



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:28 PM GMT

PDB ID : 1JJ2  
Title : Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution  
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2001-07-03  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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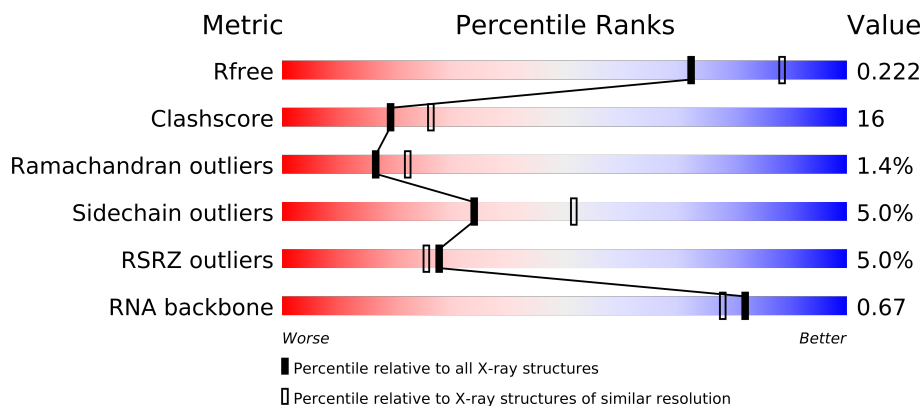
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	A	239	
4	B	337	
5	C	246	
6	D	176	
7	E	177	
8	F	119	
9	G	348	
10	H	167	
11	I	145	

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	MG	0	8007	-	X
31	MG	0	8012	-	X
31	MG	0	8042	-	X
31	MG	0	8060	-	X
31	MG	0	8066	-	X
31	MG	0	8082	-	X
31	MG	0	8087	-	X
31	MG	0	8090	-	X
31	MG	0	8099	-	X
31	MG	0	8101	-	X
31	MG	0	8103	-	X
31	MG	0	8117	-	X
33	NA	0	8302	-	X
33	NA	0	8307	-	X
33	NA	0	8314	-	X
33	NA	0	8318	-	X
33	NA	0	8320	-	X
33	NA	0	8325	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	NA	0	8326	-	X
33	NA	0	8327	-	X
33	NA	0	8329	-	X
33	NA	0	8331	-	X
33	NA	0	8340	-	X
33	NA	0	8350	-	X
33	NA	0	8355	-	X
33	NA	0	8358	-	X
33	NA	0	8359	-	X
33	NA	0	8360	-	X
33	NA	0	8361	-	X
33	NA	0	8362	-	X
33	NA	0	8363	-	X
33	NA	0	8364	-	X
33	NA	0	8366	-	X
33	NA	0	8367	-	X
33	NA	0	8369	-	X
33	NA	0	8370	-	X
33	NA	0	8371	-	X
33	NA	0	8372	-	X
33	NA	0	8373	-	X
33	NA	0	8374	-	X
33	NA	0	8376	-	X
33	NA	0	8377	-	X
33	NA	0	8379	-	X
33	NA	0	8384	-	X
33	NA	0	8385	-	X
33	NA	9	8383	-	X
33	NA	K	8380	-	X
33	NA	Q	8386	-	X
34	CL	0	8522	-	X

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98543 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.



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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	109	Total Mg 109 109	0	0
31	J	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	A	2	Total Mg 2 2	0	0
31	X	1	Total Mg 1 1	0	0
31	2	1	Total Mg 1 1	0	0
31	9	1	Total Mg 1 1	0	0
31	S	1	Total Mg 1 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	72	Total Na 72 72	0	0
33	P	1	Total Na 1 1	0	0
33	Q	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	H	2	Total Na 2 2	0	0
33	I	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	A	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	2	Total 2	Na 2	0	0
33	L	1	Total 1	Na 1	0	0
33	S	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	10	Total 10	Cl 10	0	0
34	Q	1	Total 1	Cl 1	0	0
34	K	1	Total 1	Cl 1	0	0
34	B	1	Total 1	Cl 1	0	0
34	I	3	Total 3	Cl 3	0	0
34	A	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	2	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total 1	Cd 1	0	0
35	Y	1	Total 1	Cd 1	0	0
35	T	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	2	1	Total	Cd	0	0
			1	1		
35	N	1	Total	Cd	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	5938	Total	O	0	0
			5938	5938		
36	9	135	Total	O	0	0
			135	135		
36	A	126	Total	O	0	0
			126	126		
36	B	150	Total	O	0	0
			150	150		
36	C	172	Total	O	0	0
			172	172		
36	D	53	Total	O	0	0
			53	53		
36	E	46	Total	O	0	0
			46	46		
36	F	28	Total	O	0	0
			28	28		
36	G	21	Total	O	0	0
			21	21		
36	H	74	Total	O	0	0
			74	74		
36	I	56	Total	O	0	0
			56	56		
36	J	62	Total	O	0	0
			62	62		
36	K	80	Total	O	0	0
			80	80		
36	L	127	Total	O	0	0
			127	127		
36	M	70	Total	O	0	0
			70	70		
36	N	43	Total	O	0	0
			43	43		
36	O	68	Total	O	0	0
			68	68		

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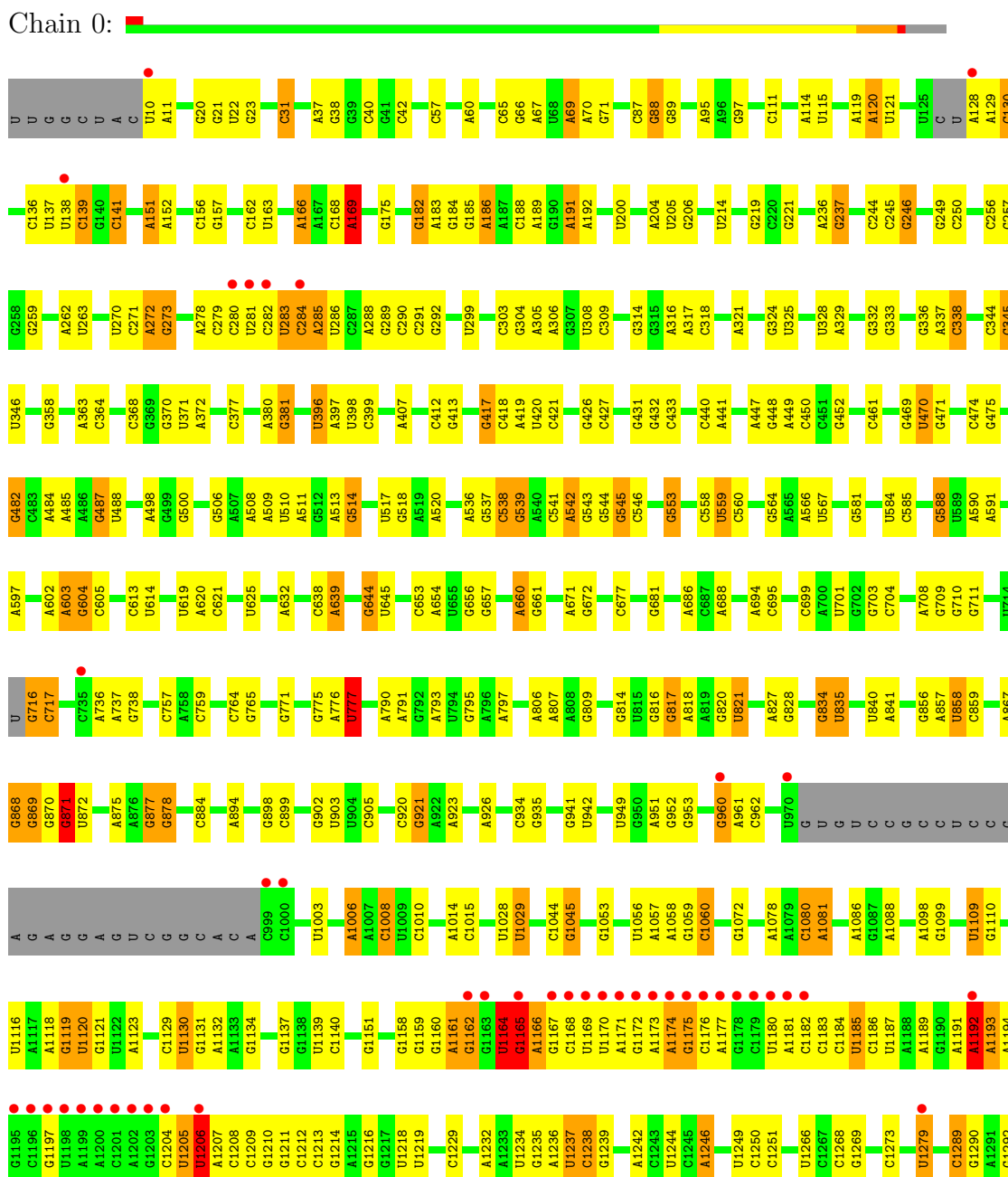
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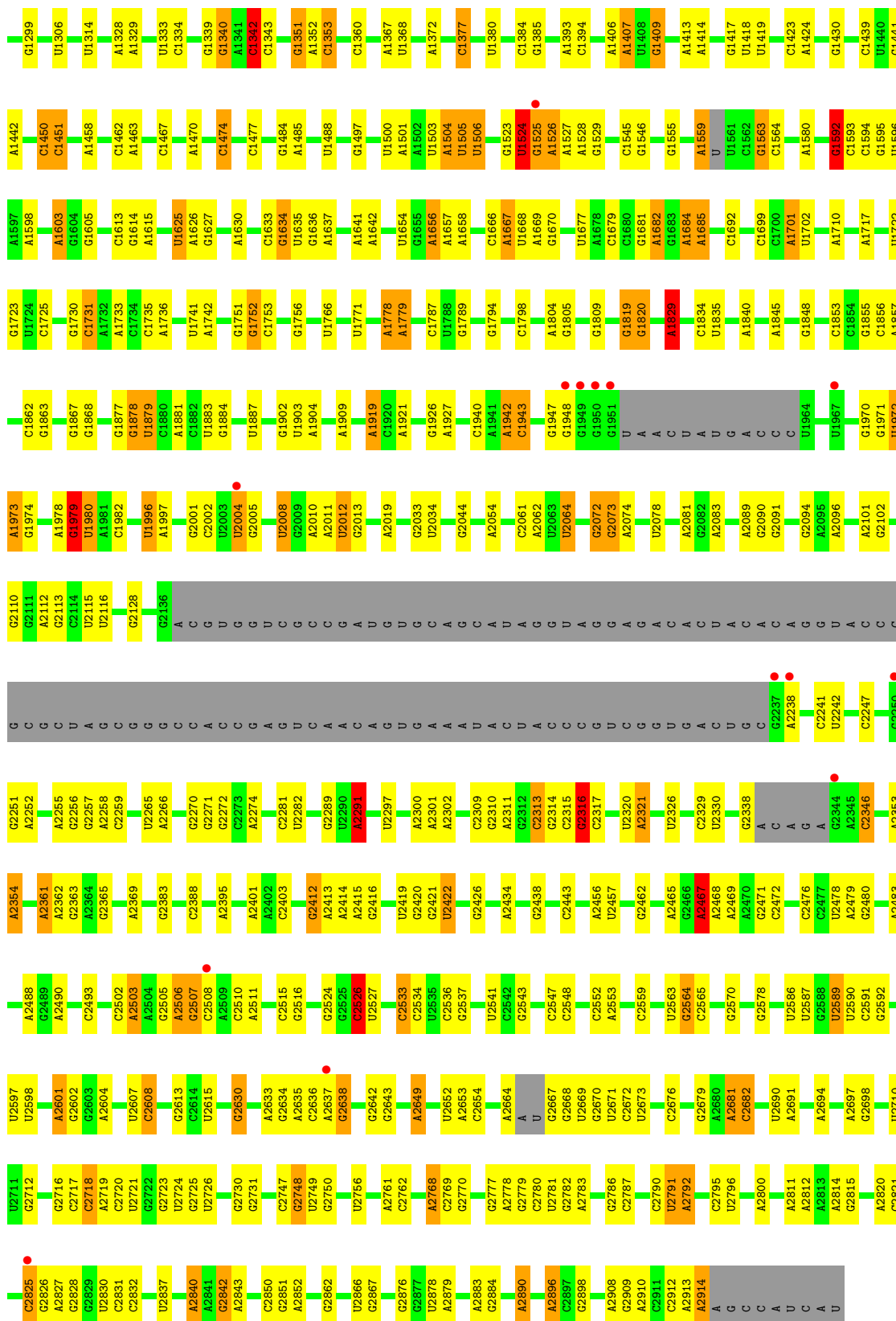
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36	P	53	Total 53	O 53	0	0
36	Q	81	Total 81	O 81	0	0
36	R	32	Total 32	O 32	0	0
36	S	39	Total 39	O 39	0	0
36	T	25	Total 25	O 25	0	0
36	U	15	Total 15	O 15	0	0
36	V	67	Total 67	O 67	0	0
36	W	29	Total 29	O 29	0	0
36	X	99	Total 99	O 99	0	0
36	Y	39	Total 39	O 39	0	0
36	Z	53	Total 53	O 53	0	0
36	1	40	Total 40	O 40	0	0
36	2	72	Total 72	O 72	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.

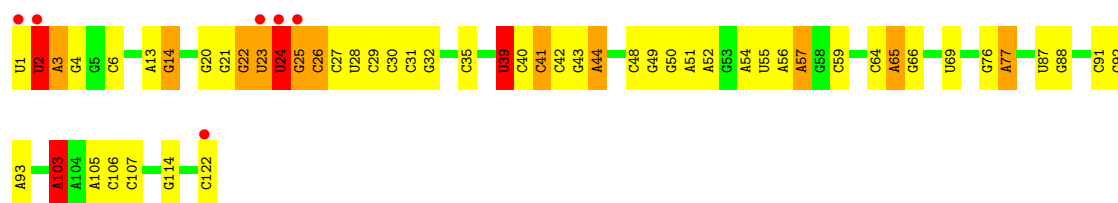
#### • Molecule 1: 23S rRNA





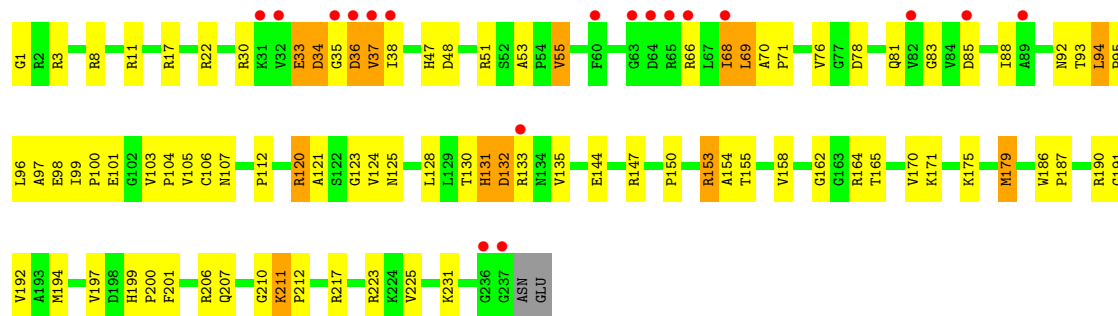
- Molecule 2: 5S rRNA

Chain 9: 



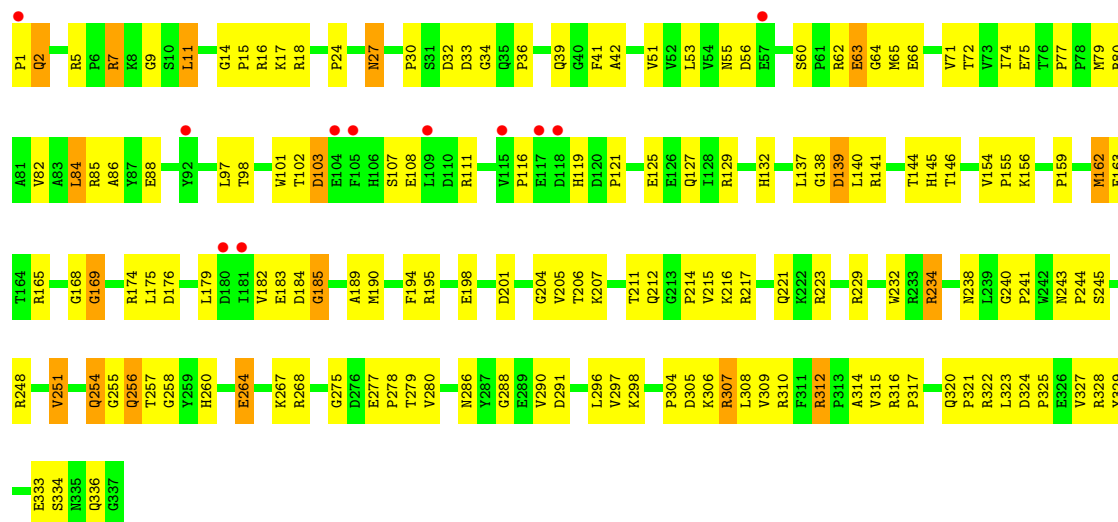
• Molecule 3: RIBOSOMAL PROTEIN L2

Chain A:



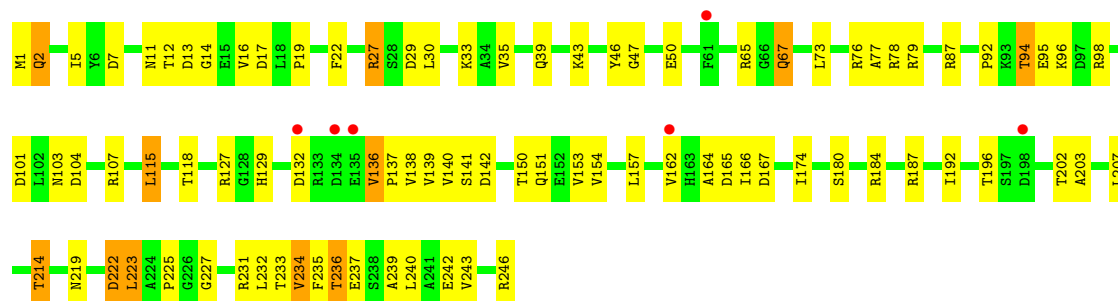
• Molecule 4: RIBOSOMAL PROTEIN L3

Chain B:



• Molecule 5: RIBOSOMAL PROTEIN L4

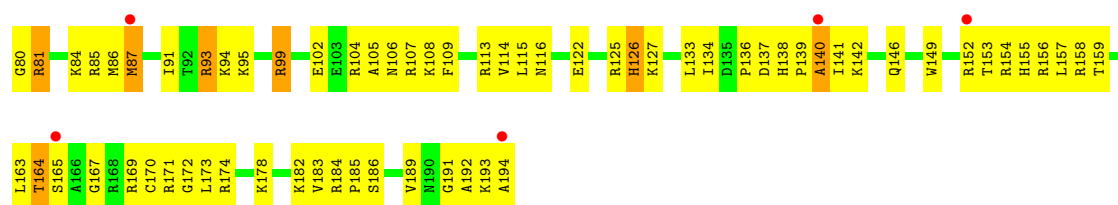
Chain C:





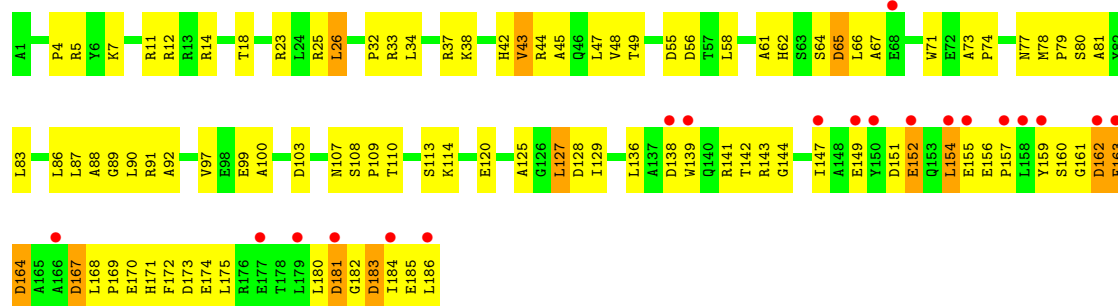






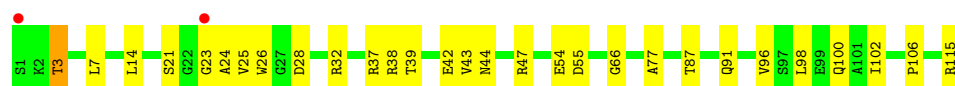
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain M:



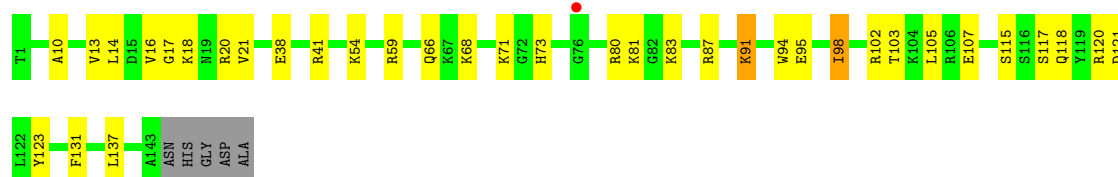
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain N:



• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain O:



• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain P:



• Molecule 19: RIBOSOMAL PROTEIN L22

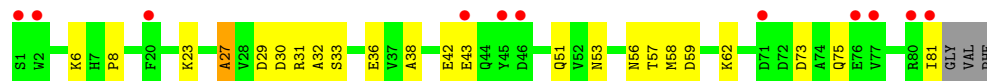
Chain Q:





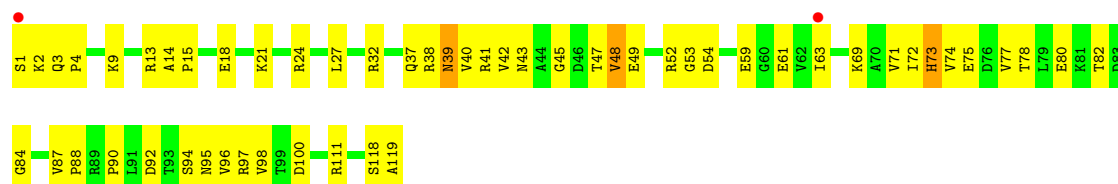
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain R:



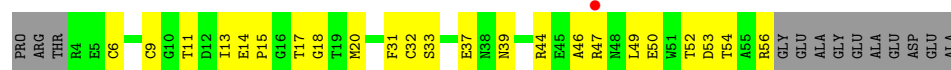
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain S:



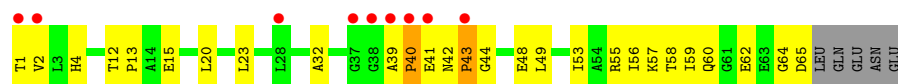
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain T:



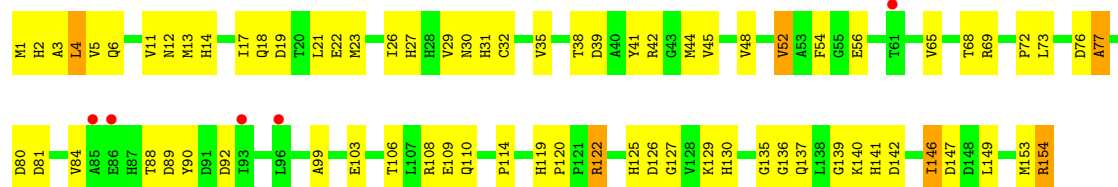
• Molecule 23: RIBOSOMAL PROTEIN L29

Chain U:



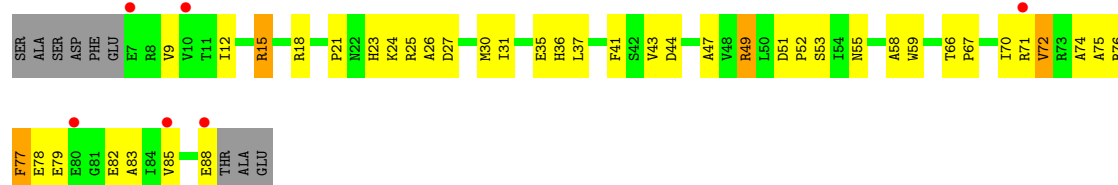
• Molecule 24: RIBOSOMAL PROTEIN L30

Chain V:



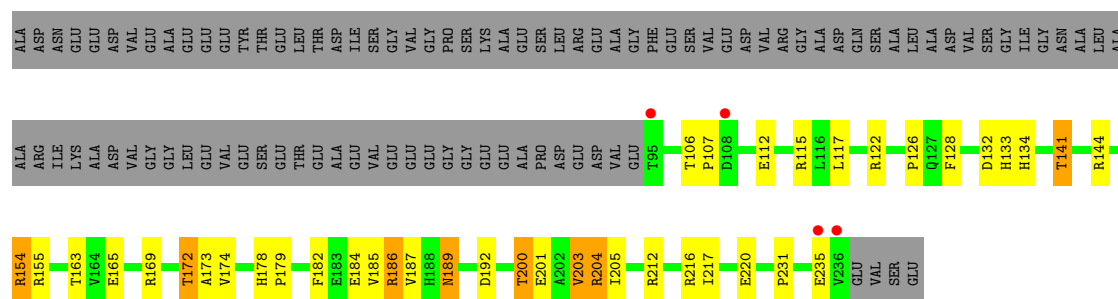
• Molecule 25: RIBOSOMAL PROTEIN L31E

Chain W:



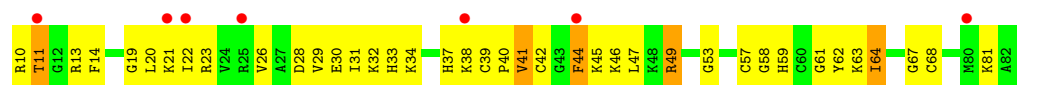
- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain X:



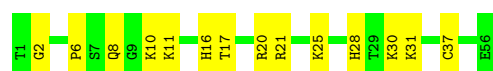
- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain Y:



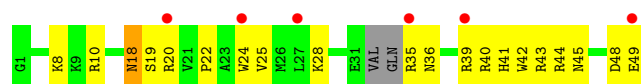
- Molecule 28: RIBOSOMAL PROTEIN L37E

Chain Z:



