.2
4	D	75	LEU	2.2
4	D	101	THR	2.2
24	X	80	GLU	2.2
30	0	282	C	2.2
22	V	41	GLU	2.2
9	I	88	GLN	2.2
30	0	1163	G	2.2
9	I	115	ASP	2.1
30	0	1965	C	2.1
22	V	3	LEU	2.1
6	F	45	ALA	2.1
5	E	100	ASP	2.1
9	I	81	GLU	2.1
30	0	2637	A	2.1
4	D	11	HIS	2.1
20	T	118	SER	2.1
4	D	64	ARG	2.1
4	D	47	GLN	2.1
6	F	25	ASP	2.1
9	I	78	ALA	2.1
30	0	1203	G	2.1
31	9	2	U	2.1

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Mol	Chain	Res	Type	RSRZ
24	X	85	VAL	2.1
1	A	31	LYS	2.1
9	I	92	VAL	2.1
1	A	237	GLY	2.0
30	0	1168	C	2.0
28	2	35	ARG	2.0
30	0	1169	U	2.0
4	D	23	VAL	2.0
25	Y	95	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
33	8AN	6	76	22/23	0.86	0.29	-	87,92,94,95	0
30	1MA	0	628	23/24	0.98	0.17	-	36,40,42,42	0
30	UR3	0	2619	21/22	0.98	0.14	-	40,41,44,47	0
30	OMU	0	2587	21/22	0.97	0.12	-	30,33,38,38	0
30	PSU	0	2621	20/21	0.98	0.15	-	36,38,42,42	0
30	OMG	0	2588	24/25	0.97	0.12	-	30,34,35,37	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
36	NA	0	8547	1/1	0.79	0.62	78.08	78,78,78,78	0
36	NA	0	8519	1/1	0.62	0.83	59.37	71,71,71,71	0
35	MG	0	8087	1/1	0.13	0.81	57.94	107,107,107,107	0
36	NA	0	8535	1/1	0.56	0.87	57.55	75,75,75,75	0
36	NA	0	8527	1/1	0.78	0.44	26.79	73,73,73,73	0
35	MG	0	8050	1/1	0.96	0.32	26.41	152,152,152,152	0
35	MG	0	8079	1/1	0.80	0.38	22.86	64,64,64,64	0
39	K	0	8401	1/1	0.49	0.82	21.78	82,82,82,82	0
35	MG	0	8071	1/1	0.93	0.41	18.66	88,88,88,88	0
36	NA	0	8562	1/1	0.84	0.36	18.19	55,55,55,55	0
39	K	0	8402	1/1	-0.03	0.91	17.71	117,117,117,117	0
37	SR	L	8969	1/1	0.75	0.45	17.24	175,175,175,175	0
36	NA	0	8523	1/1	0.95	0.23	15.16	61,61,61,61	0
35	MG	0	8010	1/1	0.47	0.42	14.06	78,78,78,78	0
36	NA	0	8521	1/1	0.95	0.34	13.52	51,51,51,51	0
36	NA	0	8512	1/1	0.94	0.44	13.19	46,46,46,46	0
35	MG	0	8076	1/1	0.96	0.28	11.92	72,72,72,72	0
36	NA	9	8572	1/1	0.60	0.25	11.87	96,96,96,96	0
35	MG	A	8051	1/1	0.94	0.98	11.85	82,82,82,82	0
36	NA	0	8520	1/1	0.90	0.23	11.80	58,58,58,58	0
36	NA	0	8556	1/1	0.89	0.80	11.57	75,75,75,75	0
36	NA	0	8567	1/1	0.72	0.34	10.87	61,61,61,61	0
35	MG	0	8029	1/1	0.92	0.24	10.86	83,83,83,83	0
35	MG	0	8009	1/1	0.98	0.32	10.63	1,1,1,1	0
36	NA	0	8568	1/1	0.91	0.43	10.33	18,18,18,18	0
36	NA	0	8565	1/1	0.88	0.37	10.03	48,48,48,48	0
36	NA	0	8533	1/1	0.96	0.28	9.74	64,64,64,64	0
36	NA	0	8507	1/1	0.95	0.26	9.64	29,29,29,29	0
35	MG	0	8028	1/1	0.96	0.22	8.99	1,1,1,1	0
36	NA	0	8563	1/1	0.94	0.30	8.43	51,51,51,51	0
35	MG	0	8047	1/1	0.87	0.26	8.07	92,92,92,92	0
37	SR	B	8987	1/1	0.86	0.39	7.43	199,199,199,199	0
36	NA	0	8553	1/1	0.88	0.25	7.30	100,100,100,100	0
36	NA	0	8552	1/1	0.89	0.26	7.25	86,86,86,86	0
35	MG	0	8062	1/1	0.93	0.30	7.22	41,41,41,41	0
36	NA	0	8550	1/1	0.88	0.25	6.56	51,51,51,51	0
36	NA	0	8557	1/1	0.14	0.21	6.52	82,82,82,82	0
35	MG	0	8002	1/1	1.00	0.28	5.81	19,19,19,19	0
36	NA	0	8559	1/1	0.85	0.16	5.75	64,64,64,64	0
37	SR	0	8949	1/1	0.99	0.16	5.51	62,62,62,62	0
35	MG	0	8041	1/1	0.94	0.19	5.39	33,33,33,33	0
35	MG	0	8014	1/1	0.94	0.18	5.37	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	NA	0	8560	1/1	0.82	0.34	4.99	134,134,134,134	0
35	MG	C	8012	1/1	0.98	0.28	4.98	17,17,17,17	0
36	NA	0	8530	1/1	0.90	0.24	4.90	49,49,49,49	0
35	MG	A	8025	1/1	0.98	0.22	4.87	39,39,39,39	0
37	SR	0	8904	1/1	0.98	0.21	4.87	55,55,55,55	0
36	NA	0	8513	1/1	0.91	0.25	4.77	53,53,53,53	0
35	MG	0	8008	1/1	0.89	0.17	4.26	9,9,9,9	0
36	NA	0	8504	1/1	0.93	0.23	4.08	31,31,31,31	0
35	MG	0	8015	1/1	0.93	0.17	3.71	41,41,41,41	0
36	NA	0	8569	1/1	0.82	0.22	3.70	32,32,32,32	0
37	SR	0	8948	1/1	0.97	0.17	3.69	65,65,65,65	0
36	NA	0	8534	1/1	0.95	0.32	3.45	68,68,68,68	0
36	NA	0	8517	1/1	0.95	0.20	3.29	36,36,36,36	0
36	NA	0	8528	1/1	0.91	0.16	3.22	55,55,55,55	0
37	SR	1	8913	1/1	0.99	0.20	2.86	54,54,54,54	0
36	NA	C	8503	1/1	0.89	0.27	2.66	31,31,31,31	0
35	MG	0	8006	1/1	0.97	0.18	2.65	8,8,8,8	0
37	SR	0	8910	1/1	0.99	0.16	2.43	47,47,47,47	0
35	MG	B	8043	1/1	0.98	0.17	2.40	29,29,29,29	0
35	MG	0	8004	1/1	0.97	0.20	2.40	21,21,21,21	0
35	MG	0	8034	1/1	0.92	0.20	2.33	30,30,30,30	0
37	SR	R	8912	1/1	1.00	0.20	2.25	64,64,64,64	0
37	SR	0	8981	1/1	0.97	0.18	2.18	117,117,117,117	0
36	NA	0	8542	1/1	0.95	0.20	2.13	31,31,31,31	0
35	MG	0	8003	1/1	0.93	0.18	2.07	14,14,14,14	0
35	MG	K	8054	1/1	0.97	0.15	1.83	15,15,15,15	0
36	NA	0	8515	1/1	0.98	0.22	1.67	26,26,26,26	0
37	SR	0	8964	1/1	0.97	0.15	1.53	102,102,102,102	0
37	SR	0	8935	1/1	0.98	0.14	1.09	73,73,73,73	0