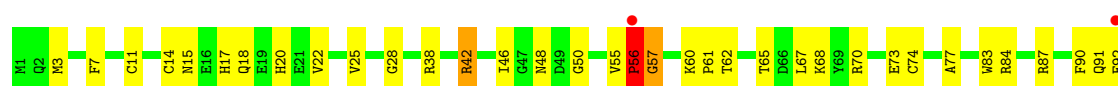
- Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 1:



- Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 2:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (15.00-2.40) 90.7 (85.48-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.189 , 0.222 0.191 , 0.222	Depositor DCC
$R_{free}$ test set	6222 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 666819 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	98543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.38	3/66076 (0.0%)	0.71	32/103052 (0.0%)
2	9	0.44	3/2905 (0.1%)	0.85	11/4528 (0.2%)
3	A	0.34	0/1787	0.66	0/2409
4	B	0.34	0/2689	0.64	0/3652
5	C	0.39	0/1883	0.67	0/2551
6	D	0.31	0/1111	0.59	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.33	0/896	0.56	0/1219
9	G	0.25	0/241	0.47	0/324
10	H	0.38	0/1246	0.74	1/1686 (0.1%)
11	I	0.33	0/1135	0.61	0/1530
12	J	0.33	0/1003	0.65	0/1351
13	K	0.34	0/1126	0.68	0/1504
14	L	0.41	0/1633	0.71	1/2180 (0.0%)
15	M	0.29	0/1473	0.64	0/1999
16	N	0.32	0/873	0.61	1/1181 (0.1%)
17	O	0.33	0/1143	0.54	0/1521
18	P	0.35	0/748	0.68	0/1005
19	Q	0.35	0/1172	0.67	0/1578
20	R	0.32	0/648	0.59	1/875 (0.1%)
21	S	0.31	0/957	0.63	0/1289
22	T	0.32	0/417	0.58	0/562
23	U	0.29	0/502	0.54	0/675
24	V	0.33	0/1218	0.62	0/1655
25	W	0.32	0/664	0.60	0/895
26	X	0.34	0/1146	0.63	0/1536
27	Y	0.37	0/575	0.69	0/763
28	Z	0.42	0/437	0.67	0/578
29	1	0.34	0/398	0.54	0/527
30	2	0.38	0/771	0.62	0/1024
All	All	0.37	6/98255 (0.0%)	0.70	47/147027 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	62
2	9	0	2
All	All	1	64

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9	3	A	C2'-O2'	-7.92	1.31	1.41
1	0	1206	U	P-OP2	6.22	1.59	1.49
2	9	3	A	O5'-C5'	6.21	1.54	1.44
1	0	1206	U	C3'-O3'	-5.28	1.34	1.42
1	0	1205	U	C3'-O3'	-5.23	1.34	1.42
2	9	3	A	C5'-C4'	-5.13	1.45	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	O5'-P-OP1	-22.95	83.17	110.70
1	0	1164	U	OP1-P-O3'	-20.79	59.47	105.20
1	0	1165	G	O5'-P-OP2	-15.10	92.11	105.70
2	9	3	A	OP1-P-O3'	-13.36	75.82	105.20
1	0	1164	U	OP2-P-O3'	-13.28	75.98	105.20
2	9	3	A	C5'-C4'-C3'	-11.15	98.16	116.00
2	9	2	U	OP2-P-O3'	-10.56	81.96	105.20
1	0	1563	G	C2'-C3'-O3'	9.58	130.57	109.50
1	0	1942	A	C5'-C4'-C3'	8.93	130.28	116.00
2	9	24	U	C2'-C3'-O3'	8.93	129.14	109.50
1	0	871	G	C5'-C4'-O4'	-8.42	99.00	109.10
1	0	1979	G	C2'-C3'-O3'	8.18	127.49	109.50
2	9	2	U	OP1-P-O3'	7.93	122.65	105.20
1	0	1819	G	C5'-C4'-C3'	7.14	127.43	116.00
2	9	39	U	N1-C1'-C2'	7.07	123.19	114.00
2	9	3	A	OP2-P-O3'	7.00	120.61	105.20
1	0	1206	U	C5'-C4'-C3'	-6.94	104.89	116.00
2	9	103	A	C5'-C4'-O4'	6.87	117.34	109.10
1	0	2316	G	C5'-C4'-C3'	-6.84	105.06	116.00
1	0	1942	A	C5'-C4'-O4'	6.80	117.26	109.10
1	0	1504	A	C1'-O4'-C4'	-6.55	104.66	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2467	A	C1'-O4'-C4'	-6.40	104.78	109.90
1	0	206	G	C5'-C4'-C3'	-6.37	105.81	116.00
1	0	2291	A	N9-C1'-C2'	6.26	122.14	114.00
1	0	1504	A	N9-C1'-C2'	6.21	122.08	114.00
1	0	1559	A	C2'-C3'-O3'	5.91	123.16	113.70
10	H	74	ASN	N-CA-C	-5.82	95.28	111.00
1	0	1942	A	C1'-O4'-C4'	-5.80	105.26	109.90
1	0	1942	A	C4'-C3'-C2'	-5.79	96.81	102.60
1	0	777	U	O4'-C1'-N1	5.70	112.76	108.20
1	0	1164	U	O3'-P-O5'	5.68	114.78	104.00
1	0	1205	U	C4'-C3'-O3'	-5.61	97.63	109.40
1	0	169	A	C5'-C4'-O4'	-5.54	102.46	109.10
1	0	1120	U	C5'-C4'-C3'	-5.52	107.17	116.00
1	0	1829	A	N9-C1'-C2'	-5.47	105.98	112.00
14	L	126	HIS	CB-CA-C	-5.44	99.53	110.40
2	9	103	A	C4'-C3'-C2'	-5.38	97.22	102.60
1	0	2313	C	C5'-C4'-O4'	5.31	115.47	109.10
1	0	1819	G	C4'-C3'-C2'	-5.30	97.30	102.60
1	0	1592	G	N9-C1'-C2'	5.27	120.85	114.00
1	0	841	A	C1'-O4'-C4'	-5.21	105.73	109.90
2	9	103	A	C1'-O4'-C4'	-5.15	105.78	109.90
2	9	24	U	C4'-C3'-C2'	5.11	107.71	102.60
1	0	1165	G	OP1-P-OP2	5.11	127.26	119.60
16	N	66	GLY	N-CA-C	5.04	125.70	113.10
20	R	27	ALA	N-CA-C	-5.03	97.41	111.00
1	0	1563	G	C4'-C3'-O3'	5.01	123.03	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1164	U	Sidechain
1	0	1192	A	Sidechain
1	0	1292	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1501	A	Sidechain
1	0	1524	U	Sidechain
1	0	1794	G	Sidechain
1	0	1809	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2012	U	Sidechain
1	0	2078	U	Sidechain
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2395	A	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2543	G	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2615	U	Sidechain
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	332	G	Sidechain
1	0	333	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	396	U	Sidechain
1	0	452	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	639	A	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
2	9	39	U	Sidechain
2	9	87	U	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29807	760	0
2	9	2600	0	1326	78	0
3	A	1754	0	1763	109	0
4	B	2624	0	2533	176	0
5	C	1858	0	1816	105	0
6	D	1094	0	1085	130	0
7	E	1357	0	1266	79	0
8	F	885	0	854	59	0
9	G	240	0	231	18	0
10	H	1215	0	1215	150	0
11	I	1119	0	1098	62	0
12	J	993	0	1027	56	0
13	K	1114	0	1072	55	0
14	L	1605	0	1676	141	0
15	M	1444	0	1401	119	0
16	N	864	0	873	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	1133	0	1127	38	0
18	P	734	0	728	18	0
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	949	0	923	52	0
22	T	410	0	364	31	0
23	U	499	0	511	28	0
24	V	1195	0	1137	91	0
25	W	654	0	653	44	0
26	X	1130	0	1133	52	0
27	Y	563	0	597	53	0
28	Z	430	0	426	22	0
29	1	393	0	406	32	0
30	2	755	0	728	36	0
31	0	109	0	0	0	0
31	2	1	0	0	0	0
31	9	1	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	S	1	0	0	0	0
31	X	1	0	0	0	0
32	0	2	0	0	0	0
33	0	72	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	2	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	2	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	I	3	0	0	1	0
34	K	1	0	0	0	0
34	L	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	2	1	0	0	0	0
35	N	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	5938	0	0	173	0
36	1	40	0	0	6	0
36	2	72	0	0	10	0
36	9	135	0	0	14	0
36	A	126	0	0	20	0
36	B	150	0	0	30	0
36	C	172	0	0	30	0
36	D	53	0	0	18	0
36	E	46	0	0	12	0
36	F	28	0	0	7	0
36	G	21	0	0	4	0
36	H	74	0	0	21	0
36	I	56	0	0	5	0
36	J	62	0	0	13	0
36	K	80	0	0	17	0
36	L	127	0	0	19	0
36	M	70	0	0	16	0
36	N	43	0	0	6	0
36	O	68	0	0	1	0
36	P	53	0	0	1	0
36	Q	81	0	0	9	0
36	R	32	0	0	5	0
36	S	39	0	0	5	0
36	T	25	0	0	6	0
36	U	15	0	0	4	0
36	V	67	0	0	10	0
36	W	29	0	0	3	0
36	X	99	0	0	15	0
36	Y	39	0	0	12	0
36	Z	53	0	0	1	0
All	All	98543	0	59503	2453	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (2453) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.14
10:H:86:ARG:NH1	10:H:133:ILE:HG13	1.62	1.12
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.35	1.07
25:W:37:LEU:HD13	25:W:85:VAL:HG21	1.29	1.06
1:0:960:G:H4'	36:0:6956:HOH:O	1.54	1.06
5:C:236:THR:HG22	5:C:239:ALA:H	1.02	1.06
1:0:1134:G:H4'	10:H:151:MET:HE1	1.34	1.05
21:S:71:VAL:HG11	21:S:90:PRO:HB3	1.39	1.03
2:9:23:U:H4'	2:9:24:U:OP2	1.54	1.02
10:H:162:SER:HB2	10:H:163:PRO:HD3	1.37	1.02
23:U:12:THR:HG22	23:U:15:GLU:HG3	1.40	1.02
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.39	1.02
1:0:156:C:H5''	14:L:171:ARG:HD3	1.39	1.01
1:0:1242:A:H5'	11:I:82:THR:HG23	1.42	1.01
1:0:871:G:C8	1:0:871:G:H5'	1.94	1.01
14:L:164:THR:HG22	14:L:167:GLY:H	1.23	1.00
1:0:1751:G:H2'	1:0:1752:G:H5''	1.43	1.00
10:H:26:LYS:HD2	10:H:28:ILE:HD12	1.41	1.00
10:H:45:GLN:HB3	10:H:163:PRO:HD2	1.38	1.00
1:0:21:G:H5'	19:Q:2:ILE:HA	1.45	0.99
2:9:6:C:H5''	15:M:37:ARG:NH1	1.78	0.99
1:0:856:G:H2'	36:0:4940:HOH:O	1.61	0.99
2:9:56:A:H2'	2:9:57:A:H5''	1.45	0.99
10:H:86:ARG:HH11	10:H:133:ILE:HG13	0.84	0.99
27:Y:10:ARG:HA	36:Y:8415:HOH:O	1.62	0.98
10:H:86:ARG:HH11	10:H:133:ILE:CG1	1.77	0.98
12:J:81:ARG:HB2	12:J:87:ARG:HH11	1.24	0.98
2:9:76:G:H3'	2:9:77:A:H5''	1.46	0.98
17:O:115:SER:H	17:O:118:GLN:HE21	1.02	0.97
12:J:10:GLN:NE2	12:J:10:GLN:H	1.60	0.97
12:J:39:GLY:HA2	36:J:4183:HOH:O	1.63	0.97
1:0:870:G:H2'	1:0:871:G:H5''	1.46	0.97
2:9:3:A:O5'	2:9:3:A:H2'	1.62	0.97
4:B:140:LEU:HA	36:B:8583:HOH:O	1.63	0.95
27:Y:38:LYS:HE2	27:Y:45:LYS:HE2	1.46	0.95
24:V:88:THR:HB	36:V:6679:HOH:O	1.66	0.95
2:9:6:C:H5''	15:M:37:ARG:HH12	1.32	0.95
14:L:102:GLU:OE1	14:L:164:THR:HG21	1.67	0.95
11:I:76:ASP:HA	36:I:5907:HOH:O	1.67	0.95
12:J:29:LEU:HB3	12:J:55:VAL:HG11	1.46	0.95
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.49	0.94
14:L:52:LEU:HD11	36:L:8616:HOH:O	1.65	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:83:LEU:HD13	15:M:175:LEU:HD23	1.48	0.94
26:X:200:THR:HG22	26:X:201:GLU:HG3	1.50	0.93
6:D:154:LYS:HD2	6:D:154:LYS:H	1.34	0.93
1:O:871:G:H8	1:O:871:G:H5'	1.30	0.93
24:V:88:THR:HG22	24:V:89:ASP:H	1.33	0.93
20:R:57:THR:HG22	20:R:59:ASP:H	1.34	0.92
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.85	0.92
24:V:137:GLN:HE21	24:V:141:HIS:HE1	1.12	0.92
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.50	0.92
5:C:236:THR:HG22	5:C:239:ALA:N	1.85	0.92
1:O:1835:U:H5	1:O:1840:A:N7	1.68	0.92
36:O:3976:HOH:O	14:L:146:GLN:HG2	1.69	0.91
14:L:106:ASN:ND2	34:L:8518:CL:CL	2.40	0.91
4:B:86:ALA:HA	36:B:8583:HOH:O	1.68	0.91
12:J:10:GLN:N	12:J:10:GLN:HE21	1.67	0.91
10:H:29:ALA:HB3	10:H:65:ARG:HH12	1.33	0.90
1:O:542:A:H5'	1:O:542:A:H8	1.35	0.90
15:M:47:LEU:HD11	15:M:127:LEU:HD21	1.52	0.89
15:M:144:GLY:O	15:M:147:ILE:HG22	1.70	0.89
15:M:23:ARG:HD3	36:M:8549:HOH:O	1.72	0.89
5:C:2:GLN:HB3	36:C:8335:HOH:O	1.73	0.89
36:O:4373:HOH:O	14:L:14:ARG:HG2	1.73	0.89
12:J:81:ARG:HB2	12:J:87:ARG:NH1	1.88	0.88
15:M:87:LEU:HD12	15:M:186:LEU:HD21	1.54	0.88
24:V:6:GLN:HB2	24:V:26:ILE:HD12	1.53	0.88
23:U:42:ASN:HB3	36:U:7247:HOH:O	1.74	0.88
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.53	0.88
3:A:199:HIS:HD2	3:A:201:PHE:H	1.20	0.88
1:O:1116:U:H3	1:O:1246:A:H62	1.20	0.87
1:O:645:U:OP2	13:K:4:LYS:HE2	1.73	0.87
24:V:88:THR:HG23	24:V:110:GLN:NE2	1.89	0.87
1:O:1164:U:H3	1:O:1192:A:H2	1.21	0.87
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.55	0.87
10:H:27:LYS:H	10:H:58:HIS:HD2	1.22	0.87
10:H:162:SER:HB2	10:H:163:PRO:CD	2.04	0.87
6:D:25:MET:HE2	6:D:41:LEU:HG	1.57	0.87
1:O:1701:A:H4'	1:O:1702:U:H5''	1.55	0.87
27:Y:38:LYS:HG2	27:Y:45:LYS:HG2	1.54	0.86
27:Y:46:LYS:HD3	27:Y:59:HIS:HB2	1.58	0.86
2:9:25:G:H3'	2:9:26:C:H5'	1.57	0.86
5:C:132:ASP:HB3	36:C:8365:HOH:O	1.75	0.86
1:O:1165:G:H4'	1:O:1174:A:O2'	1.75	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.39	0.86
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.56	0.85
2:9:23:U:H3'	36:9:8474:HOH:O	1.76	0.85
10:H:55:GLN:HE21	10:H:124:ARG:HE	1.22	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.20	0.85
1:0:2716:G:H5''	4:B:206:THR:HG21	1.59	0.85
5:C:236:THR:CG2	5:C:239:ALA:H	1.88	0.85
12:J:10:GLN:H	12:J:10:GLN:HE21	0.86	0.85
16:N:42:GLU:HB2	36:N:2176:HOH:O	1.74	0.85
1:0:1474:C:H6	1:0:1474:C:H5'	1.42	0.85
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.57	0.85
2:9:24:U:O2'	2:9:25:G:H4'	1.76	0.84
10:H:49:VAL:O	10:H:157:ILE:HG23	1.76	0.84
1:0:1329:A:H2	36:0:4193:HOH:O	1.60	0.84
1:0:381:G:H5''	36:0:3826:HOH:O	1.75	0.84
4:B:238:ASN:HD22	4:B:240:GLY:H	1.26	0.84
5:C:214:THR:HG21	36:C:8403:HOH:O	1.78	0.84
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.59	0.84
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.43	0.84
12:J:74:VAL:HG11	12:J:113:ILE:HG12	1.58	0.84
15:M:7:LYS:HE3	18:P:21:ARG:O	1.77	0.84
2:9:3:A:O5'	2:9:3:A:C2'	2.23	0.83
4:B:321:PRO:HA	36:B:8662:HOH:O	1.78	0.83
19:Q:8:ALA:HB1	19:Q:13:THR:HG21	1.59	0.83
13:K:133:VAL:HA	36:K:8572:HOH:O	1.77	0.83
7:E:97:VAL:HG12	36:E:4191:HOH:O	1.77	0.83
29:1:41:HIS:H	29:1:45:ASN:HD22	1.25	0.83
1:0:560:C:H42	1:0:597:A:H61	1.24	0.83
1:0:2717:C:H2'	1:0:2718:C:H5''	1.60	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.09	0.83
6:D:105:SER:HB2	6:D:131:THR:HG23	1.59	0.83
15:M:113:SER:HB2	36:M:8562:HOH:O	1.78	0.83
14:L:172:GLY:O	14:L:183:VAL:HG11	1.79	0.82
27:Y:58:GLY:HA3	36:Y:8439:HOH:O	1.80	0.82
8:F:91:VAL:HG12	8:F:92:GLY:H	1.45	0.82
1:0:214:U:H5'	36:0:5660:HOH:O	1.78	0.82
1:0:1184:C:H1'	36:0:6994:HOH:O	1.79	0.82
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.61	0.82
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.62	0.82
10:H:4:ALA:HB3	36:H:8364:HOH:O	1.80	0.82
1:0:870:G:C2'	1:0:871:G:H5''	2.10	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:14:LYS:HB2	12:J:45:PRO:HG2	1.61	0.82
1:O:962:C:H1'	15:M:5:ARG:NH1	1.93	0.82
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.60	0.81
13:K:79:ASP:HB3	36:K:8558:HOH:O	1.81	0.81
10:H:139:ASP:N	10:H:140:PRO:HD3	1.95	0.81
3:A:191:GLY:HA2	3:A:194:MET:CE	2.10	0.81
23:U:1:THR:HG23	23:U:2:VAL:H	1.44	0.81
1:O:1372:A:H3'	36:O:6711:HOH:O	1.79	0.81
17:O:115:SER:H	17:O:118:GLN:NE2	1.79	0.81
1:O:541:C:H2'	1:O:542:A:H5''	1.62	0.81
30:2:62:THR:HB	36:2:8550:HOH:O	1.79	0.81
2:9:25:G:H3'	2:9:26:C:C5'	2.10	0.80
1:O:1667:A:H8	1:O:1667:A:H5'	1.45	0.80
29:1:22:PRO:HB2	29:1:24:TRP:CD1	2.17	0.80
13:K:68:GLU:HA	36:K:8543:HOH:O	1.82	0.80
1:O:506:G:H22	1:O:509:A:C5'	1.94	0.80
23:U:12:THR:HG22	23:U:15:GLU:CG	2.11	0.80
14:L:152:ARG:HG3	36:L:8555:HOH:O	1.82	0.80
15:M:164:ASP:CG	15:M:167:ASP:HA	2.02	0.80
1:O:1116:U:O2'	1:O:1118:A:H2	1.65	0.80
1:O:1191:A:N1	1:O:1206:U:O4	2.14	0.80
24:V:88:THR:HG23	24:V:110:GLN:HE21	1.45	0.80
24:V:4:LEU:HD22	24:V:52:VAL:HG21	1.64	0.79
36:O:6394:HOH:O	14:L:178:LYS:HB2	1.81	0.79
1:O:346:U:H4'	36:O:6364:HOH:O	1.82	0.79
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.10	0.79
6:D:20:LYS:HA	6:D:75:LEU:O	1.82	0.79
30:2:70:ARG:HD3	36:2:8539:HOH:O	1.81	0.79
1:O:288:A:H61	1:O:364:C:H42	1.31	0.79
3:A:192:VAL:HB	36:A:8596:HOH:O	1.81	0.79
36:O:4053:HOH:O	10:H:151:MET:HE2	1.80	0.79
15:M:49:THR:HG22	15:M:56:ASP:HB2	1.64	0.79
1:O:1160:G:H5'	1:O:1161:A:C5'	2.11	0.78
21:S:61:GLU:HG3	36:S:3851:HOH:O	1.81	0.78
24:V:137:GLN:HE21	24:V:141:HIS:CE1	2.01	0.78
1:O:2710:U:H1'	36:O:7157:HOH:O	1.84	0.78
1:O:871:G:H8	1:O:871:G:C5'	1.96	0.78
24:V:88:THR:HG22	24:V:89:ASP:N	1.98	0.78
24:V:122:ARG:HG2	24:V:122:ARG:HH11	1.48	0.78
1:O:2506:A:O2'	1:O:2507:G:H8	1.65	0.78
27:Y:40:PRO:HD3	27:Y:47:LEU:HD11	1.66	0.78
1:O:1160:G:C5'	1:O:1161:A:H5'	2.10	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1119:G:H22	1:0:1246:A:H2	1.26	0.78
1:0:1701:A:H5'	36:0:5802:HOH:O	1.84	0.78
29:1:39:ARG:HG2	36:1:3143:HOH:O	1.83	0.78
5:C:236:THR:HG21	36:C:8376:HOH:O	1.82	0.78
1:0:1116:U:HO2'	1:0:1118:A:H2	0.82	0.78
36:0:6950:HOH:O	21:S:9:LYS:HB2	1.82	0.78
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.65	0.78
14:L:87:MET:HB3	30:2:46:ILE:HG21	1.65	0.78
29:1:24:TRP:CD1	36:1:6863:HOH:O	2.36	0.78
10:H:55:GLN:NE2	10:H:124:ARG:HE	1.80	0.78
1:0:544:G:H2'	1:0:545:G:H5''	1.65	0.78
6:D:27:ILE:HG22	6:D:28:GLY:H	1.48	0.77
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.65	0.77
1:0:559:U:H5'	1:0:559:U:H6	1.49	0.77
36:0:4346:HOH:O	11:I:47:THR:HB	1.83	0.77
36:0:9211:HOH:O	4:B:254:GLN:HG3	1.84	0.77
24:V:149:LEU:HG	24:V:153:MET:HE2	1.67	0.77
30:2:70:ARG:HG2	30:2:77:ALA:HB2	1.65	0.77
26:X:187:VAL:HG23	26:X:192:ASP:HB2	1.65	0.77
1:0:545:G:H8	1:0:545:G:H5'	1.48	0.77
2:9:56:A:C2'	2:9:57:A:H5''	2.14	0.77
2:9:14:G:H5'	2:9:14:G:H8	1.50	0.77
1:0:284:C:H4'	1:0:285:A:O5'	1.83	0.77
36:0:3295:HOH:O	14:L:189:VAL:HG21	1.84	0.77
10:H:33:MET:HB2	10:H:83:PHE:HB3	1.67	0.77
12:J:74:VAL:HG13	12:J:113:ILE:HG23	1.67	0.77
1:0:1625:U:H4'	36:0:4177:HOH:O	1.84	0.77
10:H:59:ASN:HD22	10:H:59:ASN:N	1.82	0.77
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.66	0.77
1:0:2890:A:H1'	22:T:56:ARG:NH2	2.00	0.77
1:0:536:A:H3'	36:0:4557:HOH:O	1.85	0.77
14:L:87:MET:HB3	30:2:46:ILE:HD13	1.66	0.76
36:0:6291:HOH:O	15:M:4:PRO:HD2	1.85	0.76
24:V:68:THR:HG23	24:V:69:ARG:HG2	1.67	0.76
27:Y:49:ARG:HD2	36:Y:8430:HOH:O	1.84	0.76
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.67	0.76
8:F:96:ALA:HA	36:F:3111:HOH:O	1.83	0.76
1:0:1130:U:H5'	36:0:7208:HOH:O	1.85	0.76
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.21	0.76
14:L:139:PRO:O	14:L:140:ALA:HB3	1.86	0.76
8:F:91:VAL:HG12	8:F:92:GLY:N	2.01	0.76
5:C:242:GLU:HG3	36:C:8384:HOH:O	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1751:G:C2'	1:0:1752:G:H5''	2.15	0.76
15:M:164:ASP:OD2	15:M:167:ASP:HA	1.85	0.76
4:B:62:ARG:HA	4:B:65:MET:HE3	1.67	0.76
14:L:35:PRO:HG2	14:L:38:VAL:HG23	1.67	0.76
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.68	0.76
36:0:3235:HOH:O	14:L:157:LEU:HD11	1.85	0.76
20:R:51:GLN:HE21	20:R:53:ASN:HD21	1.34	0.76
2:9:23:U:H6	2:9:23:U:H5''	1.50	0.75
2:9:3:A:N6	2:9:22:G:H1'	2.01	0.75
1:0:1191:A:C2	1:0:1206:U:O4	2.40	0.75
16:N:47:ARG:HH11	16:N:47:ARG:HG3	1.51	0.75
3:A:35:GLY:O	3:A:36:ASP:HB3	1.85	0.75
36:0:5814:HOH:O	6:D:99:ASP:HA	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75
10:H:59:ASN:HD22	10:H:59:ASN:H	1.34	0.75
1:0:1209:C:H4'	36:0:4791:HOH:O	1.85	0.75
11:I:93:ARG:HH11	11:I:93:ARG:HB3	1.49	0.75
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.69	0.75
1:0:541:C:C2'	1:0:542:A:H5''	2.17	0.75
19:Q:9:ASP:O	19:Q:13:THR:HB	1.87	0.74
1:0:2054:A:N3	19:Q:128:ARG:NH2	2.35	0.74
24:V:122:ARG:HH21	24:V:154:ARG:HD2	1.51	0.74
14:L:87:MET:HG2	30:2:46:ILE:HG21	1.69	0.74
26:X:189:ASN:HA	26:X:217:ILE:HD11	1.67	0.74
19:Q:18:LEU:HB2	19:Q:143:VAL:HG12	1.67	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.67	0.74
25:W:78:GLU:HG2	25:W:79:GLU:H	1.52	0.74
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.23	0.74
24:V:72:PRO:HG2	24:V:77:ALA:HB3	1.69	0.74
20:R:57:THR:HG22	20:R:59:ASP:N	2.02	0.74
23:U:39:ALA:N	23:U:40:PRO:HD2	2.03	0.74
1:0:2637:A:H5'	36:0:8785:HOH:O	1.88	0.74
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.74
1:0:21:G:C5'	19:Q:2:ILE:HA	2.17	0.74
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.70	0.74
1:0:289:G:H22	1:0:363:A:H2	1.36	0.74
19:Q:39:THR:HG22	19:Q:42:GLU:H	1.53	0.74
1:0:1634:G:H3'	36:0:3402:HOH:O	1.87	0.74
10:H:162:SER:CB	10:H:163:PRO:HD3	2.17	0.73
10:H:150:LYS:HE2	36:H:8381:HOH:O	1.89	0.73
6:D:146:LYS:NZ	15:M:107:ASN:HD21	1.86	0.73
6:D:19:GLU:O	6:D:20:LYS:HG2	1.89	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2840:A:OP1	4:B:211:THR:HG23	1.88	0.73
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.21	0.73
10:H:165:GLY:HA3	36:H:8394:HOH:O	1.87	0.73
5:C:1:MET:HG2	5:C:2:GLN:H	1.53	0.73
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.67	0.73
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.19	0.73
17:O:115:SER:OG	17:O:118:GLN:HG3	1.88	0.73
1:0:1328:A:OP1	26:X:169:ARG:HD2	1.87	0.73
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.71	0.73
30:2:65:THR:HG23	30:2:67:LEU:HG	1.70	0.73
1:0:2586:U:H3	1:0:2592:G:H22	1.35	0.73
10:H:46:VAL:HG12	10:H:146:TRP:HZ3	1.53	0.73
1:0:431:G:P	14:L:48:ARG:HH12	2.11	0.73
13:K:143:THR:HG22	13:K:144:ASP:N	2.03	0.73
5:C:236:THR:HA	36:C:8450:HOH:O	1.89	0.73
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.18	0.73
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.53	0.73
15:M:48:VAL:CG1	15:M:55:ASP:HB3	2.18	0.73
1:0:272:A:H3'	36:0:7061:HOH:O	1.88	0.73
1:0:657:G:OP1	5:C:27:ARG:NH2	2.18	0.73
3:A:131:HIS:O	3:A:132:ASP:HB2	1.89	0.72
1:0:1118:A:H3'	1:0:1118:A:C8	2.24	0.72
27:Y:37:HIS:HB2	27:Y:47:LEU:HB2	1.71	0.72
1:0:1450:C:H4'	1:0:1451:C:OP2	1.88	0.72
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.69	0.72
14:L:104:ARG:O	14:L:108:LYS:HE2	1.88	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.54	0.72
1:0:1194:A:C6	1:0:1206:U:C4	2.78	0.72
1:0:506:G:H22	1:0:509:A:H5'	1.53	0.72
24:V:65:VAL:HA	24:V:68:THR:HG22	1.72	0.72
10:H:14:TYR:H	10:H:91:HIS:CE1	2.07	0.72
10:H:142:VAL:HG13	36:H:8379:HOH:O	1.89	0.72
1:0:1666:C:H2'	1:0:1667:A:H5'	1.71	0.72