35	MG	0	8011	1/1	0.97	0.18	1.02	4,4,4,4	0
37	SR	0	8922	1/1	1.00	0.17	1.00	61,61,61,61	0
37	SR	3	8932	1/1	0.95	0.17	0.97	74,74,74,74	0
35	MG	0	8052	1/1	0.85	0.14	0.86	42,42,42,42	0
36	NA	0	8575	1/1	0.92	0.16	0.69	44,44,44,44	0
37	SR	0	8943	1/1	0.99	0.12	0.44	88,88,88,88	0
38	CL	O	8808	1/1	0.92	0.16	0.23	75,75,75,75	0
36	NA	M	8539	1/1	0.97	0.14	0.21	33,33,33,33	0
35	MG	0	8088	1/1	0.96	0.14	0.21	40,40,40,40	0
38	CL	J	8816	1/1	0.93	0.14	0.21	80,80,80,80	0
37	SR	0	8985	1/1	0.89	0.11	0.15	142,142,142,142	0
38	CL	J	8821	1/1	0.92	0.17	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
38	CL	0	8812	1/1	0.97	0.13	0.12	50,50,50,50	0
36	NA	0	8522	1/1	0.97	0.11	0.08	72,72,72,72	0
37	SR	0	8957	1/1	0.91	0.13	-0.06	124,124,124,124	0
40	CD	1	8702	1/1	0.99	0.12	-0.20	57,57,57,57	0
38	CL	M	8818	1/1	0.94	0.12	-0.57	46,46,46,46	0
36	NA	J	8538	1/1	0.99	0.12	-0.68	31,31,31,31	0
36	NA	0	8564	1/1	0.86	0.09	-0.68	35,35,35,35	0
35	MG	0	8084	1/1	0.94	0.10	-0.70	27,27,27,27	0
35	MG	0	8007	1/1	0.98	0.15	-0.75	30,30,30,30	0
36	NA	Q	8540	1/1	0.92	0.11	-0.88	66,66,66,66	0
36	NA	0	8537	1/1	0.95	0.09	-0.96	21,21,21,21	0
40	CD	Z	8703	1/1	0.99	0.10	-0.97	55,55,55,55	0
35	MG	T	8057	1/1	0.97	0.17	-1.01	31,31,31,31	0
35	MG	A	8044	1/1	0.61	0.08	-1.06	51,51,51,51	0
40	CD	U	8701	1/1	0.99	0.09	-1.07	57,57,57,57	0
37	SR	A	8929	1/1	0.95	0.09	-1.27	114,114,114,114	0
37	SR	H	8972	1/1	0.82	0.09	-1.50	132,132,132,132	0
38	CL	L	8810	1/1	0.89	0.08	-1.62	56,56,56,56	0
40	CD	3	8704	1/1	0.99	0.08	-1.70	52,52,52,52	0
37	SR	0	8962	1/1	0.60	0.11	-1.74	104,104,104,104	0
35	MG	0	8021	1/1	0.96	0.09	-1.77	24,24,24,24	0
37	SR	0	8970	1/1	0.98	0.08	-1.97	99,99,99,99	0
35	MG	0	8075	1/1	0.90	0.08	-2.02	38,38,38,38	0
38	CL	B	8819	1/1	0.92	0.11	-2.24	62,62,62,62	0
38	CL	3	8804	1/1	0.92	0.11	-2.44	60,60,60,60	0
37	SR	0	8945	1/1	0.95	0.09	-2.65	104,104,104,104	0
37	SR	0	8975	1/1	0.95	0.06	-2.78	125,125,125,125	0
37	SR	0	8992	1/1	0.90	0.05	-3.35	122,122,122,122	0
38	CL	0	8805	1/1	0.95	0.07	-5.12	60,60,60,60	0
35	MG	0	8013	1/1	0.98	0.04	-9.12	20,20,20,20	0
35	MG	Y	8086	1/1	0.95	0.05	-9.12	48,48,48,48	0
35	MG	0	8001	1/1	0.99	0.23	-	7,7,7,7	0
37	SR	0	9001	1/1	0.41	0.37	-	190,190,190,190	0
35	MG	0	8027	1/1	0.94	0.15	-	28,28,28,28	0
37	SR	0	8991	1/1	0.87	0.10	-	148,148,148,148	0
37	SR	0	8963	1/1	0.98	0.14	-	74,74,74,74	0
36	NA	0	8524	1/1	0.97	0.13	-	52,52,52,52	0
35	MG	0	8061	1/1	0.97	0.25	-	17,17,17,17	0
36	NA	0	8502	1/1	0.97	0.34	-	60,60,60,60	0
37	SR	0	8937	1/1	0.97	0.22	-	69,69,69,69	0
35	MG	0	8049	1/1	0.95	0.98	-	103,103,103,103	0
35	MG	0	8064	1/1	0.88	0.24	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	MG	0	8032	1/1	0.95	0.04	-	21,21,21,21	0
36	NA	0	8508	1/1	0.87	0.12	-	27,27,27,27	0
35	MG	0	8089	1/1	0.90	0.10	-	31,31,31,31	0
37	SR	0	8947	1/1	0.96	0.15	-	91,91,91,91	0
36	NA	0	8545	1/1	0.80	0.34	-	64,64,64,64	0
37	SR	0	8995	1/1	0.91	0.15	-	98,98,98,98	0
36	NA	0	8506	1/1	0.83	0.07	-	50,50,50,50	0
35	MG	9	8074	1/1	0.98	0.23	-	52,52,52,52	0
35	MG	0	8016	1/1	0.85	0.38	-	131,131,131,131	0
40	CD	O	8705	1/1	0.89	0.05	-	111,111,111,111	0
37	SR	0	8936	1/1	0.95	0.18	-	67,67,67,67	0
35	MG	0	8035	1/1	0.86	0.14	-	84,84,84,84	0
37	SR	0	8934	1/1	0.98	0.17	-	71,71,71,71	0
35	MG	0	8072	1/1	0.88	0.17	-	55,55,55,55	0
38	CL	0	8813	1/1	0.93	0.09	-	63,63,63,63	0
37	SR	3	8953	1/1	0.98	0.16	-	110,110,110,110	0
36	NA	0	8570	1/1	0.94	0.15	-	48,48,48,48	0
37	SR	0	8906	1/1	0.99	0.21	-	56,56,56,56	0
37	SR	Y	9002	1/1	0.91	0.11	-	124,124,124,124	0
37	SR	3	8999	1/1	1.00	0.13	-	69,69,69,69	0
35	MG	0	8005	1/1	0.94	0.25	-	25,25,25,25	0
37	SR	0	8926	1/1	0.95	0.17	-	87,87,87,87	0
37	SR	1	8952	1/1	0.98	0.20	-	67,67,67,67	0
38	CL	L	8814	1/1	0.96	0.13	-	62,62,62,62	0
36	NA	0	8548	1/1	0.99	0.17	-	26,26,26,26	0
35	MG	0	8018	1/1	1.00	0.26	-	3,3,3,3	0
37	SR	0	8986	1/1	0.91	0.10	-	108,108,108,108	0
37	SR	0	8983	1/1	0.53	0.22	-	169,169,169,169	0
35	MG	0	8031	1/1	0.97	0.05	-	41,41,41,41	0
36	NA	R	8532	1/1	0.89	0.12	-	25,25,25,25	0
36	NA	9	8543	1/1	0.66	0.16	-	65,65,65,65	0
37	SR	0	8961	1/1	-0.02	0.13	-	185,185,185,185	0
37	SR	B	8950	1/1	0.96	0.17	-	98,98,98,98	0
37	SR	0	8965	1/1	0.95	0.13	-	95,95,95,95	0
37	SR	0	8927	1/1	0.98	0.19	-	70,70,70,70	0
37	SR	0	8998	1/1	0.68	0.22	-	113,113,113,113	0
37	SR	F	9005	1/1	0.97	0.10	-	98,98,98,98	0
37	SR	0	8954	1/1	0.98	0.16	-	82,82,82,82	0
37	SR	0	9006	1/1	0.89	0.75	-	198,198,198,198	0