14:L:164:THR:HG22	14:L:167:GLY:N	2.03	0.72
1:0:31:C:H2'	36:0:7224:HOH:O	1.89	0.72
1:0:1187:U:HO2'	1:0:1189:A:H2	1.35	0.72
4:B:221:GLN:HE22	12:J:42:ASN:HD22	1.37	0.72
1:0:1594:C:OP2	17:O:120:ARG:HD2	1.89	0.72
24:V:21:LEU:HD22	24:V:26:ILE:HD11	1.72	0.71
3:A:199:HIS:CD2	3:A:201:PHE:H	2.07	0.71
1:0:877:G:H5'	1:0:878:G:OP1	1.89	0.71
17:O:115:SER:N	17:O:118:GLN:HE21	1.84	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1771:U:H4'	27:Y:20:LEU:HD21	1.71	0.71
10:H:41:THR:HA	36:H:8392:HOH:O	1.88	0.71
36:0:3192:HOH:O	14:L:79:LYS:HD3	1.90	0.71
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.54	0.71
2:9:6:C:OP1	15:M:37:ARG:NH1	2.23	0.71
14:L:106:ASN:HD22	14:L:114:VAL:HG23	1.53	0.71
22:T:14:GLU:O	22:T:17:THR:HB	1.91	0.71
10:H:26:LYS:HG2	10:H:28:ILE:H	1.55	0.71
14:L:87:MET:HB2	14:L:91:ILE:HD11	1.72	0.71
1:0:183:A:H5'	14:L:157:LEU:HD12	1.73	0.71
1:0:1170:U:O2'	1:0:1172:G:N7	2.21	0.71
10:H:47:GLU:HB3	10:H:133:ILE:CD1	2.20	0.71
14:L:87:MET:CB	30:2:46:ILE:HG21	2.20	0.71
13:K:148:GLU:HA	36:K:8571:HOH:O	1.90	0.71
3:A:210:GLY:HA3	36:A:8590:HOH:O	1.90	0.71
14:L:35:PRO:CG	14:L:38:VAL:HG23	2.20	0.71
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.05	0.71
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.71
1:0:1119:G:N2	1:0:1246:A:C2	2.55	0.71
19:Q:99:ALA:HB1	19:Q:109:MET:CE	2.20	0.71
11:I:107:ASN:HD21	11:I:109:TYR:HB2	1.56	0.71
7:E:101:GLU:HB2	7:E:116:THR:O	1.91	0.71
12:J:81:ARG:HD3	12:J:87:ARG:NH1	2.06	0.71
1:0:281:U:H2'	1:0:282:C:O4'	1.90	0.71
17:O:59:ARG:NH2	17:O:66:GLN:HE22	1.89	0.70
19:Q:18:LEU:HD12	19:Q:143:VAL:HG11	1.71	0.70
9:G:12:ILE:N	9:G:13:PRO:HD3	2.05	0.70
1:0:2896:A:H5''	36:0:5618:HOH:O	1.90	0.70
15:M:80:SER:HB2	36:M:8537:HOH:O	1.90	0.70
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
29:1:41:HIS:N	29:1:45:ASN:HD22	1.89	0.70
10:H:137:ASN:O	10:H:139:ASP:N	2.25	0.70
4:B:103:ASP:HB2	36:B:8598:HOH:O	1.89	0.70
11:I:45:VAL:HG23	11:I:130:VAL:O	1.91	0.70
16:N:14:LEU:HD23	16:N:102:ILE:HD11	1.72	0.70
26:X:187:VAL:HG23	26:X:192:ASP:CB	2.22	0.70
1:0:1973:A:H5'	1:0:1973:A:H8	1.57	0.70
10:H:3:GLY:HA2	10:H:57:ARG:HH12	1.57	0.70
13:K:136:ALA:HB3	36:K:8572:HOH:O	1.90	0.70
14:L:113:ARG:NH2	14:L:156:ARG:HG2	2.07	0.70
30:2:73:GLU:HB3	36:2:8560:HOH:O	1.91	0.70
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.21	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:139:VAL:HG13	36:C:8447:HOH:O	1.91	0.70
7:E:68:HIS:O	7:E:72:MET:HG3	1.92	0.70
1:O:2468:A:H61	30:2:48:ASN:HD21	1.38	0.70
1:O:1835:U:C5	1:O:1840:A:N7	2.58	0.69
36:C:8359:HOH:O	16:N:3:THR:HG21	1.92	0.69
2:9:39:U:H1'	2:9:44:A:H61	1.56	0.69
1:O:542:A:H5'	1:O:542:A:C8	2.24	0.69
29:1:18:ASN:HD21	29:1:40:ARG:H	1.41	0.69
1:O:1603:A:H5'	1:O:1605:G:O4'	1.92	0.69
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.75	0.69
14:L:164:THR:HG23	14:L:165:SER:N	2.06	0.69
1:O:236:A:H4'	1:O:237:G:H5'	1.75	0.69
11:I:107:ASN:ND2	11:I:109:TYR:H	1.89	0.69
12:J:22:ASP:HB2	36:J:5264:HOH:O	1.91	0.69
6:D:95:THR:O	6:D:97:GLN:N	2.23	0.69
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.26	0.69
10:H:71:TYR:C	10:H:73:GLN:H	1.96	0.69
10:H:31:PHE:HE2	10:H:87:LYS:O	1.76	0.69
5:C:140:VAL:HB	36:C:8450:HOH:O	1.93	0.69
1:O:1172:G:H1'	36:O:4485:HOH:O	1.91	0.69
2:9:29:C:H2'	2:9:30:C:H5'	1.75	0.69
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.73	0.69
9:G:12:ILE:HA	36:G:4499:HOH:O	1.93	0.69
25:W:71:ARG:HB3	25:W:88:GLU:OE1	1.93	0.69
30:2:57:GLY:HA2	36:2:8526:HOH:O	1.92	0.69
27:Y:38:LYS:HE2	27:Y:45:LYS:CE	2.22	0.68
1:O:1474:C:C6	1:O:1474:C:H5'	2.28	0.68
1:O:1377:C:H6	1:O:1377:C:H5'	1.58	0.68
1:O:182:G:H5'	36:O:4666:HOH:O	1.94	0.68
7:E:100:ASP:HB2	36:E:2789:HOH:O	1.93	0.68
10:H:47:GLU:HB3	10:H:133:ILE:HD13	1.75	0.68
6:D:37:ALA:O	6:D:40:ILE:HG12	1.94	0.68
21:S:9:LYS:HE3	21:S:13:ARG:NH1	2.09	0.68
1:O:2346:C:O2'	6:D:52:THR:HG21	1.94	0.68
12:J:34:VAL:HG22	12:J:47:ALA:HB2	1.76	0.68
36:O:6982:HOH:O	4:B:211:THR:HG21	1.93	0.68
10:H:53:PRO:HG3	10:H:127:GLY:H	1.59	0.68
1:O:1194:A:N6	1:O:1206:U:C4	2.61	0.68
24:V:149:LEU:HG	24:V:153:MET:CE	2.24	0.68
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.22	0.68
24:V:13:MET:CE	24:V:17:ILE:HG22	2.24	0.68
3:A:192:VAL:HG13	36:A:8558:HOH:O	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:236:THR:H	5:C:239:ALA:HB3	1.59	0.68
24:V:21:LEU:HB3	24:V:26:ILE:HG12	1.76	0.68
1:O:711:G:H1'	36:O:6617:HOH:O	1.93	0.68
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.74	0.68
6:D:97:GLN:HG2	6:D:97:GLN:O	1.94	0.68
14:L:52:LEU:HD21	36:L:8616:HOH:O	1.93	0.68
36:9:8462:HOH:O	15:M:147:ILE:HB	1.94	0.68
12:J:74:VAL:CG1	12:J:113:ILE:HG12	2.24	0.68
5:C:246:ARG:NE	36:C:8424:HOH:O	2.27	0.68
19:Q:39:THR:HB	19:Q:42:GLU:HG3	1.74	0.67
7:E:69:ILE:HA	7:E:72:MET:CE	2.24	0.67
11:I:74:ARG:HB3	11:I:74:ARG:HH11	1.57	0.67
24:V:21:LEU:HD22	24:V:26:ILE:CD1	2.25	0.67
14:L:139:PRO:O	14:L:140:ALA:CB	2.40	0.67
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.75	0.67
23:U:12:THR:CG2	23:U:15:GLU:HG3	2.21	0.67
3:A:33:GLU:O	3:A:34:ASP:HB2	1.94	0.67
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.75	0.67
1:O:396:U:H1'	36:O:7164:HOH:O	1.95	0.67
4:B:125:GLU:O	4:B:129:ARG:HG3	1.94	0.67
19:Q:111:ILE:HG23	19:Q:145:LEU:HD11	1.76	0.67
24:V:21:LEU:HD21	24:V:48:VAL:HG11	1.76	0.67
8:F:58:GLU:OE1	14:L:27:ARG:NH2	2.23	0.67
1:O:1819:G:H2'	1:O:1820:G:H4'	1.76	0.67
1:O:1505:U:H5'	1:O:1505:U:H6	1.58	0.67
1:O:1205:U:C2'	1:O:1206:U:H5''	2.24	0.67
1:O:1701:A:H4'	1:O:1702:U:C5'	2.24	0.67
10:H:136:VAL:HG22	10:H:137:ASN:O	1.94	0.67
1:O:282:C:H1'	1:O:368:C:N4	2.09	0.67
14:L:34:GLU:HB3	14:L:35:PRO:HD2	1.76	0.67
3:A:36:ASP:OD2	3:A:85:ASP:HB2	1.94	0.67
4:B:51:VAL:HG23	4:B:329:TYR:O	1.95	0.67
1:O:2426:G:H1'	36:O:5611:HOH:O	1.92	0.67
4:B:62:ARG:HA	4:B:65:MET:CE	2.24	0.67
23:U:64:GLY:O	23:U:65:ASP:HB2	1.93	0.67
4:B:16:ARG:NH1	36:B:8621:HOH:O	2.28	0.67
1:O:1119:G:H8	11:I:52:GLN:HE22	1.41	0.67
1:O:1209:C:H2'	1:O:1210:G:H8	1.59	0.67
24:V:13:MET:HE3	24:V:17:ILE:HG22	1.76	0.67
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.76	0.67
1:O:2748:G:H2'	36:O:7073:HOH:O	1.94	0.67
1:O:1205:U:H2'	1:O:1206:U:H5''	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:63:VAL:HG21	14:L:109:PHE:CE1	2.30	0.67
10:H:28:ILE:HA	10:H:62:GLU:OE1	1.94	0.66
5:C:162:VAL:HG13	5:C:232:LEU:HD21	1.77	0.66
27:Y:61:GLY:HA3	36:Y:8427:HOH:O	1.95	0.66
10:H:26:LYS:HD2	10:H:28:ILE:CD1	2.22	0.66
24:V:6:GLN:HB2	24:V:26:ILE:CD1	2.25	0.66
10:H:46:VAL:O	10:H:146:TRP:HH2	1.78	0.66
21:S:47:THR:HB	21:S:100:ASP:HB3	1.77	0.66
26:X:185:VAL:HG12	36:X:8572:HOH:O	1.94	0.66
2:9:14:G:H5'	2:9:14:G:C8	2.29	0.66
1:0:2508:C:H2'	36:0:6273:HOH:O	1.94	0.66
26:X:141:THR:HG23	36:X:8591:HOH:O	1.94	0.66
25:W:76:ARG:HG3	25:W:76:ARG:HH11	1.60	0.66
16:N:32:ARG:O	16:N:32:ARG:HD3	1.94	0.66
9:G:12:ILE:HG13	36:G:6833:HOH:O	1.94	0.66
1:0:1058:A:H2'	1:0:1060:C:H5''	1.77	0.66
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.96	0.66
17:O:18:LYS:O	17:O:21:VAL:HG22	1.95	0.66
1:0:1730:G:H5'	1:0:1731:C:C5	2.31	0.66
2:9:6:C:C5'	15:M:37:ARG:NH1	2.57	0.66
28:Z:25:LYS:HE2	36:1:7213:HOH:O	1.93	0.66
1:0:1766:U:O2	1:0:1778:A:H5'	1.96	0.66
1:0:2908:A:H2'	1:0:2909:G:O4'	1.96	0.66
1:0:1080:C:H4'	1:0:1081:A:OP1	1.95	0.66
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.78	0.66
14:L:138:HIS:ND1	14:L:139:PRO:O	2.22	0.66
16:N:87:THR:O	16:N:91:GLN:HG3	1.96	0.66
19:Q:44:VAL:O	19:Q:48:GLU:HG3	1.94	0.66
14:L:149:TRP:O	14:L:152:ARG:HG2	1.95	0.66
1:0:2414:A:H2'	1:0:2415:A:C8	2.30	0.66
10:H:85:ILE:HB	10:H:132:PHE:CE2	2.31	0.66
1:0:1684:A:H1'	29:1:43:ARG:HH22	1.60	0.66
1:0:2635:A:O2'	1:0:2636:C:H5'	1.96	0.66
36:0:4461:HOH:O	2:9:103:A:H4'	1.95	0.66
4:B:307:ARG:HB2	4:B:307:ARG:HH11	1.59	0.66
1:0:69:A:H5'	1:0:69:A:C8	2.31	0.66
10:H:150:LYS:HB2	10:H:157:ILE:HD12	1.78	0.65
17:O:10:ALA:HA	17:O:13:VAL:HG12	1.78	0.65
4:B:36:PRO:HA	4:B:168:GLY:CA	2.26	0.65
1:0:1191:A:H3'	1:0:1192:A:H5''	1.79	0.65
1:0:2533:C:H6	1:0:2533:C:H5'	1.61	0.65
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:1:41:HIS:H	29:1:45:ASN:ND2	1.94	0.65
4:B:204:GLY:HA3	36:B:8659:HOH:O	1.95	0.65
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.11	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.65
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.77	0.65
12:J:32:ILE:HD11	12:J:56:SER:HB3	1.77	0.65
15:M:183:ASP:OD2	15:M:186:LEU:HD12	1.95	0.65
6:D:69:ILE:O	6:D:69:ILE:HG22	1.96	0.65
1:0:2505:G:O2'	1:0:2506:A:H5'	1.97	0.65
27:Y:39:CYS:HA	27:Y:47:LEU:HD11	1.77	0.65
16:N:14:LEU:CD2	16:N:102:ILE:HD11	2.26	0.65
1:0:20:G:H21	19:Q:117:HIS:HD2	1.45	0.65
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.79	0.65
4:B:141:ARG:HD2	4:B:163:GLU:OE2	1.97	0.65
21:S:41:ARG:HH11	21:S:41:ARG:HG2	1.60	0.65
1:0:2878:U:H2'	1:0:2879:A:O4'	1.96	0.65
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.79	0.65
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.60	0.65
14:L:104:ARG:O	14:L:108:LYS:HG2	1.97	0.65
6:D:99:ASP:HB2	6:D:103:ASN:HB2	1.79	0.65
1:0:1666:C:O2'	1:0:1667:A:H5''	1.97	0.65
21:S:9:LYS:HE3	21:S:13:ARG:HH11	1.62	0.65
21:S:53:GLY:HA3	36:S:6384:HOH:O	1.94	0.65
1:0:2690:U:O2'	7:E:111:LYS:HE3	1.97	0.65
10:H:166:ASN:N	10:H:166:ASN:HD22	1.94	0.65
5:C:115:LEU:O	5:C:118:THR:HB	1.97	0.65
2:9:49:G:H5''	36:9:8462:HOH:O	1.97	0.65
24:V:4:LEU:O	24:V:32:CYS:HA	1.97	0.65
1:0:2756:U:H3	1:0:2896:A:H2	1.43	0.65
11:I:131:THR:HG22	11:I:134:GLU:H	1.61	0.65
21:S:32:ARG:NH1	21:S:38:ARG:HH12	1.95	0.65
2:9:23:U:H5''	2:9:23:U:C6	2.32	0.65
10:H:3:GLY:HA2	10:H:57:ARG:NH1	2.11	0.65
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.79	0.65
14:L:94:LYS:HE3	36:L:8582:HOH:O	1.95	0.65
36:0:7116:HOH:O	27:Y:31:ILE:HG13	1.96	0.65
1:0:299:U:H5'	36:0:6860:HOH:O	1.97	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.97	0.65
7:E:11:VAL:HG12	7:E:12:ASP:N	2.12	0.64
1:0:2783:A:H3'	36:0:4742:HOH:O	1.96	0.64
8:F:99:THR:HA	36:F:3461:HOH:O	1.96	0.64
6:D:135:VAL:HG22	6:D:136:ARG:H	1.62	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.79	0.64
1:0:603:A:H5''	1:0:604:G:OP1	1.97	0.64
25:W:72:VAL:HG22	25:W:85:VAL:HG12	1.78	0.64
10:H:27:LYS:N	10:H:58:HIS:HD2	1.92	0.64
2:9:69:U:OP1	15:M:4:PRO:HG3	1.98	0.64
14:L:80:GLY:O	14:L:81:ARG:HD3	1.97	0.64
7:E:6:GLU:HA	7:E:46:THR:HG22	1.80	0.64
23:U:44:GLY:O	23:U:48:GLU:HG2	1.98	0.64
5:C:76:ARG:HD3	36:C:8369:HOH:O	1.95	0.64
1:0:2672:C:H1'	36:B:8639:HOH:O	1.97	0.64
6:D:25:MET:CE	6:D:37:ALA:HB1	2.27	0.64
1:0:1701:A:H5''	1:0:1702:U:H3'	1.80	0.64
7:E:15:GLN:NE2	7:E:40:VAL:O	2.29	0.64
7:E:7:ILE:HD11	7:E:11:VAL:C	2.18	0.64
3:A:223:ARG:HG3	36:A:8604:HOH:O	1.97	0.64
1:0:259:G:H21	14:L:58:GLN:NE2	1.96	0.64
10:H:69:ASN:O	10:H:72:VAL:HG12	1.98	0.64
4:B:185:GLY:HA2	36:B:8638:HOH:O	1.97	0.64
24:V:154:ARG:C	36:V:4276:HOH:O	2.35	0.64
2:9:13:A:O2'	2:9:14:G:H5''	1.98	0.64
1:0:1778:A:H2'	1:0:1779:A:H5'	1.80	0.64
1:0:2676:C:H4'	11:I:70:PHE:CE1	2.33	0.64
1:0:2438:G:H5'	36:O:5690:HOH:O	1.97	0.64
20:R:43:GLU:HB3	36:R:8341:HOH:O	1.97	0.64
24:V:38:THR:HG22	36:V:3580:HOH:O	1.98	0.64
10:H:140:PRO:HB3	36:H:8379:HOH:O	1.98	0.64
1:0:2769:C:H2'	1:0:2770:G:O4'	1.98	0.64
24:V:21:LEU:HD21	24:V:48:VAL:CG1	2.27	0.63
1:0:1189:A:H3'	36:O:7217:HOH:O	1.97	0.63
1:0:1441:G:H1'	36:O:7301:HOH:O	1.97	0.63
14:L:64:ARG:HD2	36:L:8586:HOH:O	1.97	0.63
1:0:902:G:N7	13:K:18:HIS:HD2	1.97	0.63
1:0:506:G:H22	1:0:509:A:H5''	1.62	0.63
14:L:30:GLU:O	14:L:34:GLU:HG3	1.98	0.63
19:Q:39:THR:HG23	19:Q:107:GLU:O	1.99	0.63
5:C:27:ARG:HG3	5:C:29:ASP:OD1	1.99	0.63
1:0:558:C:O2'	1:0:559:U:H5''	1.98	0.63
12:J:62:PRO:HG3	12:J:65:ARG:HH21	1.64	0.63
1:0:1168:C:H2'	1:0:1169:U:O4'	1.99	0.63
5:C:142:ASP:OD1	5:C:237:GLU:HB3	1.99	0.63
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.63
6:D:55:LYS:HA	36:D:6752:HOH:O	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:962:C:H1'	15:M:5:ARG:HH12	1.62	0.63
26:X:187:VAL:CG2	26:X:192:ASP:HB2	2.28	0.63
5:C:107:ARG:NE	36:C:8457:HOH:O	2.24	0.63
6:D:99:ASP:CB	6:D:103:ASN:H	2.12	0.63
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.79	0.63
13:K:73:VAL:HG23	13:K:74:THR:H	1.62	0.63
5:C:16:VAL:HG12	5:C:17:ASP:N	2.14	0.63
14:L:87:MET:CG	30:2:46:ILE:HG21	2.29	0.63
14:L:37:VAL:CG1	14:L:63:VAL:HG11	2.28	0.63
1:O:69:A:H5'	1:O:69:A:H8	1.64	0.63
1:O:2830:U:H3'	36:O:4738:HOH:O	1.97	0.63
26:X:212:ARG:HD2	36:X:8605:HOH:O	1.99	0.63
26:X:133:HIS:HD2	36:X:8584:HOH:O	1.80	0.63
10:H:44:ALA:HA	10:H:163:PRO:O	1.99	0.62
3:A:55:VAL:HG22	3:A:68:ILE:O	1.99	0.62
1:O:1741:U:H5'	1:O:1742:A:OP1	1.99	0.62
1:O:2827:A:H2'	1:O:2828:G:O4'	1.98	0.62
4:B:145:HIS:HD2	4:B:146:THR:O	1.83	0.62
15:M:12:ARG:HD3	15:M:18:THR:OG1	1.99	0.62
21:S:24:ARG:HH21	21:S:39:ASN:HD22	1.45	0.62
1:O:2694:A:H4'	7:E:91:PHE:CE1	2.33	0.62
10:H:130:HIS:CD2	10:H:133:ILE:HD11	2.34	0.62
10:H:35:ASN:ND2	10:H:80:ASN:HA	2.13	0.62
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.80	0.62
1:O:474:C:O3'	5:C:73:LEU:HD21	1.99	0.62
1:O:2547:C:OP2	4:B:5:ARG:NH1	2.32	0.62
25:W:75:ALA:O	25:W:83:ALA:HA	1.99	0.62
1:O:2851:G:O2'	1:O:2852:A:H5'	1.99	0.62
15:M:37:ARG:NE	36:M:8535:HOH:O	2.32	0.62
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.14	0.62
10:H:2:PRO:HB2	36:H:8364:HOH:O	1.99	0.62
7:E:7:ILE:HD11	7:E:11:VAL:O	1.98	0.62
19:Q:111:ILE:HG23	19:Q:145:LEU:CD1	2.29	0.62
15:M:86:LEU:HD12	15:M:125:ALA:HB2	1.82	0.62
24:V:4:LEU:HD22	24:V:52:VAL:CG2	2.29	0.62
4:B:7:ARG:CG	4:B:7:ARG:HH11	2.10	0.62
1:O:1187:U:O2'	1:O:1189:A:H2	1.83	0.62
1:O:1008:C:H5"	10:H:16:ARG:HH12	1.64	0.62
15:M:155:GLU:O	15:M:156:GLU:HG3	2.00	0.62
1:O:470:U:O2'	28:Z:16:HIS:HD2	1.82	0.62
5:C:79:ARG:O	5:C:87:ARG:HG2	1.99	0.62
1:O:710:G:OP1	16:N:24:ALA:HB3	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2587:U:H2'	1:0:2589:U:H5''	1.82	0.62
12:J:55:VAL:HG12	12:J:56:SER:N	2.15	0.62
12:J:75:ARG:CZ	36:J:4172:HOH:O	2.46	0.62
24:V:122:ARG:NH2	24:V:154:ARG:HD2	2.14	0.62
1:0:182:G:O3'	14:L:157:LEU:HD13	1.99	0.62
19:Q:18:LEU:HB2	19:Q:143:VAL:CG1	2.29	0.62
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.81	0.62
7:E:69:ILE:HA	7:E:72:MET:HE3	1.82	0.62
1:0:2638:G:H5'	36:0:4439:HOH:O	2.00	0.62
15:M:159:TYR:HB3	15:M:162:ASP:HB2	1.82	0.62
2:9:39:U:H1'	2:9:44:A:N6	2.14	0.62
26:X:186:ARG:HG2	26:X:186:ARG:HH11	1.65	0.62
1:0:417:G:P	36:0:6944:HOH:O	2.58	0.62
6:D:149:ARG:NH1	36:D:3066:HOH:O	2.23	0.62
1:0:2578:G:H5'	1:0:2578:G:H8	1.64	0.62
2:9:25:G:C3'	2:9:26:C:H5'	2.27	0.61
11:I:103:VAL:HG12	36:I:5907:HOH:O	1.99	0.61
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.81	0.61
1:0:2346:C:O5'	1:0:2346:C:H6	1.83	0.61
1:0:338:C:H5''	36:C:8421:HOH:O	1.97	0.61
15:M:71:TRP:CE3	15:M:175:LEU:HD22	2.35	0.61
1:0:1118:A:H62	1:0:1244:U:H3	1.48	0.61
10:H:139:ASP:HA	36:H:8369:HOH:O	1.99	0.61
6:D:93:LEU:HB3	6:D:97:GLN:OE1	2.01	0.61
1:0:338:C:H4'	5:C:174:ILE:CD1	2.30	0.61
13:K:67:ARG:O	13:K:71:GLU:HG3	1.99	0.61
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.80	0.61
5:C:237:GLU:HB2	36:C:8430:HOH:O	2.00	0.61
10:H:139:ASP:H	10:H:140:PRO:HD3	1.62	0.61
6:D:35:ALA:N	36:D:5576:HOH:O	2.32	0.61
2:9:48:C:H4'	15:M:141:ARG:HH21	1.66	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
2:9:42:C:H2'	36:9:8497:HOH:O	2.00	0.61
10:H:127:GLY:O	10:H:128:ALA:HB3	2.00	0.61
13:K:72:ASN:HB2	36:K:8580:HOH:O	2.00	0.61
8:F:107:VAL:O	8:F:111:ILE:HG13	2.00	0.61
1:0:1120:U:H5''	1:0:1120:U:C6	2.36	0.61
7:E:132:THR:HB	36:E:2227:HOH:O	2.01	0.61
20:R:81:ILE:HG23	36:R:8334:HOH:O	2.00	0.61
15:M:23:ARG:NH1	36:M:8549:HOH:O	2.34	0.61
1:0:1299:G:O6	13:K:6:ARG:HD3	2.01	0.61
6:D:23:VAL:O	6:D:23:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:558:C:C2'	1:0:559:U:H5''	2.31	0.61
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.29	0.61
1:0:2779:G:H21	7:E:143:GLN:NE2	1.98	0.61
14:L:169:ARG:HD2	36:L:8590:HOH:O	2.01	0.61
15:M:184:ILE:HG22	15:M:185:GLU:HG3	1.83	0.61
25:W:74:ALA:CB	25:W:85:VAL:HG22	2.31	0.61
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.30	0.61
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.61
1:0:1189:A:H1'	1:0:1209:C:O4'	2.01	0.61
9:G:23:ILE:O	9:G:27:ILE:HG13	2.01	0.61
36:J:408:HOH:O	22:T:37:GLU:HB3	2.00	0.61
1:0:281:U:O2'	1:0:282:C:H5'	2.01	0.61
6:D:38:GLU:HB3	6:D:49:PRO:HG2	1.83	0.61
1:0:553:G:P	26:X:204:ARG:HH22	2.24	0.61
24:V:21:LEU:HD13	24:V:26:ILE:HD11	1.83	0.60
1:0:1525:G:H5'	1:0:1526:A:OP2	2.01	0.60
7:E:79:GLY:HA3	36:E:7046:HOH:O	2.00	0.60
1:0:1244:U:OP1	11:I:18:ILE:HD13	2.01	0.60
1:0:1667:A:C8	1:0:1667:A:H5'	2.34	0.60
10:H:118:PRO:HD2	36:H:8339:HOH:O	2.00	0.60
1:0:111:C:O2'	28:Z:20:ARG:HG2	2.01	0.60
8:F:110:GLU:HG2	36:F:6926:HOH:O	2.01	0.60
15:M:47:LEU:HD13	15:M:97:VAL:HG11	1.82	0.60
10:H:83:PHE:HZ	10:H:146:TRP:HE1	1.46	0.60
2:9:41:C:O4'	6:D:50:VAL:HG23	2.01	0.60
1:0:2570:G:H5''	36:0:4423:HOH:O	2.02	0.60
6:D:166:ILE:HD12	36:D:6326:HOH:O	2.01	0.60
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.60
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.60
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.66	0.60
27:Y:53:GLY:HA2	27:Y:67:GLY:O	2.00	0.60
4:B:7:ARG:CD	4:B:9:GLY:O	2.50	0.60
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.02	0.60
14:L:87:MET:CB	30:2:46:ILE:HD13	2.30	0.60
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.70	0.60
7:E:23:GLU:HG2	7:E:28:SER:CB	2.32	0.60
4:B:258:GLY:H	4:B:260:HIS:CE1	2.20	0.60
4:B:140:LEU:HD23	36:B:8583:HOH:O	2.01	0.60
9:G:12:ILE:N	9:G:13:PRO:CD	2.65	0.60
1:0:1641:A:H2'	1:0:1642:A:H5'	1.83	0.60
10:H:5:MET:HG3	36:H:8364:HOH:O	2.01	0.60
3:A:170:VAL:HG22	27:Y:22:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:447:A:OP1	21:S:2:LYS:HG2	2.02	0.60
4:B:238:ASN:HD22	4:B:240:GLY:N	2.00	0.60
23:U:39:ALA:C	23:U:41:GLU:H	2.05	0.60
23:U:55:ARG:O	23:U:59:ILE:HG12	2.02	0.60
24:V:88:THR:CG2	24:V:89:ASP:H	2.09	0.60
5:C:118:THR:O	5:C:136:VAL:HG13	2.02	0.60
7:E:81:GLU:HG2	7:E:134:SER:CB	2.32	0.60
11:I:74:ARG:CB	11:I:74:ARG:HH11	2.14	0.60
25:W:21:PRO:HG2	25:W:24:LYS:HD3	1.83	0.60
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.84	0.60
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.84	0.60
14:L:48:ARG:NH2	36:L:8562:HOH:O	2.34	0.59
25:W:15:ARG:HH11	25:W:15:ARG:HB3	1.66	0.59
15:M:151:ASP:O	15:M:154:LEU:HB2	2.02	0.59
13:K:145:LEU:O	13:K:148:GLU:HG3	2.02	0.59
25:W:25:ARG:HD2	36:W:3861:HOH:O	2.02	0.59
11:I:75:PRO:HG2	11:I:105:LEU:HD21	1.84	0.59
13:K:53:ARG:NH2	13:K:57:VAL:HG12	2.16	0.59
1:O:2310:G:OP2	10:H:114:PRO:HD2	2.01	0.59
4:B:307:ARG:CG	4:B:307:ARG:HH11	2.14	0.59
25:W:30:MET:HE1	25:W:58:ALA:HB3	1.84	0.59
15:M:38:LYS:HD2	15:M:114:LYS:HE3	1.84	0.59
5:C:12:THR:HB	36:C:8440:HOH:O	2.00	0.59
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.84	0.59
20:R:38:ALA:O	20:R:42:GLU:HG3	2.03	0.59
10:H:84:ARG:NH2	10:H:135:TRP:HH2	2.00	0.59
10:H:58:HIS:HA	10:H:61:LEU:HD23	1.84	0.59
5:C:76:ARG:HG2	5:C:78:ARG:HH12	1.66	0.59
13:K:77:ALA:HB3	36:K:8530:HOH:O	2.00	0.59
1:O:2721:U:H4'	12:J:87:ARG:HG3	1.84	0.59
29:1:22:PRO:HG2	29:1:25:VAL:CG2	2.32	0.59
19:Q:39:THR:HB	19:Q:42:GLU:CG	2.32	0.59
1:O:2270:G:H4'	3:A:223:ARG:HH12	1.67	0.59
14:L:174:ARG:HG3	36:L:8521:HOH:O	2.02	0.59
18:P:64:GLU:HG3	18:P:74:ASP:OD2	2.02	0.59
26:X:126:PRO:HG2	26:X:128:PHE:CE1	2.38	0.59
10:H:27:LYS:H	10:H:58:HIS:CD2	2.12	0.59
10:H:56:ILE:HG22	10:H:61:LEU:HD22	1.84	0.59
15:M:47:LEU:HD12	15:M:92:ALA:HB1	1.85	0.59
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.14	0.59
11:I:131:THR:HG22	11:I:133:GLY:N	2.17	0.59
6:D:95:THR:C	6:D:97:GLN:H	2.06	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:O:5309:HOH:O	14:L:170:CYS:SG	2.32	0.59
1:O:1159:G:H21	1:O:1189:A:H8	1.50	0.59
1:O:558:C:H5'	36:O:4769:HOH:O	2.03	0.59
6:D:65:GLU:HG3	36:D:6752:HOH:O	2.01	0.59
22:T:9:CYS:HA	22:T:52:THR:HG23	1.83	0.59
24:V:80:ASP:O	24:V:84:VAL:HG23	2.03	0.59
14:L:114:VAL:HG21	14:L:159:THR:HG21	1.85	0.59
1:O:1119:G:N2	1:O:1246:A:H2	1.98	0.59
13:K:133:VAL:HB	36:K:8557:HOH:O	2.02	0.59
1:O:545:G:C8	1:O:545:G:H5'	2.35	0.59
15:M:43:VAL:HG11	15:M:81:ALA:HA	1.85	0.59
1:O:1166:A:H1'	1:O:1192:A:N1	2.17	0.58
1:O:1053:G:OP1	10:H:12:PRO:HG3	2.03	0.58
1:O:2004:U:H4'	36:O:4818:HOH:O	2.03	0.58
1:O:2502:C:C2'	1:O:2503:A:H5'	2.33	0.58
1:O:1329:A:C2	36:O:4193:HOH:O	2.45	0.58
3:A:88:ILE:HG22	3:A:88:ILE:O	2.02	0.58
36:O:3172:HOH:O	14:L:79:LYS:HD2	2.02	0.58
4:B:307:ARG:CB	4:B:307:ARG:HH11	2.16	0.58
27:Y:28:ASP:O	27:Y:31:ILE:HG22	2.03	0.58
1:O:1528:A:H2'	1:O:1529:G:O4'	2.03	0.58
29:1:22:PRO:HG2	29:1:25:VAL:HG23	1.85	0.58
1:O:31:C:H4'	36:O:6950:HOH:O	2.02	0.58
1:O:285:A:H2'	1:O:286:U:O4'	2.03	0.58
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.21	0.58
1:O:316:A:H5'	21:S:54:ASP:OD2	2.02	0.58
3:A:164:ARG:NE	36:A:8591:HOH:O	2.35	0.58
2:9:92:G:H22	10:H:52:LYS:NZ	2.01	0.58
15:M:78:MET:HB2	15:M:79:PRO:HD3	1.86	0.58
30:2:25:VAL:HG22	30:2:68:LYS:HG3	1.84	0.58
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.67	0.58
28:Z:21:ARG:HD2	28:Z:37:CYS:SG	2.43	0.58
27:Y:62:TYR:CE2	27:Y:64:ILE:HG23	2.38	0.58
13:K:114:VAL:HG11	36:K:8572:HOH:O	2.02	0.58
1:O:2694:A:H4'	7:E:91:PHE:HE1	1.68	0.58
1:O:485:A:N3	1:O:487:G:H5''	2.18	0.58
1:O:1887:U:OP1	27:Y:21:LYS:HE3	2.03	0.58
3:A:175:LYS:HE2	36:A:8579:HOH:O	2.03	0.58
36:O:3353:HOH:O	10:H:11:LYS:HE2	2.03	0.58
1:O:2064:U:H5'	1:O:2652:U:O3'	2.04	0.58
15:M:62:HIS:HB3	15:M:65:ASP:OD1	2.03	0.58
10:H:45:GLN:HE21	10:H:135:TRP:HE1	1.51	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:46:VAL:HG12	10:H:146:TRP:CZ3	2.37	0.58
36:O:3496:HOH:O	21:S:82:THR:HA	2.03	0.58
26:X:144:ARG:NH1	36:X:8578:HOH:O	2.33	0.58
20:R:81:ILE:HG12	36:R:8334:HOH:O	2.03	0.58
1:O:328:U:O4'	5:C:202:THR:HG22	2.03	0.58
1:O:2862:G:H4'	4:B:336:GLN:O	2.03	0.58
14:L:108:LYS:HE3	36:L:8614:HOH:O	2.04	0.58
13:K:143:THR:CG2	13:K:144:ASP:N	2.66	0.58
7:E:172:PRO:HB3	36:E:6931:HOH:O	2.03	0.58
3:A:37:VAL:HG22	36:A:8599:HOH:O	2.04	0.58
4:B:267:LYS:HD3	36:B:8528:HOH:O	2.02	0.58
22:T:52:THR:HG22	22:T:54:THR:N	2.19	0.58
27:Y:13:ARG:NH1	36:Y:8421:HOH:O	2.37	0.58
23:U:58:THR:O	23:U:62:GLU:HG3	2.04	0.58
1:O:1118:A:H8	1:O:1119:G:H5''	1.67	0.57
13:K:143:THR:HG22	13:K:144:ASP:H	1.69	0.57
13:K:73:VAL:HG23	13:K:74:THR:N	2.19	0.57
15:M:154:LEU:O	15:M:155:GLU:HB3	2.04	0.57
1:O:1878:G:H1'	36:O:5640:HOH:O	2.03	0.57
13:K:90:ARG:NH2	13:K:121:ILE:HD11	2.19	0.57
15:M:34:LEU:HA	15:M:47:LEU:HD23	1.86	0.57
1:O:1181:A:H2'	1:O:1182:C:O4'	2.03	0.57
4:B:62:ARG:CA	4:B:65:MET:HE3	2.34	0.57
22:T:13:ILE:HG12	22:T:32:CYS:HB3	1.86	0.57
1:O:1173:A:H2'	36:O:3856:HOH:O	2.04	0.57
7:E:15:GLN:HG2	7:E:19:ASP:O	2.04	0.57
22:T:31:PHE:CG	22:T:37:GLU:HG2	2.39	0.57
22:T:52:THR:CG2	22:T:54:THR:HB	2.34	0.57
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.86	0.57
1:O:371:U:H2'	1:O:372:A:H8	1.69	0.57
4:B:175:LEU:C	4:B:175:LEU:HD23	2.24	0.57
23:U:39:ALA:N	23:U:40:PRO:CD	2.66	0.57
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.16	0.57
4:B:329:TYR:CE2	22:T:15:PRO:HG2	2.38	0.57
1:O:1120:U:H6	1:O:1120:U:H5''	1.69	0.57
36:O:7216:HOH:O	14:L:154:ARG:HB2	2.04	0.57
36:O:4077:HOH:O	5:C:50:GLU:HG2	2.03	0.57
1:O:1679:C:H5'	36:O:8834:HOH:O	2.05	0.57
8:F:37:THR:O	8:F:41:GLU:HG3	2.04	0.57
1:O:2456:A:H5'	36:O:5210:HOH:O	2.04	0.57
6:D:91:ALA:HB1	36:D:5198:HOH:O	2.03	0.57
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:164:ARG:HB2	27:Y:68:CYS:SG	2.44	0.57
3:A:53:ALA:HB3	36:A:8608:HOH:O	2.05	0.57
2:9:20:G:O2'	2:9:21:G:H5'	2.05	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.34	0.57
24:V:122:ARG:CZ	36:V:5817:HOH:O	2.53	0.57
15:M:48:VAL:HG11	15:M:55:ASP:HB3	1.85	0.57
7:E:31:ARG:NH1	36:E:5919:HOH:O	2.36	0.57
11:I:75:PRO:HG2	11:I:105:LEU:CD2	2.33	0.57
1:0:2241:C:O2'	1:0:2242:U:H5'	2.04	0.57
1:0:2630:G:O6	3:A:206:ARG:NH2	2.37	0.57
25:W:31:ILE:O	25:W:35:GLU:HG3	2.05	0.57
24:V:106:THR:OG1	24:V:109:GLU:HG3	2.04	0.57
20:R:33:SER:OG	20:R:36:GLU:HG3	2.05	0.57
12:J:115:ARG:HG3	12:J:116:GLU:N	2.19	0.57
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.57
6:D:86:THR:O	6:D:90:LEU:HG	2.05	0.57
23:U:4:HIS:HB3	36:U:6622:HOH:O	2.05	0.57
15:M:90:LEU:HB2	15:M:186:LEU:HD22	1.85	0.57
10:H:48:LEU:HG	10:H:157:ILE:HG21	1.87	0.57
14:L:38:VAL:C	14:L:63:VAL:HG13	2.24	0.57
9:G:12:ILE:HG22	9:G:12:ILE:O	2.05	0.57
4:B:162:MET:HG3	4:B:310:ARG:NH1	2.19	0.57
22:T:46:ALA:HB1	22:T:52:THR:HG21	1.87	0.57
26:X:144:ARG:NE	36:X:8615:HOH:O	2.37	0.57
1:0:2420:G:O2'	1:0:2421:G:H5'	2.04	0.57
17:O:121:ASP:HB2	36:O:198:HOH:O	2.05	0.57
1:0:449:A:N7	5:C:43:LYS:HG2	2.18	0.57
2:9:55:U:H4'	2:9:56:A:C8	2.39	0.57
2:9:76:G:C3'	2:9:77:A:H5''	2.28	0.57
1:0:2533:C:C6	1:0:2533:C:H5'	2.39	0.57
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.35	0.57
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.57
1:0:797:A:O4'	27:Y:10:ARG:N	2.37	0.57
5:C:1:MET:HG2	5:C:2:GLN:N	2.18	0.57
12:J:34:VAL:CG2	12:J:47:ALA:HB2	2.33	0.57
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.87	0.57
3:A:105:VAL:HG12	3:A:106:CYS:N	2.20	0.57
15:M:154:LEU:HG	15:M:155:GLU:H	1.68	0.57
26:X:165:GLU:HB3	36:X:8597:HOH:O	2.04	0.57
14:L:60:ILE:C	14:L:61:ILE:HD12	2.25	0.57
36:J:1387:HOH:O	22:T:20:MET:HE3	2.03	0.57
28:Z:28:HIS:CD2	28:Z:30:LYS:HB2	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:136:ARG:HD2	6:D:155:HIS:O	2.04	0.56
1:O:2419:U:H5''	1:O:2420:G:H5'	1.87	0.56
14:L:61:ILE:HG13	36:L:8624:HOH:O	2.04	0.56
8:F:101:ALA:HB2	8:F:108:LEU:CD2	2.34	0.56
10:H:14:TYR:N	10:H:91:HIS:CE1	2.74	0.56
5:C:214:THR:HG23	36:C:8436:HOH:O	2.05	0.56
20:R:51:GLN:HE21	20:R:53:ASN:ND2	2.02	0.56
10:H:166:ASN:N	10:H:166:ASN:ND2	2.52	0.56
24:V:125:HIS:CD2	24:V:127:GLY:H	2.23	0.56
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.04	0.56
6:D:103:ASN:ND2	6:D:134:LEU:H	2.03	0.56
20:R:51:GLN:NE2	20:R:53:ASN:HD21	2.00	0.56
1:O:289:G:N2	1:O:363:A:H2	2.00	0.56
6:D:93:LEU:HG	36:D:3862:HOH:O	2.05	0.56
8:F:99:THR:O	8:F:100:ASP:HB2	2.05	0.56
1:O:2676:C:H4'	11:I:70:PHE:HE1	1.70	0.56
10:H:75:SER:HB3	10:H:79:ALA:HB1	1.88	0.56
4:B:82:VAL:HG12	4:B:82:VAL:O	2.05	0.56
24:V:31:HIS:HB3	36:V:5420:HOH:O	2.05	0.56
24:V:81:ASP:OD1	24:V:92:ASP:HB2	2.04	0.56
26:X:220:GLU:HG2	36:X:8551:HOH:O	2.04	0.56
1:O:738:G:H3'	36:O:6569:HOH:O	2.05	0.56
1:O:200:U:H2'	36:O:9957:HOH:O	2.03	0.56
25:W:12:ILE:HD12	25:W:36:HIS:ND1	2.20	0.56
3:A:121:ALA:O	3:A:124:VAL:HG22	2.05	0.56
1:O:2718:C:H6	1:O:2718:C:H5'	1.70	0.56
1:O:183:A:C5'	14:L:157:LEU:HD12	2.36	0.56
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.56
1:O:380:A:H5''	14:L:48:ARG:NH2	2.21	0.56
15:M:64:SER:C	15:M:66:LEU:H	2.09	0.56
21:S:9:LYS:CE	21:S:13:ARG:NH1	2.68	0.56
1:O:280:C:H2'	1:O:281:U:O4'	2.06	0.56
1:O:2890:A:H1'	22:T:56:ARG:HH21	1.70	0.56
11:I:130:VAL:HG12	11:I:131:THR:N	2.19	0.56
17:O:13:VAL:HG21	17:O:41:ARG:HG2	1.87	0.56
1:O:2548:C:OP2	4:B:5:ARG:NH2	2.39	0.56
6:D:49:PRO:HG3	36:D:5828:HOH:O	2.05	0.56
16:N:96:VAL:HA	36:N:4258:HOH:O	2.04	0.56
1:O:1116:U:O2'	1:O:1118:A:C2	2.48	0.56
19:Q:106:GLY:HA2	19:Q:109:MET:HE3	1.87	0.56
17:O:38:GLU:HA	17:O:41:ARG:NH1	2.21	0.56
1:O:2781:U:H1'	7:E:139:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:2815:G:OP2	11:I:99:GLU:HG2	2.06	0.56
22:T:11:THR:HG22	22:T:53:ASP:OD2	2.06	0.56
10:H:109:ASP:HB2	36:H:8345:HOH:O	2.05	0.56
10:H:47:GLU:HG2	10:H:133:ILE:HD12	1.87	0.56
15:M:159:TYR:HE2	15:M:163:PHE:HE2	1.54	0.56
14:L:37:VAL:HG13	14:L:63:VAL:HG11	1.88	0.56
12:J:62:PRO:HG3	12:J:65:ARG:NH2	2.20	0.56
4:B:215:VAL:HB	4:B:234:ARG:HH12	1.70	0.56
24:V:108:ARG:HE	24:V:114:PRO:HG3	1.71	0.56
1:O:797:A:C4'	27:Y:10:ARG:N	2.69	0.56
1:O:1119:G:H8	11:I:52:GLN:NE2	2.04	0.56
25:W:78:GLU:CG	25:W:79:GLU:H	2.18	0.56
9:G:63:ARG:O	9:G:67:LEU:HG	2.05	0.56
10:H:39:GLY:O	10:H:41:THR:N	2.39	0.56
1:O:2081:A:H4'	11:I:69:TYR:CE1	2.41	0.56
18:P:11:ARG:HD3	36:P:5620:HOH:O	2.04	0.56
1:O:1134:G:H4'	10:H:151:MET:CE	2.23	0.56
3:A:212:PRO:HB2	36:A:8562:HOH:O	2.06	0.56
1:O:1209:C:H2'	1:O:1210:G:C8	2.39	0.56
1:O:2821:C:H4'	4:B:116:PRO:HB3	1.88	0.56
36:O:5761:HOH:O	3:A:22:ARG:HG2	2.06	0.56
6:D:11:HIS:C	6:D:13:MET:H	2.09	0.56
15:M:87:LEU:CD1	15:M:186:LEU:HD21	2.33	0.55
19:Q:18:LEU:HD12	19:Q:143:VAL:CG1	2.36	0.55
6:D:10:PHE:CG	6:D:11:HIS:N	2.74	0.55
29:I:35:ARG:HB2	36:I:2691:HOH:O	2.06	0.55
5:C:16:VAL:HG12	5:C:17:ASP:H	1.69	0.55
1:O:1667:A:H2'	1:O:1668:U:C6	2.41	0.55
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.88	0.55
25:W:25:ARG:HG2	36:W:5356:HOH:O	2.05	0.55
15:M:11:ARG:NH2	36:M:8521:HOH:O	2.39	0.55
5:C:98:ARG:NH1	36:C:8357:HOH:O	2.36	0.55
1:O:1086:A:C6	24:V:11:VAL:HG11	2.41	0.55
36:O:6547:HOH:O	3:A:211:LYS:HG2	2.06	0.55
27:Y:58:GLY:CA	36:Y:8439:HOH:O	2.47	0.55
1:O:567:U:H5''	36:V:5817:HOH:O	2.06	0.55
1:O:1524:U:OP1	1:O:1524:U:H4'	2.06	0.55
1:O:2604:A:H5'	36:O:5307:HOH:O	2.06	0.55
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.88	0.55
13:K:104:ASP:HB3	36:K:8563:HOH:O	2.07	0.55
1:O:263:U:O4'	8:F:59:ILE:HD13	2.05	0.55
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:2:18:GLN:OE1	30:2:73:GLU:HB3	2.05	0.55
7:E:11:VAL:HG13	7:E:23:GLU:O	2.05	0.55
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.42	0.55
26:X:144:ARG:CZ	36:X:8615:HOH:O	2.53	0.55
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.88	0.55
1:0:1185:U:H2'	1:0:1186:C:C6	2.41	0.55
10:H:139:ASP:N	10:H:140:PRO:CD	2.68	0.55
14:L:94:LYS:CE	36:L:8582:HOH:O	2.54	0.55
10:H:97:LYS:HD3	10:H:117:LYS:HE2	1.88	0.55
26:X:216:ARG:HD3	36:X:8571:HOH:O	2.05	0.55
9:G:64:ASN:N	9:G:64:ASN:HD22	2.03	0.55
36:0:5728:HOH:O	4:B:2:GLN:HA	2.05	0.55
14:L:164:THR:HB	36:L:8519:HOH:O	2.07	0.55
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.37	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
11:I:133:GLY:O	11:I:137:GLU:HG3	2.07	0.55
6:D:174:VAL:HG13	36:D:6555:HOH:O	2.07	0.55
1:0:2064:U:H5'	1:0:2652:U:H4'	1.88	0.55
6:D:36:ASN:HA	36:D:7500:HOH:O	2.07	0.55
6:D:62:ASP:HA	36:D:4233:HOH:O	2.06	0.55
36:0:8907:HOH:O	14:L:94:LYS:HE2	2.06	0.55
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.06	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.55
1:0:1477:C:H5'	1:0:1868:G:C5'	2.36	0.55
15:M:61:ALA:HB3	15:M:88:ALA:HB2	1.89	0.55
21:S:111:ARG:HB3	21:S:119:ALA:HB2	1.89	0.55
14:L:74:ARG:HG3	14:L:74:ARG:HH11	1.72	0.55
2:9:55:U:H4'	2:9:56:A:H8	1.70	0.55
24:V:21:LEU:HB3	24:V:26:ILE:CG1	2.36	0.55
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.72	0.55
1:0:2898:G:H4'	4:B:288:GLY:HA2	1.88	0.55
25:W:43:VAL:CG1	25:W:47:ALA:HB3	2.37	0.55
6:D:58:VAL:HG12	6:D:59:GLY:N	2.22	0.55
1:0:1299:G:N2	36:0:4193:HOH:O	2.39	0.55
10:H:59:ASN:H	10:H:59:ASN:ND2	2.04	0.55
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.55
1:0:1123:A:C6	1:0:1238:C:H5'	2.42	0.55
1:0:1137:G:H1'	36:0:3386:HOH:O	2.06	0.55
1:0:1615:A:H5'	36:0:3690:HOH:O	2.07	0.55
1:0:57:C:H5''	36:0:6278:HOH:O	2.06	0.55
26:X:235:GLU:CD	26:X:235:GLU:H	2.10	0.55
6:D:154:LYS:H	6:D:154:LYS:CD	2.10	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:2717:C:O2'	1:O:2718:C:H5''	2.06	0.55
15:M:49:THR:CG2	15:M:56:ASP:HB2	2.36	0.55
11:I:107:ASN:HD22	11:I:109:TYR:H	1.52	0.55
6:D:51:ARG:HD3	36:D:7636:HOH:O	2.07	0.55
8:F:101:ALA:HB2	8:F:108:LEU:HD22	1.88	0.55
11:I:99:GLU:HA	36:I:7377:HOH:O	2.06	0.55
1:O:1669:A:H2'	1:O:1670:G:C8	2.42	0.55
19:Q:25:PHE:CE2	19:Q:29:LYS:HE2	2.42	0.55
20:R:23:LYS:HE2	36:R:8329:HOH:O	2.06	0.55
17:O:80:ARG:HG2	17:O:87:ARG:CZ	2.37	0.55
15:M:170:GLU:O	15:M:174:GLU:HG3	2.07	0.55
16:N:38:ARG:NH1	36:N:7674:HOH:O	2.40	0.55
26:X:189:ASN:C	26:X:189:ASN:HD22	2.10	0.54
30:2:17:HIS:O	30:2:18:GLN:HG3	2.07	0.54
25:W:74:ALA:HB2	25:W:85:VAL:HG13	1.88	0.54
8:F:58:GLU:CD	14:L:27:ARG:HH22	2.10	0.54
1:O:138:U:H5''	1:O:139:C:OP2	2.08	0.54
26:X:112:GLU:CD	26:X:115:ARG:NH1	2.60	0.54
17:O:16:VAL:HG12	17:O:17:GLY:N	2.22	0.54
4:B:7:ARG:NH1	4:B:11:LEU:HD22	2.22	0.54
14:L:55:LYS:HB2	14:L:60:ILE:CD1	2.38	0.54
14:L:61:ILE:HA	36:L:8624:HOH:O	2.07	0.54
19:Q:33:ARG:NH1	36:Q:8541:HOH:O	2.39	0.54
10:H:129:ASN:HD22	10:H:129:ASN:N	2.04	0.54
1:O:2502:C:H2'	1:O:2503:A:H5'	1.89	0.54
1:O:21:G:H5''	19:Q:1:GLY:O	2.07	0.54
1:O:542:A:H2'	1:O:543:G:O4'	2.07	0.54
1:O:1118:A:C8	1:O:1118:A:C3'	2.87	0.54
1:O:283:U:H5''	1:O:284:C:P	2.47	0.54
14:L:37:VAL:HG21	14:L:108:LYS:CG	2.38	0.54
1:O:1189:A:H1'	1:O:1209:C:H1'	1.89	0.54
1:O:1268:C:O2'	26:X:169:ARG:HB2	2.07	0.54
13:K:143:THR:HG22	13:K:145:LEU:H	1.72	0.54
19:Q:119:VAL:HG12	19:Q:119:VAL:O	2.07	0.54
23:U:39:ALA:O	23:U:41:GLU:N	2.41	0.54
25:W:9:VAL:HG22	25:W:88:GLU:OE2	2.07	0.54
1:O:2795:C:O2'	1:O:2796:U:H5'	2.06	0.54
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.89	0.54
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.89	0.54
2:9:25:G:H2'	36:9:8458:HOH:O	2.08	0.54
12:J:87:ARG:CZ	36:J:4854:HOH:O	2.55	0.54
2:9:49:G:H2'	2:9:50:G:O4'	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:110:THR:HB	15:M:113:SER:OG	2.07	0.54
1:O:1189:A:O2'	1:O:1208:C:H2'	2.07	0.54
10:H:53:PRO:HA	10:H:125:VAL:O	2.07	0.54
4:B:85:ARG:NH1	36:B:8639:HOH:O	2.41	0.54
36:O:9462:HOH:O	25:W:23:HIS:HD2	1.90	0.54
16:N:39:THR:O	16:N:115:ARG:NH2	2.40	0.54
1:O:2488:A:H61	1:O:2534:C:H42	1.55	0.54
14:L:164:THR:CG2	14:L:165:SER:N	2.71	0.54
24:V:139:GLY:O	24:V:141:HIS:HD2	1.90	0.54
11:I:93:ARG:HB3	11:I:93:ARG:NH1	2.22	0.54
1:O:244:C:OP2	8:F:38:LYS:HE3	2.08	0.54
1:O:2094:G:H4'	4:B:245:SER:HB3	1.89	0.54
1:O:1333:U:H2'	1:O:1334:C:C6	2.43	0.54
1:O:797:A:H5'	27:Y:10:ARG:HG2	1.90	0.54
27:Y:38:LYS:HD3	36:Y:8425:HOH:O	2.06	0.54
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.33	0.54
17:O:103:THR:O	17:O:107:GLU:HG3	2.08	0.54
1:O:2265:U:H2'	1:O:2266:A:C8	2.43	0.54
4:B:7:ARG:HG2	4:B:7:ARG:NH1	2.15	0.54
5:C:77:ALA:O	5:C:78:ARG:HG3	2.07	0.54
3:A:100:PRO:HG2	3:A:103:VAL:CG2	2.34	0.54
1:O:282:C:H1'	1:O:368:C:H42	1.71	0.54
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.90	0.54
10:H:35:ASN:HD21	10:H:80:ASN:HA	1.73	0.54
1:O:1384:C:H5'	25:W:30:MET:HG2	1.90	0.54
26:X:106:THR:HG23	26:X:107:PRO:HD2	1.90	0.54
12:J:30:LYS:O	12:J:55:VAL:HG13	2.07	0.54
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.90	0.54
1:O:2289:G:H21	1:O:2291:A:H2	1.52	0.54
2:9:44:A:O4'	6:D:76:ARG:NE	2.41	0.54
10:H:71:TYR:C	10:H:73:GLN:N	2.59	0.54
1:O:1730:G:H5'	1:O:1731:C:C6	2.43	0.54
4:B:162:MET:CE	4:B:308:LEU:HD21	2.38	0.54
8:F:47:LEU:HD22	8:F:108:LEU:CD1	2.38	0.54
1:O:2815:G:N7	11:I:80:LYS:NZ	2.55	0.54
1:O:951:A:C2'	1:O:952:G:H5'	2.38	0.54
4:B:248:ARG:O	4:B:251:VAL:CG1	2.56	0.54
10:H:45:GLN:HG3	10:H:135:TRP:NE1	2.23	0.53
6:D:99:ASP:O	6:D:159:PRO:HG3	2.07	0.53
14:L:172:GLY:C	14:L:183:VAL:HG11	2.26	0.53
4:B:297:VAL:HB	36:B:8610:HOH:O	2.08	0.53
1:O:500:G:H21	19:Q:98:ASN:HD21	1.56	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:81:GLU:O	6:D:85:GLN:HG3	2.08	0.53
1:0:1044:C:H3'	1:0:1045:G:H5''	1.90	0.53
1:0:1919:A:H4'	36:0:4360:HOH:O	2.08	0.53
1:0:2301:A:H5''	1:0:2302:A:H5'	1.89	0.53
27:Y:30:GLU:HA	27:Y:33:HIS:CB	2.39	0.53
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.37	0.53
11:I:107:ASN:C	11:I:107:ASN:HD22	2.12	0.53
36:0:8593:HOH:O	4:B:214:PRO:HD2	2.08	0.53
1:0:2812:A:N7	36:0:7048:HOH:O	2.34	0.53
10:H:147:ARG:HA	10:H:150:LYS:NZ	2.24	0.53
29:1:19:SER:HB3	36:1:4479:HOH:O	2.09	0.53
8:F:39:SER:CB	8:F:45:ALA:HB2	2.39	0.53
29:1:48:ASP:O	29:1:49:GLU:HB2	2.08	0.53
15:M:154:LEU:HG	15:M:155:GLU:N	2.22	0.53
1:0:775:G:OP1	28:Z:16:HIS:HE1	1.91	0.53
1:0:2526:C:O2'	1:0:2527:U:H5'	2.08	0.53
2:9:3:A:OP2	2:9:3:A:C8	2.61	0.53
13:K:143:THR:CG2	13:K:144:ASP:H	2.20	0.53
1:0:272:A:H5'	1:0:273:G:OP2	2.08	0.53
9:G:12:ILE:HD12	36:G:692:HOH:O	2.07	0.53
4:B:16:ARG:NE	36:B:8555:HOH:O	2.25	0.53
6:D:57:THR:HG23	6:D:63:ILE:CB	2.38	0.53
12:J:82:ARG:NH2	12:J:115:ARG:HG2	2.23	0.53
8:F:47:LEU:HB2	8:F:108:LEU:HD11	1.90	0.53
7:E:36:PRO:HD3	11:I:127:ILE:HD12	1.90	0.53
17:O:91:LYS:O	17:O:95:GLU:HG3	2.08	0.53
11:I:19:MET:HE3	11:I:132:LEU:HD11	1.89	0.53
24:V:19:ASP:O	24:V:23:MET:HG3	2.09	0.53
8:F:91:VAL:CG1	8:F:92:GLY:H	2.18	0.53
3:A:132:ASP:OD1	3:A:133:ARG:N	2.41	0.53
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.23	0.53
6:D:38:GLU:OE2	6:D:51:ARG:CZ	2.57	0.53
27:Y:11:THR:OG1	27:Y:23:ARG:HB2	2.09	0.53
30:2:60:LYS:HG3	30:2:61:PRO:HD2	1.90	0.53
1:0:703:G:O2'	1:0:704:C:H5'	2.09	0.53
1:0:2591:C:H2'	1:0:2592:G:O4'	2.09	0.53
5:C:27:ARG:HG2	5:C:30:LEU:HG	1.91	0.53
17:O:105:LEU:HD21	17:O:137:LEU:HD21	1.91	0.53
23:U:56:ILE:O	23:U:60:GLN:HG3	2.08	0.53