35	MG	0	8070	1/1	0.80	0.23	-	63,63,63,63	0
35	MG	0	8058	1/1	0.99	0.20	-	1,1,1,1	0
37	SR	T	8939	1/1	0.99	0.14	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	9	9003	1/1	0.92	0.04	-	144,144,144,144	0
36	NA	0	8573	1/1	0.46	0.20	-	79,79,79,79	0
37	SR	0	8928	1/1	0.91	0.11	-	92,92,92,92	0
35	MG	0	8065	1/1	0.87	0.39	-	102,102,102,102	0
35	MG	0	8022	1/1	0.99	0.21	-	11,11,11,11	0
37	SR	0	8988	1/1	0.96	0.10	-	114,114,114,114	0
37	SR	0	8940	1/1	0.98	0.17	-	51,51,51,51	0
37	SR	0	8996	1/1	0.80	0.13	-	158,158,158,158	0
36	NA	0	8536	1/1	0.88	0.18	-	63,63,63,63	0
37	SR	0	8923	1/1	0.94	0.21	-	72,72,72,72	0
35	MG	0	8077	1/1	0.92	0.19	-	41,41,41,41	0
38	CL	0	8822	1/1	0.88	0.34	-	66,66,66,66	0
35	MG	0	8038	1/1	0.68	0.24	-	97,97,97,97	0
37	SR	9	8980	1/1	0.87	0.07	-	132,132,132,132	0
37	SR	0	9007	1/1	0.80	0.59	-	195,195,195,195	0
37	SR	0	8931	1/1	1.00	0.20	-	80,80,80,80	0
37	SR	0	8990	1/1	0.93	0.55	-	177,177,177,177	0
35	MG	0	8083	1/1	0.99	0.11	-	29,29,29,29	0
37	SR	0	8951	1/1	0.98	0.09	-	105,105,105,105	0
38	CL	J	8801	1/1	0.93	0.13	-	62,62,62,62	0
37	SR	H	8907	1/1	0.99	0.14	-	48,48,48,48	0
37	SR	9	8968	1/1	0.78	0.10	-	117,117,117,117	0
36	NA	0	8505	1/1	0.99	0.54	-	29,29,29,29	0
35	MG	0	8019	1/1	0.99	0.16	-	1,1,1,1	0
36	NA	0	8561	1/1	0.98	0.19	-	66,66,66,66	0
36	NA	0	8526	1/1	0.69	0.10	-	55,55,55,55	0
36	NA	0	8509	1/1	0.91	0.34	-	80,80,80,80	0
35	MG	0	8069	1/1	0.93	0.17	-	120,120,120,120	0
37	SR	0	8903	1/1	0.98	0.21	-	55,55,55,55	0
35	MG	0	8055	1/1	0.99	0.27	-	26,26,26,26	0
38	CL	0	8803	1/1	0.91	0.07	-	51,51,51,51	0
35	MG	0	8067	1/1	0.99	0.33	-	33,33,33,33	0
35	MG	0	8091	1/1	0.90	0.11	-	76,76,76,76	0
37	SR	0	8997	1/1	0.97	0.04	-	116,116,116,116	0
37	SR	0	8967	1/1	0.92	0.07	-	103,103,103,103	0
37	SR	0	8979	1/1	0.82	1.99	-	184,184,184,184	0
35	MG	0	8037	1/1	0.94	0.16	-	64,64,64,64	0
35	MG	0	8048	1/1	0.98	0.26	-	49,49,49,49	0
35	MG	0	8092	1/1	0.81	0.70	-	76,76,76,76	0
37	SR	0	8966	1/1	0.96	0.15	-	85,85,85,85	0
37	SR	0	8955	1/1	0.90	0.08	-	127,127,127,127	0
37	SR	0	8994	1/1	-0.13	0.79	-	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
35	MG	0	8053	1/1	0.94	0.15	-	33,33,33,33	0
35	MG	0	8090	1/1	0.56	0.59	-	130,130,130,130	0