12:J:58:THR:HG22	12:J:59:LYS:HG3	1.91	0.53
1:0:920:C:H5''	1:0:921:G:O5'	2.08	0.53
21:S:49:GLU:HB3	21:S:59:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:76:VAL:HG23	27:Y:63:LYS:HB3	1.89	0.53
28:Z:8:GLN:HE22	28:Z:11:LYS:NZ	2.07	0.53
24:V:141:HIS:HB2	24:V:146:ILE:HG12	1.89	0.53
1:O:2717:C:H2'	1:O:2718:C:C5'	2.35	0.53
14:L:185:PRO:HG2	14:L:189:VAL:HG11	1.91	0.53
23:U:64:GLY:O	23:U:65:ASP:CB	2.57	0.53
4:B:42:ALA:HB1	4:B:308:LEU:HD11	1.89	0.53
1:O:1523:G:H2'	1:O:1524:U:C6	2.44	0.53
36:O:9045:HOH:O	17:O:81:LYS:HG2	2.08	0.53
8:F:22:VAL:HG21	8:F:104:ALA:HB2	1.90	0.53
19:Q:106:GLY:HA2	19:Q:109:MET:CE	2.39	0.53
27:Y:30:GLU:HA	27:Y:33:HIS:HB3	1.90	0.53
22:T:14:GLU:OE1	22:T:15:PRO:HD2	2.09	0.53
24:V:41:TYR:O	24:V:45:VAL:HG13	2.09	0.53
4:B:119:HIS:O	4:B:121:PRO:HD3	2.09	0.53
19:Q:132:ARG:NH1	36:Q:8580:HOH:O	2.41	0.53
7:E:166:VAL:HG12	36:E:3134:HOH:O	2.08	0.53
10:H:144:GLU:OE1	10:H:144:GLU:HA	2.08	0.53
2:9:23:U:H3'	2:9:24:U:H5''	1.91	0.53
1:O:2507:G:H2'	1:O:2510:C:H42	1.74	0.53
1:O:2896:A:OP1	25:W:15:ARG:NH1	2.42	0.53
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.90	0.53
1:O:2072:G:C6	1:O:2533:C:H1'	2.44	0.53
1:O:2638:G:H1'	36:O:7295:HOH:O	2.08	0.53
8:F:19:ALA:O	8:F:22:VAL:HG22	2.09	0.53
36:O:8627:HOH:O	5:C:103:ASN:HB3	2.08	0.53
26:X:178:HIS:CG	26:X:179:PRO:HD2	2.44	0.53
1:O:1299:G:H5'	36:O:3580:HOH:O	2.09	0.53
19:Q:104:PHE:HB2	19:Q:109:MET:HE1	1.90	0.53
8:F:100:ASP:HB3	36:F:5691:HOH:O	2.09	0.53
8:F:2:VAL:HG11	14:L:23:LEU:HD23	1.89	0.53
1:O:1306:U:OP1	5:C:184:ARG:HD2	2.09	0.53
1:O:1353:C:P	36:O:4189:HOH:O	2.67	0.53
13:K:125:PHE:CZ	13:K:140:VAL:HG13	2.44	0.53
5:C:180:SER:HB2	36:C:8444:HOH:O	2.09	0.53
5:C:246:ARG:NH2	36:C:8424:HOH:O	2.41	0.52
4:B:138:GLY:O	4:B:139:ASP:O	2.26	0.52
1:O:2787:C:H5	36:O:4141:HOH:O	1.91	0.52
6:D:99:ASP:HB2	6:D:103:ASN:H	1.75	0.52
6:D:99:ASP:HB3	6:D:103:ASN:H	1.74	0.52
6:D:163:VAL:HA	36:D:6326:HOH:O	2.09	0.52
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.36	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:109:LEU:HD13	12:J:113:ILE:HD11	1.91	0.52
11:I:45:VAL:HG21	11:I:129:PHE:CD1	2.45	0.52
1:0:2415:A:C2	15:M:25:ARG:HB3	2.44	0.52
4:B:17:LYS:O	4:B:260:HIS:HD2	1.93	0.52
26:X:184:GLU:OE1	26:X:204:ARG:NH1	2.42	0.52
25:W:30:MET:CE	25:W:58:ALA:HB3	2.39	0.52
3:A:164:ARG:CZ	36:A:8591:HOH:O	2.57	0.52
1:0:317:A:H5''	21:S:52:ARG:HD2	1.91	0.52
16:N:7:LEU:HD22	36:N:5650:HOH:O	2.09	0.52
3:A:211:LYS:HD3	36:A:8613:HOH:O	2.09	0.52
10:H:55:GLN:HE22	10:H:91:HIS:CD2	2.27	0.52
16:N:47:ARG:HG3	16:N:47:ARG:NH1	2.22	0.52
19:Q:39:THR:HB	19:Q:42:GLU:CD	2.30	0.52
1:0:184:G:H5''	14:L:153:THR:HG22	1.91	0.52
1:0:949:U:O2'	18:P:40:HIS:HE1	1.93	0.52
20:R:56:ASN:O	29:1:8:LYS:HE2	2.09	0.52
1:0:2329:C:O2'	1:0:2330:U:H5'	2.10	0.52
6:D:105:SER:CB	6:D:131:THR:HG23	2.35	0.52
18:P:40:HIS:CE1	18:P:94:GLN:HA	2.45	0.52
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.52
14:L:77:PHE:HD2	36:L:8526:HOH:O	1.91	0.52
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.52
27:Y:11:THR:CG2	27:Y:23:ARG:HB2	2.40	0.52
19:Q:17:MET:HE1	19:Q:19:ARG:NH2	2.24	0.52
30:2:87:ARG:NH1	36:2:8525:HOH:O	2.43	0.52
2:9:23:U:C3'	2:9:24:U:H5''	2.39	0.52
6:D:146:LYS:NZ	15:M:107:ASN:ND2	2.56	0.52
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.43	0.52
7:E:22:VAL:O	7:E:28:SER:HA	2.10	0.52
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.40	0.52
1:0:2524:G:H21	1:0:2526:C:N4	2.07	0.52
19:Q:132:ARG:CZ	36:Q:8580:HOH:O	2.57	0.52
3:A:94:LEU:N	3:A:94:LEU:HD23	2.24	0.52
15:M:37:ARG:NH2	36:M:8535:HOH:O	2.43	0.52
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.52
5:C:246:ARG:CZ	36:C:8424:HOH:O	2.56	0.52
4:B:310:ARG:NH2	36:B:8558:HOH:O	2.41	0.52
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.92	0.52
11:I:88:PRO:O	11:I:94:GLY:HA3	2.10	0.52
15:M:169:PRO:O	15:M:172:PHE:HB3	2.10	0.52
1:0:2090:G:H2'	1:0:2091:G:C8	2.44	0.52
3:A:179:MET:HG2	3:A:186:TRP:CB	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:960:G:H2'	1:0:960:G:N3	2.25	0.52
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.40	0.52
27:Y:29:VAL:O	27:Y:33:HIS:HB2	2.10	0.52
1:0:182:G:O3'	14:L:157:LEU:CD1	2.57	0.52
6:D:94:ALA:O	6:D:95:THR:O	2.27	0.52
8:F:99:THR:HG23	8:F:99:THR:O	2.09	0.52
1:0:1878:G:O2'	1:0:1879:U:C6	2.60	0.52
1:0:1197:G:N2	36:0:5753:HOH:O	2.43	0.52
12:J:10:GLN:NE2	12:J:10:GLN:N	2.42	0.52
1:0:88:G:H5'	1:0:88:G:H8	1.75	0.52
1:0:1497:G:H4'	1:0:1627:G:O2'	2.10	0.52
14:L:12:TRP:CE2	14:L:20:ILE:HD11	2.45	0.52
1:0:1213:C:O2'	1:0:1214:G:H5'	2.10	0.52
14:L:182:LYS:HB2	14:L:194:ALA:HB2	1.92	0.52
1:0:1503:U:H2'	1:0:1504:A:O4'	2.10	0.52
14:L:137:ASP:HA	14:L:142:LYS:HE3	1.91	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.75	0.52
20:R:57:THR:CG2	20:R:58:MET:N	2.73	0.52
6:D:27:ILE:HG22	6:D:28:GLY:N	2.20	0.52
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.40	0.52
1:0:2768:A:O2'	1:0:2769:C:H5'	2.10	0.52
36:9:8514:HOH:O	15:M:107:ASN:HB3	2.09	0.52
1:0:2837:U:H2'	36:0:6360:HOH:O	2.10	0.52
8:F:46:GLU:N	36:F:3461:HOH:O	2.42	0.52
1:0:710:G:P	16:N:24:ALA:HB3	2.50	0.52
4:B:175:LEU:O	4:B:175:LEU:HD23	2.09	0.52
19:Q:29:LYS:HB3	36:Q:8530:HOH:O	2.08	0.52
1:0:2300:A:H4'	1:0:2301:A:O5'	2.10	0.52
7:E:43:ASP:HA	36:E:5864:HOH:O	2.10	0.52
5:C:151:GLN:O	5:C:154:VAL:HB	2.10	0.52
13:K:149:ARG:O	13:K:150:GLN:HB2	2.10	0.52
2:9:1:U:O3'	2:9:3:A:H5'	2.10	0.51
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.71	0.51
1:0:88:G:C6	29:1:24:TRP:CZ3	2.98	0.51
1:0:1450:C:C4'	1:0:1451:C:OP2	2.57	0.51
6:D:135:VAL:HG22	6:D:136:ARG:N	2.25	0.51
22:T:33:SER:O	22:T:37:GLU:HG3	2.10	0.51
6:D:50:VAL:O	6:D:71:ALA:HA	2.10	0.51
4:B:305:ASP:O	4:B:306:LYS:HB2	2.11	0.51
15:M:157:PRO:HA	36:M:8527:HOH:O	2.09	0.51
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.93	0.51
1:0:1462:C:H2'	1:0:1463:A:C8	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:37:LEU:CD1	25:W:85:VAL:HG21	2.20	0.51
14:L:114:VAL:HB	14:L:159:THR:HG23	1.90	0.51
1:O:2506:A:O2'	1:O:2507:G:O5'	2.27	0.51
14:L:37:VAL:HG21	14:L:108:LYS:HG3	1.91	0.51
14:L:81:ARG:HG3	14:L:85:ARG:HB2	1.91	0.51
3:A:170:VAL:HG13	27:Y:22:ILE:HG21	1.92	0.51
26:X:144:ARG:NH2	36:X:8615:HOH:O	2.44	0.51
36:O:7089:HOH:O	30:2:60:LYS:HG3	2.11	0.51
18:P:75:ILE:CD1	18:P:84:ILE:HD11	2.41	0.51
1:O:2812:A:C2	1:O:2814:A:N6	2.68	0.51
1:O:283:U:H5''	1:O:284:C:OP2	2.11	0.51
2:9:29:C:C2'	2:9:30:C:H5'	2.40	0.51
1:O:470:U:O2'	28:Z:16:HIS:CD2	2.62	0.51
1:O:1878:G:H4'	36:O:3624:HOH:O	2.10	0.51
1:O:538:C:H5''	1:O:539:G:C8	2.45	0.51
2:9:49:G:O2'	2:9:50:G:H5'	2.10	0.51
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.92	0.51
10:H:59:ASN:ND2	10:H:59:ASN:N	2.55	0.51
3:A:34:ASP:OD1	3:A:35:GLY:N	2.40	0.51
21:S:80:GLU:OE2	21:S:84:GLY:HA2	2.11	0.51
26:X:155:ARG:NH1	36:X:8559:HOH:O	2.44	0.51
14:L:84:LYS:HE2	36:L:8576:HOH:O	2.10	0.51
25:W:74:ALA:HB1	25:W:85:VAL:HG22	1.92	0.51
1:O:1118:A:C8	1:O:1119:G:H5''	2.45	0.51
19:Q:18:LEU:HG	19:Q:91:LEU:HD13	1.91	0.51
7:E:69:ILE:HA	7:E:72:MET:HE2	1.92	0.51
6:D:65:GLU:HA	36:D:6752:HOH:O	2.09	0.51
6:D:11:HIS:O	6:D:12:GLU:HB3	2.10	0.51
1:O:1236:A:H2'	1:O:1237:U:O4'	2.11	0.51
36:O:5650:HOH:O	29:1:20:ARG:HB3	2.11	0.51
23:U:49:LEU:O	23:U:53:ILE:HG13	2.11	0.51
2:9:23:U:H6	2:9:23:U:C5'	2.21	0.51
15:M:71:TRP:HE3	15:M:175:LEU:HD22	1.76	0.51
8:F:91:VAL:CG1	8:F:92:GLY:N	2.72	0.51
14:L:87:MET:HB2	14:L:91:ILE:CD1	2.39	0.51
12:J:106:GLY:HA3	36:J:5264:HOH:O	2.09	0.51
24:V:38:THR:HG22	24:V:39:ASP:N	2.26	0.51
6:D:58:VAL:CG1	6:D:59:GLY:N	2.72	0.51
19:Q:132:ARG:HG2	19:Q:133:ALA:N	2.26	0.51
21:S:92:ASP:OD1	21:S:94:SER:HB3	2.11	0.51
1:O:2251:G:H2'	1:O:2252:A:C8	2.46	0.51
1:O:1972:U:H2'	1:O:1973:A:C5'	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:113:ARG:HH21	14:L:156:ARG:HG2	1.74	0.51
1:0:475:G:OP1	5:C:73:LEU:HD22	2.11	0.51
22:T:52:THR:HG22	22:T:54:THR:HB	1.93	0.51
16:N:96:VAL:HG13	16:N:100:GLN:HB2	1.93	0.51
6:D:170:TYR:O	6:D:171:ASP:HB3	2.10	0.51
6:D:25:MET:CE	6:D:41:LEU:HG	2.34	0.51
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.28	0.51
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.76	0.51
10:H:75:SER:C	10:H:79:ALA:HB2	2.31	0.51
13:K:57:VAL:O	13:K:57:VAL:HG12	2.11	0.51
4:B:156:LYS:HE3	36:B:8635:HOH:O	2.09	0.51
1:0:1470:A:OP1	14:L:93:ARG:HD2	2.11	0.51
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.51
2:9:6:C:C5'	15:M:37:ARG:HH12	2.12	0.51
14:L:52:LEU:HD13	14:L:116:ASN:HB3	1.93	0.51
26:X:187:VAL:HB	36:X:8572:HOH:O	2.10	0.51
3:A:93:THR:HG23	3:A:154:ALA:O	2.11	0.51
1:0:1044:C:H5''	36:0:8542:HOH:O	2.10	0.51
1:0:1862:C:H1'	36:0:6742:HOH:O	2.10	0.51
15:M:182:GLY:O	15:M:183:ASP:O	2.28	0.51
17:O:10:ALA:HA	17:O:13:VAL:CG1	2.41	0.51
1:0:2672:C:O2'	1:0:2673:U:H5'	2.11	0.51
10:H:75:SER:O	10:H:79:ALA:HB2	2.11	0.51
15:M:152:GLU:C	15:M:154:LEU:H	2.13	0.51
1:0:1787:C:OP1	17:O:68:LYS:HE2	2.11	0.51
25:W:18:ARG:NH1	36:W:4132:HOH:O	2.41	0.51
1:0:1592:G:O2'	1:0:1593:C:O4'	2.27	0.51
24:V:119:HIS:HD2	24:V:120:PRO:O	1.94	0.51
15:M:180:LEU:O	15:M:181:ASP:HB3	2.10	0.51
24:V:5:VAL:O	24:V:52:VAL:HG22	2.11	0.50
1:0:1180:U:H2'	1:0:1181:A:O4'	2.11	0.50
1:0:1194:A:N6	1:0:1206:U:O4	2.44	0.50
4:B:41:PHE:CE1	4:B:79:MET:HG3	2.45	0.50
10:H:71:TYR:O	10:H:73:GLN:N	2.44	0.50
25:W:43:VAL:HG12	25:W:44:ASP:N	2.25	0.50
4:B:14:GLY:HA2	4:B:15:PRO:C	2.31	0.50
1:0:2842:G:H2'	1:0:2843:A:H5'	1.92	0.50
24:V:122:ARG:HH22	24:V:154:ARG:C	2.15	0.50
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.26	0.50
24:V:38:THR:HG22	24:V:39:ASP:H	1.77	0.50
1:0:2363:G:O3'	18:P:11:ARG:NH1	2.44	0.50
27:Y:19:GLY:O	27:Y:23:ARG:HG2	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2361:A:H8	1:0:2361:A:H5'	1.76	0.50
1:0:899:C:H5'	36:0:9711:HOH:O	2.11	0.50
14:L:69:LYS:HG2	14:L:127:LYS:HG3	1.93	0.50
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.50
1:0:1733:A:H4'	4:B:212:GLN:HA	1.92	0.50
12:J:74:VAL:HG12	12:J:75:ARG:HG3	1.92	0.50
14:L:63:VAL:HG21	14:L:109:PHE:CZ	2.47	0.50
6:D:146:LYS:HZ3	15:M:107:ASN:HD21	1.57	0.50
4:B:168:GLY:O	4:B:169:GLY:O	2.30	0.50
21:S:49:GLU:OE2	21:S:97:ARG:HD2	2.10	0.50
13:K:97:VAL:HG12	13:K:98:GLU:O	2.12	0.50
10:H:65:ARG:HB3	36:H:8383:HOH:O	2.12	0.50
12:J:87:ARG:NE	36:J:4854:HOH:O	2.44	0.50
10:H:48:LEU:HD13	10:H:146:TRP:HB3	1.93	0.50
11:I:74:ARG:O	11:I:78:ILE:HG12	2.11	0.50
1:0:818:A:O2'	27:Y:13:ARG:HD3	2.11	0.50
13:K:61:ALA:HA	36:K:8563:HOH:O	2.12	0.50
4:B:63:GLU:HG3	4:B:63:GLU:O	2.11	0.50
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.47	0.50
36:0:3572:HOH:O	4:B:27:ASN:HB2	2.10	0.50
10:H:56:ILE:HG21	10:H:61:LEU:HD13	1.94	0.50
4:B:320:GLN:HG3	4:B:321:PRO:HD2	1.94	0.50
24:V:125:HIS:HD2	24:V:127:GLY:H	1.58	0.50
12:J:28:GLU:HB3	12:J:59:LYS:HB2	1.93	0.50
4:B:27:ASN:H	4:B:27:ASN:HD22	1.59	0.50
2:9:35:C:H5''	36:9:8452:HOH:O	2.12	0.50
30:2:56:PRO:N	36:2:8549:HOH:O	2.43	0.50
5:C:233:THR:HG22	5:C:234:VAL:N	2.26	0.50
2:9:54:A:O2'	2:9:55:U:H5'	2.12	0.50
1:0:1834:C:H2'	1:0:1840:A:N6	2.26	0.50
3:A:194:MET:CE	3:A:199:HIS:HB2	2.42	0.50
4:B:333:GLU:HB2	22:T:14:GLU:OE2	2.10	0.50
1:0:2004:U:H2'	1:0:2004:U:O2	2.10	0.50
1:0:371:U:H2'	1:0:372:A:C8	2.45	0.50
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.94	0.50
1:0:188:C:H5''	14:L:163:LEU:HD21	1.94	0.50
15:M:77:ASN:OD1	15:M:80:SER:HB2	2.12	0.50
2:9:92:G:H2'	2:9:93:A:C8	2.47	0.50
15:M:139:TRP:N	36:M:8572:HOH:O	2.45	0.50
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.77	0.50
26:X:186:ARG:NH1	26:X:186:ARG:HG2	2.26	0.50
4:B:248:ARG:HG2	36:B:8577:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:43:PRO:HG3	14:L:62:VAL:HG21	1.94	0.50
22:T:39:ASN:ND2	22:T:44:ARG:HH11	2.10	0.50
1:O:1559:A:H1'	36:O:5381:HOH:O	2.11	0.50
1:O:1717:A:H5''	17:O:54:LYS:HB2	1.94	0.50
12:J:29:LEU:HB3	12:J:55:VAL:CG1	2.30	0.50
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.41	0.50
27:Y:30:GLU:O	27:Y:33:HIS:HB3	2.12	0.50
25:W:78:GLU:HG2	25:W:79:GLU:N	2.25	0.50
1:O:2756:U:N3	1:O:2896:A:H2	2.09	0.50
6:D:57:THR:HG23	6:D:63:ILE:CG2	2.41	0.50
1:O:1527:A:H1'	1:O:1528:A:C8	2.46	0.50
26:X:107:PRO:HB3	26:X:182:PHE:CE2	2.47	0.50
10:H:47:GLU:CB	10:H:133:ILE:HD13	2.42	0.49
6:D:99:ASP:CB	6:D:103:ASN:HB2	2.41	0.49
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.42	0.49
10:H:147:ARG:HA	10:H:150:LYS:HZ2	1.77	0.49
25:W:41:PHE:O	25:W:43:VAL:HG23	2.11	0.49
1:O:920:C:H5'	1:O:921:G:C4	2.47	0.49
1:O:2434:A:O3'	30:2:28:GLY:HA3	2.12	0.49
1:O:2320:U:H4'	1:O:2321:A:O4'	2.12	0.49
1:O:175:G:H2'	14:L:192:ALA:HB3	1.94	0.49
1:O:1996:U:O2'	1:O:1997:A:H5'	2.12	0.49
22:T:47:ARG:CG	36:T:4381:HOH:O	2.60	0.49
7:E:10:ASP:HA	36:E:3707:HOH:O	2.11	0.49
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.12	0.49
17:O:71:LYS:O	17:O:71:LYS:HG3	2.12	0.49
1:O:1164:U:N3	1:O:1192:A:H2	2.02	0.49
1:O:380:A:OP2	14:L:9:ARG:HD2	2.11	0.49
1:O:1972:U:H2'	1:O:1973:A:H5'	1.95	0.49
1:O:1060:C:H6	1:O:1060:C:H5'	1.77	0.49
19:Q:29:LYS:HD3	36:Q:8530:HOH:O	2.11	0.49
1:O:1656:A:H2'	1:O:1657:A:O4'	2.12	0.49
28:Z:10:LYS:HG3	36:Z:8430:HOH:O	2.11	0.49
1:O:344:C:H2'	1:O:345:G:O4'	2.11	0.49
1:O:644:G:N3	1:O:644:G:H5'	2.27	0.49
1:O:1289:C:O2'	1:O:1290:G:H5'	2.12	0.49
1:O:1500:U:P	17:O:41:ARG:HH22	2.35	0.49
1:O:654:A:OP2	16:N:38:ARG:HD3	2.12	0.49
1:O:1266:U:H4'	26:X:115:ARG:HH21	1.76	0.49
26:X:107:PRO:HB3	26:X:182:PHE:CD2	2.48	0.49
1:O:1056:U:H2'	1:O:1057:A:O4'	2.12	0.49
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:559:U:H5'	1:0:559:U:C6	2.39	0.49
12:J:45:PRO:HB2	36:J:7169:HOH:O	2.13	0.49
1:0:656:G:OP2	16:N:37:ARG:HD2	2.12	0.49
1:0:407:A:H5'	36:0:5542:HOH:O	2.12	0.49
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.49
36:0:6950:HOH:O	21:S:9:LYS:HD2	2.12	0.49
3:A:128:LEU:HG	36:A:8576:HOH:O	2.11	0.49
1:0:396:U:OP2	30:2:38:ARG:NH1	2.44	0.49
1:0:538:C:OP2	26:X:134:HIS:HE1	1.96	0.49
22:T:44:ARG:HB3	36:T:3805:HOH:O	2.11	0.49
14:L:155:HIS:CE1	14:L:158:ARG:HE	2.29	0.49
1:0:1595:G:O2'	1:0:1596:U:H5'	2.12	0.49
5:C:219:ASN:O	5:C:222:ASP:OD1	2.30	0.49
21:S:71:VAL:HG11	21:S:90:PRO:CB	2.28	0.49
1:0:1010:C:H4'	15:M:4:PRO:HB2	1.95	0.49
11:I:42:GLU:O	11:I:131:THR:HG23	2.12	0.49
7:E:11:VAL:CG1	7:E:12:ASP:N	2.75	0.49
10:H:130:HIS:CG	10:H:133:ILE:HD11	2.46	0.49
15:M:73:ALA:HB2	15:M:163:PHE:CZ	2.48	0.49
11:I:47:THR:HG22	11:I:48:GLY:N	2.28	0.49
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.47	0.49
13:K:148:GLU:HB2	36:K:8587:HOH:O	2.11	0.49
14:L:78:ASN:C	14:L:79:LYS:HG2	2.33	0.49
4:B:279:THR:OG1	4:B:290:VAL:HB	2.12	0.49
22:T:52:THR:HG22	22:T:54:THR:H	1.77	0.49
30:2:55:VAL:HB	30:2:56:PRO:HD2	1.95	0.49
24:V:126:ASP:HB3	24:V:135:GLY:O	2.12	0.49
22:T:47:ARG:HG3	36:T:4381:HOH:O	2.13	0.49
1:0:2472:C:O2'	1:0:2634:G:H4'	2.12	0.49
1:0:1192:A:N3	36:0:3910:HOH:O	2.45	0.49
1:0:1204:C:C4	1:0:1205:U:C5	3.00	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.49
24:V:65:VAL:HA	24:V:68:THR:CG2	2.42	0.49
27:Y:26:VAL:O	27:Y:30:GLU:HG3	2.13	0.49
1:0:1172:G:H5'	36:0:6784:HOH:O	2.13	0.49
1:0:2756:U:N3	1:0:2896:A:C2	2.72	0.49
5:C:246:ARG:NH1	36:C:8372:HOH:O	2.46	0.49
1:0:2316:G:H4'	36:0:5611:HOH:O	2.12	0.49
21:S:38:ARG:NH1	36:S:6217:HOH:O	2.45	0.49
1:0:447:A:O2'	1:0:448:G:H5'	2.13	0.49
4:B:27:ASN:HB3	36:B:8632:HOH:O	2.12	0.49
36:0:5713:HOH:O	29:1:44:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:7:ARG:HD2	4:B:9:GLY:O	2.12	0.49
13:K:120:LEU:HD12	13:K:133:VAL:HG21	1.95	0.49
4:B:41:PHE:CD2	4:B:190:MET:HE3	2.47	0.49
11:I:45:VAL:HG22	11:I:46:ILE:N	2.27	0.49
15:M:139:TRP:HA	15:M:139:TRP:CE3	2.48	0.49
7:E:92:PRO:HB2	36:E:4917:HOH:O	2.12	0.49
2:9:24:U:H4'	2:9:25:G:OP1	2.13	0.48
1:0:820:G:C6	3:A:171:LYS:HB2	2.48	0.48
24:V:84:VAL:HG12	36:V:6679:HOH:O	2.13	0.48
26:X:189:ASN:ND2	26:X:192:ASP:H	2.11	0.48
1:0:281:U:H3'	36:0:6729:HOH:O	2.13	0.48
27:Y:30:GLU:HB3	27:Y:34:LYS:HE3	1.95	0.48
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.42	0.48
3:A:130:THR:HG22	3:A:131:HIS:O	2.12	0.48
2:9:41:C:C6	6:D:50:VAL:HG21	2.47	0.48
14:L:182:LYS:HD2	14:L:193:LYS:HB2	1.95	0.48
1:0:256:C:H2'	1:0:257:G:O4'	2.13	0.48
29:1:24:TRP:NE1	36:1:6863:HOH:O	2.43	0.48
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.96	0.48
1:0:1730:G:C5'	1:0:1731:C:C6	2.96	0.48
21:S:41:ARG:NH1	21:S:41:ARG:HG2	2.28	0.48
1:0:2256:G:H2'	1:0:2257:G:C5'	2.43	0.48
14:L:5:TYR:HE2	14:L:46:LEU:HD13	1.78	0.48
4:B:248:ARG:O	4:B:251:VAL:HG12	2.13	0.48
1:0:1234:U:N3	4:B:244:PRO:HB3	2.29	0.48
19:Q:68:HIS:CD2	19:Q:76:ASP:HB2	2.48	0.48
5:C:150:THR:HA	5:C:203:ALA:O	2.14	0.48
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.43	0.48
8:F:113:ASP:O	8:F:117:GLU:HG3	2.13	0.48
1:0:681:G:N3	1:0:681:G:H5'	2.29	0.48
14:L:115:LEU:HD13	14:L:116:ASN:HB2	1.95	0.48
1:0:2768:A:H5''	36:0:3935:HOH:O	2.13	0.48
36:0:5044:HOH:O	14:L:58:GLN:HG3	2.13	0.48
28:Z:28:HIS:CD2	28:Z:31:LYS:HG3	2.48	0.48
26:X:172:THR:HG22	26:X:173:ALA:N	2.29	0.48
20:R:73:ASP:OD1	20:R:75:GLN:HB2	2.13	0.48
26:X:200:THR:HG22	26:X:201:GLU:CG	2.33	0.48
26:X:126:PRO:HG2	26:X:128:PHE:CZ	2.47	0.48
6:D:10:PHE:CD1	6:D:11:HIS:N	2.81	0.48
14:L:74:ARG:NH1	14:L:74:ARG:HG3	2.28	0.48
1:0:2044:G:OP1	25:W:23:HIS:HE1	1.97	0.48
1:0:1699:C:H4'	36:0:5960:HOH:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:62:ALA:HB2	13:K:103:ALA:CB	2.43	0.48
10:H:26:LYS:HD3	10:H:89:PRO:CG	2.42	0.48
1:O:1192:A:H3'	1:O:1193:A:H5'	1.94	0.48
21:S:41:ARG:NH1	21:S:42:VAL:O	2.46	0.48
1:O:2256:G:H2'	1:O:2257:G:H5'	1.95	0.48
1:O:1484:G:H2'	36:O:8618:HOH:O	2.13	0.48
1:O:1940:C:H4'	36:O:6871:HOH:O	2.12	0.48
1:O:168:C:O2'	1:O:169:A:H5'	2.13	0.48
1:O:278:A:H2'	1:O:279:C:O4'	2.14	0.48
5:C:140:VAL:HG12	5:C:141:SER:N	2.29	0.48
15:M:37:ARG:CZ	36:M:8535:HOH:O	2.62	0.48
27:Y:38:LYS:HG3	36:Y:8431:HOH:O	2.14	0.48
24:V:3:ALA:O	24:V:54:PHE:HA	2.14	0.48
2:9:42:C:O2	6:D:76:ARG:NH1	2.47	0.48
1:O:2420:G:H4'	36:O:3602:HOH:O	2.13	0.48
4:B:207:LYS:HG2	4:B:304:PRO:HB3	1.94	0.48
1:O:121:U:OP2	29:1:10:ARG:NH2	2.39	0.48
7:E:77:THR:OG1	7:E:78:GLU:N	2.45	0.48
10:H:26:LYS:HD3	10:H:89:PRO:HG3	1.95	0.48
27:Y:46:LYS:NZ	36:Y:8442:HOH:O	2.46	0.48
1:O:1666:C:C2'	1:O:1667:A:C5'	2.92	0.48
1:O:2896:A:N3	1:O:2896:A:H2'	2.29	0.48
30:2:48:ASN:ND2	30:2:50:GLY:H	2.11	0.48
1:O:1819:G:H2'	1:O:1820:G:C4'	2.44	0.48
1:O:2837:U:H1'	4:B:307:ARG:HH12	1.79	0.48
2:9:91:C:H2'	2:9:92:G:O4'	2.13	0.48
1:O:2326:U:H4'	1:O:2412:G:H4'	1.96	0.48
26:X:122:ARG:NH2	36:X:8536:HOH:O	2.46	0.48
6:D:67:ASP:OD2	6:D:69:ILE:HD11	2.13	0.48
10:H:55:GLN:HE21	10:H:124:ARG:NE	2.02	0.48
12:J:75:ARG:HG2	12:J:90:PHE:CD2	2.49	0.48
24:V:122:ARG:CG	24:V:122:ARG:HH11	2.19	0.48
17:O:59:ARG:HH22	17:O:66:GLN:HE22	1.60	0.48
21:S:41:ARG:O	21:S:43:ASN:ND2	2.47	0.48
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.43	0.48
1:O:450:C:OP1	5:C:184:ARG:NH2	2.31	0.48
1:O:1028:U:H1'	36:O:3157:HOH:O	2.14	0.48
6:D:101:THR:HG22	36:D:7400:HOH:O	2.14	0.48
7:E:95:VAL:O	7:E:126:ILE:HD13	2.13	0.48
24:V:130:HIS:O	24:V:136:GLY:HA3	2.14	0.48
1:O:2073:G:OP2	1:O:2490:A:H5'	2.14	0.48
15:M:58:LEU:HD12	15:M:58:LEU:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:46:VAL:O	10:H:146:TRP:CH2	2.63	0.48
4:B:162:MET:CE	4:B:310:ARG:HD3	2.44	0.48
1:0:1477:C:H5'	1:0:1868:G:H5''	1.95	0.48
1:0:941:G:O2'	1:0:942:U:H5'	2.13	0.48
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.48
21:S:73:HIS:CD2	21:S:88:PRO:HG3	2.49	0.48
1:0:1003:U:O2'	10:H:90:PHE:HE1	1.96	0.48
1:0:1667:A:H2'	1:0:1668:U:H6	1.78	0.47
15:M:171:HIS:CE1	36:M:8569:HOH:O	2.67	0.47
4:B:144:THR:HG22	4:B:145:HIS:N	2.28	0.47
3:A:36:ASP:O	3:A:38:ILE:N	2.47	0.47
1:0:656:G:H5'	16:N:3:THR:HG22	1.96	0.47
15:M:79:PRO:HG3	15:M:142:THR:O	2.14	0.47
1:0:584:U:H3'	36:0:5614:HOH:O	2.12	0.47
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.47
1:0:2443:C:H3'	36:0:9984:HOH:O	2.14	0.47
15:M:32:PRO:HD2	15:M:99:GLU:O	2.14	0.47
6:D:167:GLU:OE2	6:D:173:GLU:HG2	2.13	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.47
1:0:2791:U:H1'	1:0:2792:A:H5''	1.95	0.47
36:0:6749:HOH:O	14:L:13:LYS:HE2	2.13	0.47
1:0:1409:G:H5'	36:0:3237:HOH:O	2.14	0.47
2:9:64:C:H2'	2:9:65:A:H5'	1.97	0.47
1:0:1909:A:N1	1:0:2128:G:H1'	2.28	0.47
10:H:157:ILE:CG2	10:H:158:ASN:N	2.77	0.47
1:0:182:G:H4'	14:L:157:LEU:HD13	1.96	0.47
6:D:94:ALA:HB3	6:D:174:VAL:HA	1.96	0.47
26:X:154:ARG:HH12	26:X:155:ARG:HG3	1.79	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.96	0.47
10:H:84:ARG:CZ	10:H:135:TRP:HH2	2.26	0.47
1:0:1166:A:H61	1:0:1180:U:H3	1.61	0.47
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.43	0.47
7:E:31:ARG:HH12	7:E:68:HIS:CE1	2.32	0.47
8:F:58:GLU:HA	8:F:61:MET:HG3	1.96	0.47
1:0:1500:U:OP2	17:O:41:ARG:NH2	2.48	0.47
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.14	0.47
15:M:184:ILE:HG22	15:M:185:GLU:N	2.27	0.47
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.47
21:S:18:GLU:O	21:S:21:LYS:HG2	2.15	0.47
9:G:20:VAL:O	9:G:24:VAL:HG23	2.15	0.47
18:P:30:VAL:O	18:P:30:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:163:PRO:O	10:H:164:ALA:HB2	2.14	0.47
36:O:4483:HOH:O	10:H:57:ARG:HG3	2.14	0.47
1:O:2769:C:H2'	1:O:2770:G:C5'	2.44	0.47
22:T:17:THR:HG22	22:T:18:GLY:N	2.30	0.47
25:W:76:ARG:HG3	25:W:76:ARG:NH1	2.28	0.47
25:W:76:ARG:O	25:W:77:PHE:HB3	2.14	0.47
3:A:51:ARG:NH2	3:A:69:LEU:HD13	2.28	0.47
8:F:46:GLU:O	8:F:73:PRO:HD2	2.14	0.47
6:D:59:GLY:C	6:D:61:PHE:H	2.18	0.47
17:O:105:LEU:CD2	17:O:137:LEU:HD21	2.45	0.47
30:2:3:MET:O	30:2:90:PHE:HA	2.14	0.47
17:O:98:ILE:HD12	17:O:102:ARG:NE	2.30	0.47
1:O:432:G:O2'	1:O:433:C:H5'	2.14	0.47
4:B:32:ASP:HA	36:B:8575:HOH:O	2.13	0.47
21:S:63:ILE:HD11	21:S:75:GLU:HB2	1.95	0.47
1:O:2670:G:O2'	1:O:2671:U:H5'	2.15	0.47
10:H:132:PHE:O	10:H:133:ILE:HD13	2.13	0.47
10:H:149:ALA:C	10:H:151:MET:H	2.17	0.47
15:M:90:LEU:CB	15:M:186:LEU:HD22	2.44	0.47
10:H:150:LYS:HG2	36:H:8381:HOH:O	2.14	0.47
7:E:132:THR:O	7:E:132:THR:HG23	2.15	0.47
10:H:111:MET:O	10:H:114:PRO:HD3	2.14	0.47
1:O:2488:A:H2	36:O:6800:HOH:O	1.96	0.47
1:O:621:C:H5'	26:X:132:ASP:OD2	2.15	0.47
25:W:70:ILE:O	25:W:70:ILE:HG23	2.14	0.47
10:H:86:ARG:HD3	10:H:130:HIS:HD2	1.80	0.47
1:O:2720:C:O2	12:J:87:ARG:NH2	2.48	0.47
24:V:110:GLN:NE2	24:V:110:GLN:HA	2.30	0.47
36:9:8462:HOH:O	15:M:147:ILE:HD12	2.14	0.47
10:H:150:LYS:HE2	36:H:8377:HOH:O	2.14	0.47
6:D:146:LYS:HZ1	15:M:107:ASN:HD21	1.60	0.47
5:C:107:ARG:NH2	36:C:8457:HOH:O	2.39	0.47
10:H:127:GLY:O	10:H:128:ALA:CB	2.63	0.47
4:B:168:GLY:N	4:B:174:ARG:HD3	2.29	0.47
13:K:53:ARG:HH22	13:K:57:VAL:HG12	1.79	0.47
1:O:1878:G:O2'	1:O:1879:U:P	2.73	0.47
26:X:115:ARG:NE	36:X:8557:HOH:O	2.47	0.47
1:O:2361:A:H5''	36:O:8523:HOH:O	2.15	0.47
8:F:117:GLU:C	8:F:119:ARG:H	2.18	0.47
1:O:671:A:O2'	1:O:672:G:H2'	2.15	0.47
1:O:581:G:H5'	36:O:7219:HOH:O	2.14	0.47
7:E:21:THR:HG23	7:E:30:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1681:G:H5''	1:0:1682:A:H5'	1.96	0.47
1:0:2724:U:H2'	1:0:2725:G:O4'	2.14	0.47
1:0:119:A:H2'	1:0:120:A:H5''	1.95	0.47
7:E:108:LEU:HB3	36:E:1306:HOH:O	2.15	0.47
1:0:1181:A:C2	1:0:1192:A:C8	3.03	0.47
14:L:173:LEU:HD23	14:L:183:VAL:HG12	1.97	0.47
29:1:18:ASN:ND2	29:1:40:ARG:H	2.09	0.47
25:W:9:VAL:HG13	25:W:88:GLU:OE2	2.15	0.47
15:M:143:ARG:HA	15:M:172:PHE:CD2	2.50	0.47
1:0:1003:U:O2	10:H:90:PHE:CZ	2.68	0.47
1:0:2563:U:H2'	1:0:2565:C:O5'	2.14	0.47
1:0:2010:A:H2'	36:0:5476:HOH:O	2.15	0.47
14:L:57:LYS:HE2	14:L:140:ALA:O	2.14	0.47
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.80	0.47
17:O:16:VAL:CG1	17:O:17:GLY:N	2.78	0.47
22:T:49:LEU:HD11	36:T:3805:HOH:O	2.15	0.47
1:0:2353:A:H4'	1:0:2354:A:O5'	2.13	0.47
1:0:291:C:H2'	1:0:292:G:O4'	2.15	0.47
1:0:189:A:OP1	14:L:171:ARG:NH2	2.47	0.47
1:0:1185:U:H5'	36:0:6994:HOH:O	2.15	0.47
10:H:136:VAL:HG23	36:H:8343:HOH:O	2.14	0.47
4:B:79:MET:HE3	4:B:144:THR:HG21	1.97	0.47
4:B:307:ARG:HD3	36:B:8524:HOH:O	2.15	0.47
4:B:82:VAL:HG12	4:B:101:TRP:CE3	2.50	0.47
1:0:1250:C:O2'	1:0:1251:C:H5'	2.15	0.47
13:K:101:ASP:C	13:K:103:ALA:H	2.18	0.47
1:0:1753:C:O2	4:B:229:ARG:NH2	2.46	0.47
4:B:80:ARG:HD3	36:B:8611:HOH:O	2.15	0.47
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.45	0.47
30:2:7:PHE:HE2	30:2:22:VAL:HG21	1.80	0.47
24:V:21:LEU:CD2	24:V:48:VAL:HG11	2.43	0.46
10:H:150:LYS:NZ	36:H:8377:HOH:O	2.47	0.46
1:0:283:U:H5	1:0:284:C:N4	2.12	0.46
1:0:1741:U:O2'	1:0:2723:G:H4'	2.15	0.46
1:0:1120:U:H5'	1:0:1121:G:OP2	2.15	0.46
5:C:13:ASP:OD1	5:C:13:ASP:O	2.33	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.15	0.46
7:E:34:TRP:O	11:I:127:ILE:HD11	2.15	0.46
16:N:25:VAL:HG23	16:N:26:TRP:N	2.30	0.46
2:9:24:U:C6	36:9:8477:HOH:O	2.56	0.46
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.39	0.46
1:0:1505:U:C6	1:0:1505:U:H5'	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:603:A:H4'	1:0:604:G:O5'	2.15	0.46
3:A:223:ARG:NH1	36:A:8518:HOH:O	2.48	0.46
1:0:1167:G:O2'	1:0:1168:C:H5'	2.15	0.46
24:V:41:TYR:HA	24:V:44:MET:HE3	1.97	0.46
16:N:25:VAL:HG23	16:N:26:TRP:H	1.80	0.46
6:D:153:THR:HG22	36:D:5234:HOH:O	2.15	0.46
10:H:47:GLU:CB	10:H:133:ILE:CD1	2.91	0.46
15:M:37:ARG:HD3	15:M:37:ARG:HA	1.71	0.46
17:O:38:GLU:HA	17:O:41:ARG:HH11	1.78	0.46
6:D:55:LYS:O	6:D:56:ARG:HB2	2.14	0.46
26:X:112:GLU:OE2	26:X:115:ARG:NH1	2.49	0.46
24:V:41:TYR:CD2	24:V:44:MET:HE3	2.50	0.46
13:K:21:ARG:N	36:K:8531:HOH:O	2.48	0.46
1:0:204:A:C2'	1:0:205:U:H5'	2.45	0.46
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.98	0.46
8:F:60:VAL:HG12	8:F:60:VAL:O	2.16	0.46
11:I:46:ILE:HA	36:I:1123:HOH:O	2.15	0.46
1:0:585:C:H6	36:O:5614:HOH:O	1.97	0.46
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.97	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.50	0.46
12:J:66:ARG:HH11	12:J:66:ARG:HG2	1.80	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46
15:M:89:GLY:O	15:M:92:ALA:HB3	2.15	0.46
24:V:4:LEU:HD23	24:V:54:PHE:HB3	1.97	0.46
15:M:7:LYS:HE2	36:M:8514:HOH:O	2.14	0.46
1:0:1439:C:OP1	29:1:41:HIS:HE1	1.97	0.46
14:L:37:VAL:HG12	14:L:63:VAL:HG11	1.97	0.46
11:I:70:PHE:CD2	11:I:70:PHE:O	2.68	0.46
12:J:4:LEU:HD22	12:J:116:GLU:HB3	1.98	0.46
4:B:241:PRO:HD2	36:B:8661:HOH:O	2.14	0.46
15:M:100:ALA:O	15:M:129:ILE:HG23	2.16	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
14:L:167:GLY:O	14:L:171:ARG:HG3	2.15	0.46
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.45	0.46
5:C:214:THR:HB	36:C:8325:HOH:O	2.16	0.46
1:0:1419:U:H2'	1:0:1685:A:C2	2.51	0.46
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.97	0.46
21:S:27:LEU:HD23	21:S:98:VAL:HB	1.98	0.46
12:J:101:ASN:O	12:J:102:GLU:HB2	2.15	0.46
18:P:66:LYS:HB2	18:P:70:ALA:O	2.16	0.46
2:9:107:C:H5	36:9:8436:HOH:O	1.97	0.46
1:0:2730:G:O2'	1:0:2731:G:H5'	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:128:A:H3'	1:0:128:A:C8	2.50	0.46
1:0:2502:C:C4'	10:H:151:MET:HG2	2.46	0.46
2:9:3:A:H61	2:9:22:G:H1'	1.75	0.46
10:H:157:ILE:HG22	10:H:158:ASN:N	2.30	0.46
11:I:93:ARG:HH11	11:I:93:ARG:CB	2.23	0.46
1:0:656:G:H5'	16:N:3:THR:CG2	2.46	0.46
25:W:9:VAL:HG13	25:W:88:GLU:OE1	2.16	0.46
8:F:101:ALA:HA	36:F:5413:HOH:O	2.16	0.46
2:9:88:G:OP1	24:V:130:HIS:NE2	2.46	0.46
4:B:75:GLU:C	4:B:77:PRO:HD3	2.35	0.46
6:D:128:LEU:N	36:D:6007:HOH:O	2.49	0.46
20:R:8:PRO:HD2	23:U:32:ALA:HA	1.98	0.46
1:0:2831:C:H2'	1:0:2832:C:H5'	1.98	0.46
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.15	0.46
1:0:1119:G:H2'	11:I:52:GLN:NE2	2.31	0.46
4:B:7:ARG:NH1	4:B:11:LEU:CD2	2.79	0.46
1:0:88:G:C6	29:1:24:TRP:CE3	3.04	0.46
14:L:38:VAL:HG12	14:L:38:VAL:O	2.15	0.46
1:0:431:G:OP1	14:L:48:ARG:NH1	2.49	0.46
24:V:38:THR:HB	36:V:5390:HOH:O	2.15	0.46
1:0:474:C:O3'	5:C:73:LEU:CD2	2.64	0.46
8:F:107:VAL:HG23	36:F:6617:HOH:O	2.16	0.46
22:T:9:CYS:CA	22:T:52:THR:HG23	2.45	0.46
28:Z:28:HIS:HD2	28:Z:30:LYS:H	1.62	0.46
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.51	0.46
25:W:66:THR:HG23	25:W:67:PRO:HD2	1.98	0.46
1:0:2403:C:H3'	36:0:4722:HOH:O	2.16	0.46
1:0:2649:A:H5'	1:0:2649:A:H8	1.80	0.46
10:H:134:ALA:HB3	10:H:142:VAL:HG21	1.97	0.46
1:0:1603:A:H5''	1:0:1605:G:H5'	1.97	0.46
1:0:2415:A:H2'	1:0:2416:G:H5'	1.96	0.46
4:B:55:ASN:HB3	4:B:64:GLY:H	1.81	0.46
11:I:19:MET:CE	11:I:132:LEU:HD11	2.46	0.46
1:0:2883:A:H2'	1:0:2884:G:O4'	2.16	0.46
1:0:1592:G:HO2'	1:0:1593:C:C4'	2.29	0.46
1:0:1789:G:O6	17:O:73:HIS:HE1	1.98	0.46
10:H:141:ASN:HA	36:H:8365:HOH:O	2.16	0.46
4:B:102:THR:HG21	4:B:182:VAL:O	2.16	0.46
1:0:1735:C:O2'	1:0:1736:A:H5'	2.15	0.46
2:9:3:A:H2	2:9:21:G:N3	2.14	0.46
15:M:5:ARG:HG3	18:P:18:PRO:CB	2.46	0.46
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:39:U:H3'	2:9:40:C:H5''	1.98	0.46
1:0:475:G:C5'	5:C:73:LEU:HD23	2.46	0.46
2:9:31:C:H2'	2:9:32:G:O4'	2.16	0.46
1:0:2679:G:H2'	1:0:2681:A:OP2	2.16	0.46
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.45	0.46
1:0:820:G:C5	3:A:171:LYS:HB2	2.51	0.45
1:0:88:G:N7	29:1:28:LYS:HD2	2.30	0.45
1:0:2768:A:H3'	36:0:3935:HOH:O	2.15	0.45
4:B:221:GLN:HE22	12:J:42:ASN:ND2	2.08	0.45
23:U:55:ARG:NH2	36:U:4428:HOH:O	2.40	0.45
4:B:72:THR:HB	36:B:8610:HOH:O	2.15	0.45
3:A:48:ASP:HB3	36:A:8608:HOH:O	2.17	0.45
26:X:154:ARG:NH1	26:X:155:ARG:HG3	2.31	0.45
1:0:1418:U:OP1	29:1:42:TRP:HB3	2.16	0.45
12:J:79:PRO:HB2	36:J:782:HOH:O	2.15	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.16	0.45
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.31	0.45
10:H:84:ARG:CZ	10:H:135:TRP:CH2	2.99	0.45
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.46	0.45
10:H:150:LYS:HA	10:H:153:VAL:HG22	1.97	0.45
4:B:60:SER:C	4:B:62:ARG:H	2.18	0.45
17:O:120:ARG:NH2	17:O:123:TYR:CD2	2.84	0.45
30:2:73:GLU:HB2	36:2:8527:HOH:O	2.16	0.45
21:S:40:VAL:HG22	21:S:41:ARG:N	2.31	0.45
8:F:28:ALA:HB3	8:F:99:THR:O	2.15	0.45
20:R:32:ALA:HA	20:R:36:GLU:OE1	2.16	0.45
1:0:2559:C:H4'	36:0:6780:HOH:O	2.16	0.45
1:0:2297:U:H1'	36:0:4686:HOH:O	2.17	0.45
22:T:50:GLU:CD	36:T:7349:HOH:O	2.53	0.45
18:P:25:PRO:HA	18:P:26:PRO:HD3	1.84	0.45
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.45
10:H:26:LYS:HA	10:H:58:HIS:CD2	2.51	0.45
15:M:86:LEU:O	15:M:90:LEU:HG	2.16	0.45
1:0:1666:C:C2'	1:0:1667:A:H5'	2.44	0.45
1:0:776:A:OP1	28:Z:28:HIS:HE1	2.00	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
23:U:57:LYS:HA	23:U:60:GLN:HE21	1.81	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.16	0.45
11:I:90:LYS:HB2	34:I:8502:CL:CL	2.53	0.45
20:R:6:LYS:HB2	20:R:27:ALA:O	2.15	0.45
1:0:2401:A:H5'	36:0:9000:HOH:O	2.16	0.45
1:0:821:U:H5''	36:0:9559:HOH:O	2.14	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:33:LYS:HE2	36:C:8362:HOH:O	2.16	0.45
6:D:166:ILE:O	6:D:169:THR:N	2.49	0.45
15:M:71:TRP:N	36:M:8540:HOH:O	2.49	0.45
30:2:65:THR:HB	30:2:83:TRP:H	1.81	0.45
4:B:280:VAL:HG13	4:B:333:GLU:O	2.17	0.45
4:B:16:ARG:NH2	36:B:8555:HOH:O	2.44	0.45
1:0:1730:G:C5'	1:0:1731:C:H6	2.29	0.45
15:M:154:LEU:CG	15:M:155:GLU:H	2.26	0.45
36:0:6931:HOH:O	21:S:2:LYS:HE2	2.14	0.45
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.97	0.45
1:0:2912:C:H2'	1:0:2913:A:O4'	2.17	0.45
10:H:81:TYR:C	10:H:81:TYR:CD1	2.89	0.45
4:B:205:VAL:O	4:B:307:ARG:NE	2.49	0.45
24:V:11:VAL:O	24:V:12:ASN:HB2	2.16	0.45
4:B:1:PRO:O	4:B:2:GLN:HB2	2.16	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
5:C:234:VAL:HG22	5:C:234:VAL:O	2.17	0.45
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.99	0.45
1:0:1218:U:H2'	1:0:1219:U:C6	2.51	0.45
4:B:275:GLY:O	4:B:291:ASP:HA	2.17	0.45
12:J:27:ARG:HD2	36:J:4747:HOH:O	2.17	0.45
1:0:797:A:H4'	27:Y:10:ARG:N	2.31	0.45
2:9:2:U:OP2	2:9:3:A:H5'	2.16	0.45
1:0:1268:C:O2'	1:0:1269:G:H5'	2.15	0.45
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.30	0.45
12:J:98:VAL:HG22	12:J:102:GLU:C	2.36	0.45
12:J:78:LYS:HA	12:J:79:PRO:HD3	1.86	0.45
1:0:1314:U:H2'	36:0:5390:HOH:O	2.16	0.45
3:A:8:ARG:HG2	36:A:8553:HOH:O	2.16	0.45
8:F:50:VAL:HG11	8:F:60:VAL:HG11	1.97	0.45
5:C:162:VAL:HG12	5:C:162:VAL:O	2.17	0.45
1:0:1086:A:N6	24:V:11:VAL:HG11	2.32	0.45
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.17	0.45
4:B:127:GLN:HG3	36:B:8647:HOH:O	2.16	0.45
24:V:129:LYS:HG2	36:V:1990:HOH:O	2.17	0.45
1:0:420:U:H2'	1:0:421:C:C6	2.52	0.45
18:P:31:GLU:CD	18:P:93:ARG:HH12	2.20	0.45
1:0:814:G:H4'	36:0:9643:HOH:O	2.16	0.45
7:E:93:MET:HE1	7:E:165:GLY:N	2.32	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.46	0.45
21:S:45:GLY:C	36:S:3851:HOH:O	2.55	0.45
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:39:GLN:O	5:C:43:LYS:HD3	2.17	0.45
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.99	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.16	0.45
19:Q:84:ALA:O	19:Q:88:PHE:HD1	1.99	0.45
1:0:1176:C:H1'	36:0:3439:HOH:O	2.16	0.45
1:0:514:G:O5'	1:0:514:G:H8	1.99	0.45
1:0:1183:C:N4	36:0:3910:HOH:O	2.48	0.45
7:E:32:ARG:O	7:E:33:LEU:HD23	2.16	0.45
15:M:167:ASP:O	15:M:168:LEU:HD23	2.17	0.45
1:0:566:A:H2'	1:0:567:U:O4'	2.17	0.45
27:Y:33:HIS:HE1	27:Y:49:ARG:NE	2.15	0.45
14:L:67:ILE:CD1	14:L:104:ARG:HD2	2.47	0.45
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.45
1:0:1684:A:O2'	1:0:1685:A:H5''	2.17	0.45
1:0:1168:C:H5	36:0:7027:HOH:O	1.99	0.45
10:H:113:ALA:N	10:H:114:PRO:CD	2.80	0.45
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.17	0.45
7:E:20:ILE:HD12	7:E:33:LEU:HD12	2.00	0.45
23:U:1:THR:HG23	23:U:2:VAL:N	2.22	0.45
36:0:5586:HOH:O	27:Y:34:LYS:HE2	2.17	0.45
29:1:18:ASN:HD22	29:1:18:ASN:HA	1.59	0.45
23:U:55:ARG:NE	36:U:4428:HOH:O	2.37	0.45
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.47	0.45
1:0:926:A:O2'	13:K:41:HIS:HD2	2.00	0.45
2:9:51:A:H5'	15:M:160:SER:HB3	1.99	0.45
3:A:17:ARG:HD2	36:A:8542:HOH:O	2.17	0.45
11:I:142:ASN:O	11:I:144:THR:N	2.50	0.45
1:0:2642:G:H2'	1:0:2643:G:O4'	2.17	0.45
5:C:153:VAL:O	5:C:157:LEU:HG	2.17	0.45
1:0:1162:G:H2'	36:0:6102:HOH:O	2.17	0.45
5:C:164:ALA:O	5:C:167:ASP:HB2	2.17	0.45
1:0:1636:G:O2'	1:0:1637:A:H5'	2.16	0.45
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.17	0.45
21:S:74:VAL:HB	21:S:77:VAL:HG21	1.99	0.45
1:0:1182:C:H1'	1:0:1192:A:H8	1.82	0.44
12:J:75:ARG:HE	12:J:94:ALA:HB3	1.82	0.44
24:V:122:ARG:NE	36:V:5817:HOH:O	2.50	0.44
9:G:27:ILE:HD12	9:G:70:ALA:HB1	1.99	0.44
1:0:2467:A:O2'	1:0:2468:A:H2'	2.17	0.44
8:F:28:ALA:CB	8:F:99:THR:HG23	2.47	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
11:I:63:ILE:HG22	11:I:64:GLY:N	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2326:U:H4'	1:0:2412:G:C4'	2.47	0.44
1:0:2777:G:O2'	1:0:2778:A:H5'	2.17	0.44
19:Q:14:ALA:HB3	19:Q:147:LEU:HB2	1.99	0.44
1:0:870:G:C3'	1:0:871:G:H5''	2.47	0.44
2:9:2:U:OP2	2:9:2:U:H4'	2.17	0.44
10:H:14:TYR:N	10:H:91:HIS:HE1	2.16	0.44
1:0:2505:G:H8	36:0:5154:HOH:O	2.00	0.44
30:2:84:ARG:HD3	36:2:8550:HOH:O	2.17	0.44
14:L:186:SER:O	14:L:189:VAL:HG12	2.17	0.44
6:D:76:ARG:O	6:D:77:ASP:HB2	2.18	0.44
24:V:13:MET:HE1	24:V:18:GLN:HA	2.00	0.44
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.47	0.44
1:0:2515:C:H2'	1:0:2516:G:O4'	2.17	0.44
3:A:165:THR:HG22	36:A:8620:HOH:O	2.17	0.44
36:0:7244:HOH:O	5:C:94:THR:HG21	2.16	0.44
19:Q:125:ARG:HG2	36:Q:8540:HOH:O	2.17	0.44
14:L:122:GLU:HB2	14:L:126:HIS:O	2.17	0.44
4:B:198:GLU:HB3	36:B:8601:HOH:O	2.16	0.44
10:H:31:PHE:HA	10:H:85:ILE:CG2	2.48	0.44
15:M:47:LEU:CD1	15:M:97:VAL:HG11	2.47	0.44
4:B:125:GLU:OE2	4:B:129:ARG:NH1	2.50	0.44
4:B:36:PRO:HA	4:B:168:GLY:HA2	1.95	0.44
10:H:35:ASN:ND2	10:H:79:ALA:O	2.51	0.44
21:S:52:ARG:HB2	21:S:95:ASN:HB3	1.99	0.44
1:0:2388:C:H5'	18:P:83:THR:O	2.17	0.44
11:I:22:VAL:O	11:I:26:VAL:HG23	2.16	0.44
27:Y:59:HIS:HA	36:Y:8442:HOH:O	2.18	0.44
28:Z:25:LYS:HD2	29:1:49:GLU:H	1.82	0.44
17:O:10:ALA:CA	17:O:13:VAL:HG12	2.45	0.44
15:M:154:LEU:O	15:M:155:GLU:CB	2.66	0.44
1:0:2456:A:H2'	1:0:2457:U:C6	2.52	0.44
24:V:108:ARG:HE	24:V:114:PRO:CG	2.30	0.44
13:K:125:PHE:CE1	13:K:140:VAL:HG13	2.53	0.44
7:E:152:THR:HG21	7:E:165:GLY:HA2	1.99	0.44
1:0:2338:G:H2'	6:D:129:ASP:OD1	2.17	0.44
1:0:1555:G:H4'	1:0:1630:A:H2	1.83	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.52	0.44
5:C:236:THR:O	5:C:237:GLU:C	2.55	0.44
6:D:169:THR:O	6:D:170:TYR:HB2	2.17	0.44
10:H:57:ARG:O	10:H:61:LEU:HD22	2.18	0.44
15:M:91:ARG:HG3	15:M:186:LEU:HD23	1.99	0.44
10:H:43:PRO:HD2	10:H:137:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:187:VAL:HG12	26:X:205:ILE:HA	1.99	0.44
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.26	0.44
28:Z:25:LYS:O	28:Z:25:LYS:HG2	2.18	0.44
1:0:2781:U:H2'	1:0:2782:G:H5'	2.00	0.44
15:M:11:ARG:HG3	15:M:14:ARG:NH1	2.33	0.44
19:Q:25:PHE:CE2	19:Q:29:LYS:CE	3.00	0.44
24:V:42:ARG:O	24:V:45:VAL:HG22	2.17	0.44