37	SR	0	8942	1/1	0.88	0.31	-	155,155,155,155	0
35	MG	0	8093	1/1	0.96	0.07	-	27,27,27,27	0
38	CL	0	8815	1/1	0.90	0.09	-	69,69,69,69	0
37	SR	0	8920	1/1	0.55	0.92	-	200,200,200,200	0
36	NA	0	8549	1/1	0.85	0.16	-	36,36,36,36	0
35	MG	0	8017	1/1	0.38	0.22	-	123,123,123,123	0
37	SR	0	8971	1/1	0.53	0.13	-	191,191,191,191	0
36	NA	0	8525	1/1	0.79	0.18	-	53,53,53,53	0
35	MG	0	8026	1/1	0.96	0.11	-	43,43,43,43	0
37	SR	0	8901	1/1	0.92	0.19	-	48,48,48,48	0
37	SR	0	9004	1/1	0.88	0.18	-	121,121,121,121	0
35	MG	0	8063	1/1	0.72	0.28	-	69,69,69,69	0
38	CL	Y	8817	1/1	0.80	0.13	-	55,55,55,55	0
37	SR	0	8921	1/1	0.98	0.14	-	58,58,58,58	0
35	MG	0	8078	1/1	0.13	0.41	-	115,115,115,115	0
35	MG	0	8030	1/1	0.72	0.25	-	167,167,167,167	0
38	CL	Q	8811	1/1	0.78	0.24	-	86,86,86,86	0
37	SR	0	8958	1/1	0.99	0.15	-	77,77,77,77	0
37	SR	0	8956	1/1	0.95	0.16	-	111,111,111,111	0
35	MG	0	8033	1/1	0.95	0.11	-	44,44,44,44	0
36	NA	0	8529	1/1	0.90	0.08	-	24,24,24,24	0
34	PHE	6	77	11/12	0.86	0.34	-	88,88,90,90	0
36	NA	0	8554	1/1	0.93	0.25	-	42,42,42,42	0
36	NA	9	8544	1/1	0.71	0.54	-	73,73,73,73	0
35	MG	0	8059	1/1	0.84	0.16	-	88,88,88,88	0
36	NA	0	8531	1/1	0.98	0.15	-	41,41,41,41	0
38	CL	N	8807	1/1	0.92	0.07	-	70,70,70,70	0
36	NA	0	8511	1/1	0.62	0.18	-	35,35,35,35	0
37	SR	0	8924	1/1	0.99	0.23	-	80,80,80,80	0
35	MG	0	8036	1/1	0.93	0.16	-	50,50,50,50	0
35	MG	0	8068	1/1	0.99	0.13	-	50,50,50,50	0
36	NA	0	8566	1/1	0.87	0.35	-	54,54,54,54	0
37	SR	0	8919	1/1	0.96	0.15	-	92,92,92,92	0
35	MG	0	8082	1/1	0.98	0.14	-	70,70,70,70	0
37	SR	A	8930	1/1	0.97	0.16	-	78,78,78,78	0
37	SR	0	8973	1/1	0.93	0.12	-	98,98,98,98	0
37	SR	0	8989	1/1	0.06	0.29	-	200,200,200,200	0
35	MG	0	8039	1/1	0.90	0.23	-	40,40,40,40	0
37	SR	0	8982	1/1	0.92	0.09	-	116,116,116,116	0
37	SR	0	8925	1/1	0.99	0.17	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	MG	0	8040	1/1	0.62	0.34	-	70,70,70,70	0
35	MG	0	8085	1/1	0.72	0.71	-	92,92,92,92	0
35	MG	0	8073	1/1	0.94	0.13	-	58,58,58,58	0
37	SR	0	8984	1/1	0.96	0.15	-	92,92,92,92	0
35	MG	0	8045	1/1	0.89	0.64	-	119,119,119,119	0
36	NA	0	8574	1/1	0.97	0.35	-	43,43,43,43	0
36	NA	0	8571	1/1	0.78	0.41	-	85,85,85,85	0
38	CL	J	8802	1/1	0.99	0.12	-	69,69,69,69	0
37	SR	0	8909	1/1	0.99	0.16	-	56,56,56,56	0
35	MG	0	8046	1/1	0.93	0.44	-	72,72,72,72	0
35	MG	0	8081	1/1	0.80	0.55	-	91,91,91,91	0
37	SR	0	8946	1/1	0.96	0.20	-	98,98,98,98	0
35	MG	0	8020	1/1	0.96	0.20	-	24,24,24,24	0
37	SR	0	8974	1/1	0.99	0.23	-	125,125,125,125	0
35	MG	0	8023	1/1	0.92	0.23	-	25,25,25,25	0
37	SR	T	8911	1/1	0.98	0.12	-	58,58,58,58	0
35	MG	B	8042	1/1	0.61	0.19	-	103,103,103,103	0
36	NA	0	8555	1/1	0.94	0.39	-	52,52,52,52	0
37	SR	0	8916	1/1	0.96	0.14	-	64,64,64,64	0
37	SR	0	8917	1/1	0.99	0.17	-	67,67,67,67	0
37	SR	0	8918	1/1	0.98	0.19	-	53,53,53,53	0
37	SR	0	8976	1/1	0.85	0.23	-	117,117,117,117	0
37	SR	0	8914	1/1	0.95	0.27	-	88,88,88,88	0
35	MG	2	8060	1/1	0.68	0.21	-	45,45,45,45	0
35	MG	0	8080	1/1	0.93	0.09	-	45,45,45,45	0
37	SR	0	8944	1/1	0.64	0.17	-	155,155,155,155	0
36	NA	0	8558	1/1	0.93	0.91	-	67,67,67,67	0
37	SR	0	8960	1/1	0.99	0.08	-	98,98,98,98	0
36	NA	H	8518	1/1	0.97	0.29	-	69,69,69,69	0
37	SR	0	8978	1/1	0.98	0.17	-	71,71,71,71	0
37	SR	0	9008	1/1	0.96	0.21	-	90,90,90,90	0
37	SR	0	8959	1/1	0.69	0.06	-	120,120,120,120	0
36	NA	0	8551	1/1	0.90	0.10	-	32,32,32,32	0
35	MG	0	8066	1/1	0.68	0.80	-	98,98,98,98	0
36	NA	0	8541	1/1	0.63	0.20	-	103,103,103,103	0
37	SR	0	8941	1/1	0.99	0.22	-	77,77,77,77	0
38	CL	R	8806	1/1	0.97	0.09	-	44,44,44,44	0
34	ACA	6	78	8/9	0.62	0.52	-	88,90,91,91	0
36	NA	0	8516	1/1	0.80	0.54	-	65,65,65,65	0
37	SR	0	9000	1/1	0.84	0.27	-	147,147,147,147	0
37	SR	0	8915	1/1	0.95	0.14	-	84,84,84,84	0
37	SR	0	8993	1/1	0.86	0.04	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	8902	1/1	0.99	0.19	-	39,39,39,39	0
36	NA	0	8546	1/1	0.94	0.78	-	97,97,97,97	0
36	NA	0	8501	1/1	0.95	0.16	-	107,107,107,107	0
38	CL	A	8809	1/1	0.95	0.14	-	51,51,51,51	0
37	SR	A	8977	1/1	0.96	0.16	-	95,95,95,95	0
36	NA	0	8514	1/1	0.69	0.24	-	83,83,83,83	0
37	SR	0	8938	1/1	0.97	0.11	-	95,95,95,95	0
38	CL	Y	8820	1/1	0.94	0.06	-	48,48,48,48	0
37	SR	0	8905	1/1	0.93	0.25	-	61,61,61,61	0
35	MG	0	8056	1/1	0.90	0.38	-	94,94,94,94	0
35	MG	0	8024	1/1	0.96	0.37	-	69,69,69,69	0
37	SR	0	8908	1/1	0.99	0.16	-	64,64,64,64	0
36	NA	S	8510	1/1	0.80	0.65	-	80,80,80,80	0
37	SR	0	8933	1/1	0.86	0.30	-	126,126,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.