1:0:1006:A:N1	1:0:2311:A:H1'	2.33	0.44
13:K:128:GLY:O	13:K:132:LYS:HG3	2.17	0.44
6:D:140:ARG:O	6:D:144:ARG:HG2	2.17	0.44
10:H:110:GLY:N	36:H:8393:HOH:O	2.50	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.32	0.44
15:M:161:GLY:O	15:M:162:ASP:C	2.55	0.44
6:D:95:THR:C	6:D:97:GLN:N	2.68	0.44
36:O:6063:HOH:O	27:Y:22:ILE:HG13	2.17	0.44
5:C:13:ASP:N	36:C:8440:HOH:O	2.50	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
13:K:92:ASP:OD1	13:K:94:ARG:HB2	2.17	0.44
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.44
12:J:55:VAL:CG1	12:J:56:SER:N	2.81	0.44
15:M:182:GLY:N	36:M:8573:HOH:O	2.51	0.44
1:0:1119:G:C8	11:I:52:GLN:NE2	2.85	0.44
6:D:23:VAL:O	6:D:23:VAL:CG2	2.64	0.44
28:Z:8:GLN:HE22	28:Z:11:LYS:HZ2	1.65	0.44
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.99	0.44
11:I:6:PHE:O	11:I:8:ALA:N	2.51	0.44
1:0:1211:G:O2'	1:0:1212:C:H5'	2.17	0.44
1:0:130:C:H5'	36:O:4724:HOH:O	2.17	0.44
1:0:2005:G:OP2	1:0:2005:G:H3'	2.18	0.44
21:S:71:VAL:CG1	21:S:72:ILE:N	2.80	0.44
24:V:26:ILE:HG13	24:V:26:ILE:O	2.18	0.44
24:V:5:VAL:HG22	24:V:32:CYS:HB2	2.00	0.44
24:V:122:ARG:CG	24:V:122:ARG:NH1	2.80	0.44
4:B:146:THR:O	4:B:159:PRO:HB3	2.17	0.44
26:X:106:THR:CG2	26:X:107:PRO:HD2	2.47	0.44
27:Y:11:THR:HG23	27:Y:11:THR:O	2.17	0.44
7:E:84:MET:HE1	7:E:133:VAL:HG21	1.98	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.48	0.44
5:C:7:ASP:OD1	5:C:11:ASN:O	2.36	0.44
1:0:590:A:H2'	1:0:591:A:H5'	2.00	0.44
36:O:5034:HOH:O	4:B:298:LYS:HD3	2.17	0.44
1:0:2812:A:H1'	36:O:5305:HOH:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:183:VAL:HG12	14:L:184:ARG:N	2.32	0.44
36:O:5789:HOH:O	17:O:59:ARG:HD3	2.17	0.44
1:O:2064:U:H4'	1:O:2653:A:OP1	2.18	0.44
1:O:1980:U:O2	1:O:2008:U:H4'	2.18	0.44
24:V:90:TYR:N	24:V:90:TYR:CD1	2.85	0.44
14:L:107:ARG:NH1	36:L:8577:HOH:O	2.48	0.44
15:M:108:SER:HA	15:M:109:PRO:HD3	1.79	0.44
1:O:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:O:2769:C:H2'	1:O:2770:G:H5'	2.00	0.43
1:O:338:C:H4'	5:C:174:ILE:HD12	1.99	0.43
1:O:314:G:N2	1:O:316:A:H3'	2.33	0.43
13:K:121:ILE:HG12	13:K:141:GLU:HB2	1.99	0.43
1:O:816:G:H5'	1:O:1598:A:H4'	1.98	0.43
11:I:26:VAL:HG13	11:I:36:VAL:HG11	1.99	0.43
3:A:135:VAL:N	36:A:8598:HOH:O	2.50	0.43
8:F:21:GLU:O	8:F:24:ARG:HG3	2.17	0.43
1:O:321:A:H1'	36:O:6554:HOH:O	2.18	0.43
1:O:2383:G:H1'	36:O:6223:HOH:O	2.17	0.43
1:O:1902:G:H2'	1:O:1903:U:O4'	2.18	0.43
14:L:125:ARG:NH1	36:L:8596:HOH:O	2.50	0.43
1:O:40:C:H4'	36:O:6522:HOH:O	2.18	0.43
1:O:42:C:H1'	36:O:4186:HOH:O	2.18	0.43
10:H:26:LYS:HG2	10:H:28:ILE:N	2.29	0.43
27:Y:57:CYS:SG	27:Y:59:HIS:HB3	2.58	0.43
13:K:6:ARG:NH2	36:K:8548:HOH:O	2.47	0.43
7:E:7:ILE:HG22	7:E:45:ASP:O	2.19	0.43
6:D:173:GLU:HG3	6:D:174:VAL:N	2.33	0.43
21:S:38:ARG:HG3	21:S:38:ARG:HH11	1.82	0.43
14:L:55:LYS:O	14:L:60:ILE:HD12	2.18	0.43
1:O:1669:A:H2'	1:O:1670:G:H8	1.82	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.53	0.43
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.99	0.43
2:9:59:C:H6	2:9:59:C:O5'	2.01	0.43
1:O:1423:C:O2'	1:O:1424:A:H5'	2.18	0.43
3:A:1:GLY:HA2	3:A:197:VAL:HG23	2.00	0.43
2:9:56:A:C3'	2:9:57:A:H5''	2.49	0.43
4:B:254:GLN:HG2	4:B:255:GLY:N	2.32	0.43
13:K:53:ARG:NH2	13:K:57:VAL:CG1	2.82	0.43
5:C:14:GLY:N	36:C:8440:HOH:O	2.49	0.43
1:O:2419:U:H5''	1:O:2420:G:C5'	2.47	0.43
1:O:2782:G:O6	1:O:2790:C:H5''	2.18	0.43
1:O:2832:C:H5	36:O:6736:HOH:O	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:31:C:H1'	36:9:8392:HOH:O	2.18	0.43
1:0:2083:A:N6	11:I:90:LYS:HE2	2.33	0.43
24:V:90:TYR:CE2	24:V:99:ALA:HB2	2.54	0.43
2:9:4:G:OP1	2:9:59:C:O2'	2.33	0.43
20:R:29:ASP:OD1	20:R:31:ARG:HG3	2.19	0.43
1:0:1342:C:O2'	1:0:1343:C:H5'	2.18	0.43
1:0:1109:U:O4	11:I:21:ARG:HA	2.18	0.43
27:Y:38:LYS:CE	27:Y:45:LYS:HE2	2.34	0.43
15:M:67:ALA:HA	15:M:71:TRP:H	1.83	0.43
11:I:39:VAL:CG1	11:I:107:ASN:HB2	2.49	0.43
25:W:15:ARG:NH1	25:W:15:ARG:HB3	2.32	0.43
4:B:307:ARG:NH1	4:B:307:ARG:CG	2.79	0.43
13:K:72:ASN:OD1	13:K:75:LEU:HD12	2.19	0.43
22:T:13:ILE:HG12	22:T:32:CYS:CB	2.47	0.43
25:W:12:ILE:HG23	25:W:36:HIS:CG	2.53	0.43
1:0:653:C:H2'	1:0:654:A:C8	2.53	0.43
3:A:179:MET:HG2	3:A:186:TRP:CG	2.53	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.43
1:0:426:G:H2'	1:0:427:C:O4'	2.18	0.43
13:K:65:ASP:CG	13:K:111:ALA:HB3	2.38	0.43
24:V:22:GLU:HG2	24:V:27:HIS:CD2	2.54	0.43
10:H:30:GLN:H	10:H:65:ARG:NH1	2.17	0.43
11:I:103:VAL:CG1	36:I:5907:HOH:O	2.64	0.43
1:0:1206:U:H2'	1:0:1207:A:O4'	2.18	0.43
13:K:130:ARG:HA	36:K:8557:HOH:O	2.18	0.43
3:A:105:VAL:CG1	3:A:106:CYS:N	2.81	0.43
4:B:279:THR:CG2	4:B:280:VAL:N	2.81	0.43
1:0:1973:A:H5'	1:0:1973:A:C8	2.44	0.43
21:S:24:ARG:HH21	21:S:39:ASN:ND2	2.13	0.43
13:K:90:ARG:NH1	13:K:119:THR:HG21	2.34	0.43
1:0:1235:G:C1'	11:I:63:ILE:HG23	2.48	0.43
26:X:117:LEU:HD12	26:X:174:VAL:HG11	2.01	0.43
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.49	0.43
36:O:8729:HOH:O	3:A:11:ARG:HD3	2.19	0.43
27:Y:41:VAL:HG12	27:Y:42:CYS:N	2.33	0.43
30:2:91:GLN:O	30:2:92:GLU:HB2	2.18	0.43
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.99	0.43
29:1:36:ASN:HB3	29:1:39:ARG:NE	2.34	0.43
1:0:1467:C:OP1	14:L:35:PRO:HB2	2.19	0.43
14:L:38:VAL:O	14:L:63:VAL:HG13	2.18	0.43
13:K:146:GLY:C	13:K:148:GLU:H	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:F:28:ALA:HB3	8:F:99:THR:HG23	2.00	0.43
1:0:2851:G:C2'	1:0:2852:A:H5'	2.49	0.43
2:9:92:G:H22	10:H:52:LYS:HZ2	1.65	0.43
14:L:25:TRP:HE3	14:L:26:HIS:HD2	1.66	0.43
23:U:23:LEU:HD12	23:U:56:ILE:HD12	2.00	0.43
1:0:1787:C:H4'	1:0:2883:A:O4'	2.18	0.43
1:0:716:G:C2'	1:0:717:C:O5'	2.67	0.43
1:0:559:U:H2'	1:0:560:C:O4'	2.19	0.43
26:X:187:VAL:HB	26:X:203:VAL:HG22	1.99	0.43
14:L:153:THR:O	14:L:156:ARG:HG3	2.18	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
10:H:113:ALA:N	10:H:114:PRO:HD3	2.33	0.43
6:D:84:LEU:HA	6:D:87:ALA:HB3	2.01	0.43
1:0:1592:G:O2'	1:0:1593:C:O5'	2.36	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
8:F:26:THR:HG21	8:F:103:ALA:HB2	1.99	0.43
6:D:99:ASP:HB2	6:D:103:ASN:CB	2.47	0.43
14:L:146:GLN:NE2	36:L:8643:HOH:O	2.51	0.43
24:V:48:VAL:CG1	24:V:48:VAL:O	2.65	0.43
6:D:23:VAL:HG23	6:D:41:LEU:HD22	1.99	0.43
1:0:88:G:N1	29:1:24:TRP:CE3	2.87	0.43
7:E:80:TRP:O	7:E:134:SER:HA	2.18	0.43
27:Y:34:LYS:HE2	36:Y:8426:HOH:O	2.18	0.43
1:0:1328:A:C8	26:X:169:ARG:HD3	2.54	0.43
15:M:149:GLU:O	15:M:152:GLU:HB2	2.19	0.43
27:Y:13:ARG:NH1	27:Y:14:PHE:CE2	2.87	0.43
5:C:33:LYS:HD2	36:C:8459:HOH:O	2.18	0.43
1:0:716:G:H2'	1:0:717:C:O5'	2.19	0.43
1:0:1857:A:N6	1:0:2247:C:H1'	2.34	0.43
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.43
3:A:103:VAL:HA	3:A:104:PRO:HD3	1.89	0.43
3:A:105:VAL:HG13	3:A:155:THR:O	2.19	0.43
1:0:777:U:O2'	28:Z:11:LYS:HG2	2.19	0.43
2:9:27:C:H1'	36:9:8431:HOH:O	2.19	0.43
1:0:1194:A:C6	1:0:1206:U:N3	2.87	0.43
4:B:320:GLN:HG3	4:B:321:PRO:CD	2.48	0.43
15:M:163:PHE:HE1	15:M:171:HIS:HD1	1.67	0.43
6:D:77:ASP:HB3	6:D:78:GLU:H	1.58	0.43
1:0:396:U:H5'	30:2:42:ARG:NH1	2.34	0.43
28:Z:25:LYS:HZ3	28:Z:25:LYS:HG2	1.75	0.43
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.01	0.43
4:B:74:ILE:HG13	36:B:8610:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:84:LEU:C	6:D:86:THR:H	2.22	0.43
19:Q:29:LYS:NZ	36:Q:8538:HOH:O	2.52	0.43
21:S:49:GLU:HB3	21:S:59:GLU:HG3	2.01	0.43
8:F:21:GLU:HA	8:F:24:ARG:HE	1.83	0.43
20:R:29:ASP:OD1	20:R:31:ARG:NH1	2.52	0.43
14:L:49:ALA:C	14:L:54:TYR:HB3	2.39	0.43
1:O:2365:G:H4'	18:P:45:PRO:O	2.18	0.43
1:O:2274:A:H1'	14:L:86:MET:SD	2.59	0.43
4:B:277:GLU:N	4:B:278:PRO:HD2	2.33	0.43
16:N:21:SER:OG	16:N:106:PRO:HB2	2.19	0.43
24:V:88:THR:CG2	24:V:89:ASP:N	2.69	0.42
6:D:67:ASP:O	6:D:69:ILE:HG13	2.18	0.42
12:J:34:VAL:HB	36:J:7169:HOH:O	2.19	0.42
4:B:62:ARG:CB	4:B:65:MET:HE3	2.49	0.42
1:O:1634:G:H2'	1:O:1635:U:C6	2.54	0.42
1:O:869:G:OP1	14:L:79:LYS:HE2	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
12:J:99:ASP:OD1	12:J:101:ASN:N	2.51	0.42
4:B:268:ARG:NE	36:B:8612:HOH:O	2.51	0.42
1:O:514:G:OP1	1:O:514:G:H2'	2.19	0.42
21:S:3:GLN:HA	21:S:4:PRO:HD3	1.83	0.42
14:L:134:ILE:HG23	14:L:141:ILE:HD13	2.01	0.42
12:J:55:VAL:HG12	12:J:56:SER:H	1.83	0.42
24:V:139:GLY:O	24:V:141:HIS:CD2	2.71	0.42
11:I:75:PRO:HD3	11:I:136:SER:OG	2.18	0.42
1:O:736:A:H2'	1:O:737:A:O4'	2.19	0.42
23:U:20:LEU:HD22	23:U:60:GLN:HE22	1.84	0.42
1:O:834:G:H3'	1:O:835:U:H4'	2.00	0.42
1:O:834:G:H4'	1:O:835:U:OP2	2.19	0.42
1:O:564:G:H1'	36:O:5829:HOH:O	2.20	0.42
25:W:26:ALA:HB1	25:W:59:TRP:CE2	2.54	0.42
23:U:12:THR:OG1	23:U:13:PRO:HD2	2.20	0.42
11:I:130:VAL:CG1	11:I:131:THR:N	2.81	0.42
1:O:488:U:O2'	21:S:82:THR:HG21	2.20	0.42
7:E:9:GLU:HG3	7:E:10:ASP:N	2.33	0.42
1:O:2608:C:H2'	36:O:3085:HOH:O	2.19	0.42
1:O:1406:A:H4'	1:O:1407:A:H5''	2.00	0.42
13:K:1:THR:N	36:K:8540:HOH:O	2.53	0.42
10:H:62:GLU:HA	36:H:8383:HOH:O	2.19	0.42
24:V:54:PHE:CZ	24:V:140:LYS:HB2	2.54	0.42
1:O:1173:A:H4'	1:O:1174:A:C8	2.54	0.42
24:V:76:ASP:O	24:V:77:ALA:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:280:VAL:CG1	4:B:334:SER:HA	2.49	0.42
9:G:64:ASN:N	9:G:64:ASN:ND2	2.66	0.42
25:W:43:VAL:CG1	25:W:44:ASP:N	2.81	0.42
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.48	0.42
15:M:139:TRP:HA	15:M:139:TRP:HE3	1.84	0.42
18:P:32:GLU:O	18:P:93:ARG:NH2	2.53	0.42
12:J:125:ALA:C	12:J:127:ALA:H	2.21	0.42
15:M:33:ARG:NH1	15:M:103:ASP:OD2	2.46	0.42
2:9:20:G:H3'	36:9:8434:HOH:O	2.19	0.42
15:M:47:LEU:HD12	15:M:92:ALA:CB	2.48	0.42
1:0:289:G:O2'	1:0:290:C:H5'	2.20	0.42
1:0:2289:G:N2	1:0:2291:A:C2	2.80	0.42
6:D:57:THR:HA	6:D:63:ILE:HA	2.00	0.42
22:T:52:THR:HG21	22:T:54:THR:HB	2.00	0.42
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.42
1:0:2842:G:C2'	1:0:2843:A:H5'	2.49	0.42
7:E:9:GLU:HA	36:E:5240:HOH:O	2.18	0.42
1:0:661:G:C5	1:0:686:A:C2	3.07	0.42
15:M:44:ARG:HG3	15:M:45:ALA:N	2.35	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
16:N:43:VAL:HG12	16:N:44:ASN:O	2.19	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.55	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.42
6:D:19:GLU:O	6:D:133:ASN:HB3	2.20	0.42
10:H:136:VAL:HG22	10:H:137:ASN:N	2.35	0.42
15:M:73:ALA:HB1	15:M:74:PRO:CD	2.49	0.42
15:M:42:HIS:CG	15:M:62:HIS:HE1	2.38	0.42
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.91	0.42
1:0:1123:A:C2	1:0:1129:C:H4'	2.54	0.42
2:9:64:C:C2'	2:9:65:A:H5'	2.49	0.42
16:N:26:TRP:CE3	16:N:26:TRP:HA	2.53	0.42
24:V:1:MET:HB2	24:V:103:GLU:HG2	2.00	0.42
1:0:1367:A:H2'	1:0:1368:U:O4'	2.20	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.19	0.42
27:Y:32:LYS:HB3	27:Y:32:LYS:HE2	1.76	0.42
5:C:16:VAL:CG1	5:C:17:ASP:N	2.81	0.42
21:S:69:LYS:O	21:S:71:VAL:HG23	2.20	0.42
6:D:44:ILE:HG12	6:D:83:PHE:CE1	2.53	0.42
1:0:545:G:H2'	1:0:546:C:O4'	2.20	0.42
9:G:19:GLU:O	9:G:23:ILE:HG13	2.20	0.42
8:F:58:GLU:HA	8:F:61:MET:HE2	2.01	0.42
1:0:1236:A:C8	11:I:63:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:42:ARG:HA	14:L:43:PRO:HD3	1.85	0.42
14:L:191:GLY:O	14:L:192:ALA:HB3	2.20	0.42
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.42
11:I:71:TYR:CD1	11:I:72:PRO:HD2	2.54	0.42
5:C:35:VAL:HG21	5:C:227:GLY:HA2	2.00	0.42
1:0:2001:G:O2'	1:0:2002:C:H5'	2.20	0.42
1:0:1804:A:H2'	1:0:1805:G:C8	2.54	0.42
1:0:1279:U:H5''	36:0:9100:HOH:O	2.20	0.42
28:Z:2:GLY:O	28:Z:6:PRO:HG2	2.19	0.42
15:M:120:GLU:HG3	15:M:136:LEU:HD13	2.02	0.42
1:0:2502:C:H4'	10:H:151:MET:HG2	2.02	0.42
14:L:99:ARG:HD2	14:L:167:GLY:HA2	2.01	0.42
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.35	0.42
3:A:33:GLU:CD	3:A:33:GLU:H	2.23	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.42
7:E:31:ARG:NH1	7:E:68:HIS:CD2	2.88	0.42
1:0:2415:A:N3	15:M:26:LEU:HD13	2.35	0.42
10:H:117:LYS:HB2	36:H:8339:HOH:O	2.19	0.42
1:0:2653:A:H2'	1:0:2654:C:C6	2.55	0.42
1:0:1878:G:O2'	1:0:1879:U:H6	2.03	0.42
6:D:86:THR:HG23	36:D:7477:HOH:O	2.20	0.42
1:0:2820:A:H2'	1:0:2821:C:O4'	2.19	0.42
19:Q:132:ARG:NH2	36:Q:8580:HOH:O	2.52	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.85	0.42
1:0:644:G:H1'	36:0:5924:HOH:O	2.19	0.42
1:0:2681:A:H4'	1:0:2682:C:H5'	2.02	0.42
10:H:94:ARG:NH2	36:H:8332:HOH:O	2.50	0.42
1:0:1883:U:O2'	1:0:1884:G:H5'	2.19	0.42
1:0:249:G:O2'	1:0:250:C:H5'	2.20	0.42
16:N:54:GLU:O	16:N:55:ASP:HB2	2.20	0.42
5:C:139:VAL:CG1	36:C:8447:HOH:O	2.61	0.42
1:0:306:A:P	21:S:38:ARG:HH21	2.43	0.42
22:T:9:CYS:O	22:T:52:THR:HG23	2.20	0.42
1:0:1855:G:H8	3:A:144:GLU:OE2	2.03	0.42
15:M:127:LEU:HA	15:M:127:LEU:HD12	1.85	0.42
1:0:1175:G:H1'	1:0:1193:A:H2'	2.02	0.42
29:1:19:SER:O	29:1:36:ASN:ND2	2.53	0.42
1:0:1524:U:O2'	1:0:1525:G:OP2	2.34	0.42
1:0:2257:G:H4'	1:0:2259:C:C2	2.55	0.42
1:0:2649:A:H5'	1:0:2649:A:C8	2.55	0.42
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.42
12:J:72:VAL:HG11	12:J:121:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:V:146:ILE:HA	24:V:146:ILE:HD13	1.88	0.41
10:H:13:ALA:HA	10:H:91:HIS:CE1	2.55	0.41
19:Q:96:VAL:HG13	19:Q:106:GLY:HA3	2.02	0.41
1:O:88:G:H2'	1:O:89:G:C8	2.54	0.41
3:A:200:PRO:HD3	36:A:8521:HOH:O	2.20	0.41
4:B:145:HIS:CD2	4:B:146:THR:O	2.68	0.41
9:G:67:LEU:O	9:G:71:LEU:HG	2.20	0.41
1:O:1058:A:H2'	1:O:1060:C:C5'	2.47	0.41
1:O:2578:G:C8	1:O:2578:G:H5'	2.51	0.41
28:Z:28:HIS:HD2	28:Z:31:LYS:H	1.68	0.41
18:P:40:HIS:HD2	18:P:60:THR:OG1	2.03	0.41
8:F:26:THR:HG21	8:F:103:ALA:CB	2.48	0.41
4:B:315:VAL:HG23	4:B:316:ARG:HG2	2.01	0.41
1:O:1385:G:O3'	25:W:49:ARG:NH1	2.52	0.41
1:O:1139:U:H2'	1:O:1140:C:C6	2.55	0.41
24:V:29:VAL:O	24:V:30:ASN:HB2	2.19	0.41
21:S:37:GLN:OE1	21:S:118:SER:HA	2.19	0.41
1:O:613:C:H2'	1:O:614:U:H6	1.85	0.41
1:O:2115:U:H2'	1:O:2116:U:C6	2.55	0.41
1:O:2601:A:N1	12:J:38:SER:HB2	2.35	0.41
2:9:24:U:C5	36:9:8477:HOH:O	2.72	0.41
1:O:820:G:O2'	1:O:856:G:H4'	2.20	0.41
10:H:83:PHE:HE1	10:H:146:TRP:CZ2	2.39	0.41
15:M:73:ALA:N	36:M:8569:HOH:O	2.53	0.41
2:9:28:U:H2'	2:9:29:C:C6	2.55	0.41
1:O:2821:C:H4'	4:B:116:PRO:CB	2.49	0.41
15:M:61:ALA:CB	15:M:88:ALA:HB2	2.50	0.41
4:B:305:ASP:O	4:B:306:LYS:CB	2.67	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.21	0.41
1:O:1003:U:O2	10:H:90:PHE:HZ	2.03	0.41
14:L:125:ARG:CZ	36:L:8596:HOH:O	2.68	0.41
1:O:757:C:OP1	13:K:27:ARG:HD2	2.20	0.41
14:L:65:VAL:HG21	14:L:105:ALA:HB2	2.01	0.41
1:O:806:A:H2'	1:O:807:A:O4'	2.20	0.41
1:O:440:C:H2'	1:O:441:A:C8	2.55	0.41
36:O:3538:HOH:O	18:P:13:LYS:HE3	2.19	0.41
3:A:30:ARG:HB3	3:A:30:ARG:HE	1.68	0.41
1:O:2712:G:H5'	36:J:4183:HOH:O	2.19	0.41
10:H:46:VAL:CG1	10:H:146:TRP:HZ3	2.29	0.41
10:H:83:PHE:CE1	10:H:146:TRP:NE1	2.87	0.41
25:W:76:ARG:HA	25:W:82:GLU:O	2.20	0.41
21:S:38:ARG:HG3	21:S:38:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2589:U:H2'	1:0:2590:U:C6	2.55	0.41
15:M:143:ARG:HH12	15:M:173:ASP:CG	2.21	0.41
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.85	0.41
26:X:154:ARG:HH11	26:X:154:ARG:HB3	1.84	0.41
1:0:1593:C:OP1	17:O:117:SER:CB	2.68	0.41
17:O:94:TRP:CZ2	17:O:98:ILE:HG13	2.55	0.41
1:0:858:U:H2'	1:0:859:C:C6	2.55	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.21	0.41
1:0:303:C:H2'	1:0:304:G:O4'	2.21	0.41
36:O:3589:HOH:O	8:F:31:LYS:HE3	2.19	0.41
21:S:78:THR:HB	21:S:87:VAL:O	2.21	0.41
2:9:105:A:H2'	2:9:106:C:O4'	2.20	0.41
1:0:2667:G:H1'	1:0:2914:A:N3	2.34	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.41
1:0:2668:G:H2'	1:0:2669:U:C6	2.55	0.41
1:0:1881:A:OP1	3:A:199:HIS:HE1	2.04	0.41
15:M:163:PHE:O	15:M:164:ASP:O	2.37	0.41
4:B:41:PHE:HB3	4:B:190:MET:CE	2.50	0.41
4:B:60:SER:C	4:B:62:ARG:N	2.73	0.41
23:U:39:ALA:C	23:U:41:GLU:N	2.74	0.41
4:B:258:GLY:N	4:B:260:HIS:CE1	2.86	0.41
3:A:223:ARG:NE	36:A:8575:HOH:O	2.54	0.41
1:0:553:G:P	26:X:204:ARG:NH2	2.93	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.41
5:C:65:ARG:HG3	5:C:67:GLN:HB2	2.03	0.41
1:0:1413:A:H2'	1:0:1414:A:O4'	2.20	0.41
8:F:34:ASN:HA	14:L:4:ALA:HB2	2.02	0.41
20:R:30:ASP:HA	20:R:62:LYS:HE3	2.03	0.41
1:0:1545:C:H2'	1:0:1546:G:O4'	2.21	0.41
21:S:71:VAL:HG12	21:S:72:ILE:N	2.34	0.41
24:V:146:ILE:HG22	24:V:147:ASP:N	2.35	0.41
23:U:42:ASN:O	23:U:44:GLY:N	2.53	0.41
1:0:1205:U:O2	1:0:1205:U:H2'	2.20	0.41
12:J:90:PHE:CD1	12:J:90:PHE:N	2.89	0.41
1:0:262:A:OP2	8:F:91:VAL:HG11	2.20	0.41
15:M:159:TYR:CE2	15:M:163:PHE:HE2	2.36	0.41
1:0:588:G:O6	24:V:154:ARG:NH1	2.53	0.41
7:E:101:GLU:OE2	7:E:115:ARG:HD3	2.21	0.41
16:N:14:LEU:HD23	16:N:102:ILE:CD1	2.48	0.41
1:0:2346:C:H4'	6:D:52:THR:HG22	2.03	0.41
4:B:71:VAL:CG1	4:B:296:LEU:HB3	2.48	0.41
25:W:30:MET:HE1	25:W:55:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2421:G:H3'	1:0:2422:U:C5'	2.51	0.41
28:Z:28:HIS:CD2	28:Z:31:LYS:H	2.38	0.41
36:0:9135:HOH:O	8:F:38:LYS:HE2	2.20	0.41
7:E:35:TYR:HA	11:I:127:ILE:HD12	2.03	0.41
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.41
16:N:26:TRP:HE3	16:N:26:TRP:HA	1.84	0.41
36:0:3919:HOH:O	3:A:11:ARG:CZ	2.69	0.41
1:0:1406:A:N1	36:0:5553:HOH:O	2.37	0.41
1:0:793:A:H5''	17:O:83:LYS:HG2	2.03	0.41
1:0:1926:G:H2'	1:0:1927:A:C8	2.56	0.41
16:N:23:GLY:C	36:N:3062:HOH:O	2.58	0.41
13:K:89:PHE:N	36:K:8570:HOH:O	2.54	0.41
1:0:903:U:OP2	13:K:11:ARG:NH1	2.51	0.41
16:N:98:LEU:HD12	16:N:98:LEU:HA	1.88	0.41
1:0:1752:G:H2'	36:0:7080:HOH:O	2.19	0.41
24:V:6:GLN:HA	24:V:52:VAL:HG23	2.02	0.41
10:H:48:LEU:CD1	10:H:157:ILE:HG21	2.50	0.41
9:G:63:ARG:N	36:G:2569:HOH:O	2.53	0.41
14:L:78:ASN:O	14:L:79:LYS:HG2	2.21	0.41
1:0:2346:C:H4'	6:D:52:THR:CG2	2.50	0.41
36:0:3697:HOH:O	26:X:186:ARG:HD2	2.21	0.41
16:N:77:ALA:HA	16:N:96:VAL:O	2.20	0.41
1:0:513:A:H3'	36:0:3363:HOH:O	2.20	0.41
21:S:1:SER:N	36:S:5837:HOH:O	2.53	0.41
10:H:62:GLU:O	10:H:66:VAL:HG23	2.21	0.41
23:U:1:THR:HG23	23:U:2:VAL:HG23	2.02	0.41
3:A:36:ASP:HB2	3:A:83:GLY:HA3	2.03	0.41
24:V:14:HIS:HB2	24:V:17:ILE:HD12	2.03	0.41
1:0:677:C:H4'	5:C:246:ARG:NH2	2.36	0.41
4:B:205:VAL:HA	4:B:260:HIS:O	2.21	0.41
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.35	0.41
1:0:1525:G:C5'	1:0:1526:A:OP2	2.68	0.41
21:S:48:VAL:HG22	21:S:97:ARG:O	2.21	0.41
21:S:48:VAL:HG13	21:S:49:GLU:N	2.35	0.41
1:0:660:A:H4'	1:0:661:G:O5'	2.21	0.41
7:E:37:ASP:OD1	11:I:125:SER:HB3	2.21	0.41
1:0:305:A:C5	1:0:329:A:C2	3.09	0.41
18:P:16:ASN:HA	18:P:16:ASN:HD22	1.71	0.41
2:9:3:A:H61	2:9:22:G:C1'	2.34	0.41
1:0:771:G:OP2	14:L:79:LYS:HE3	2.21	0.41
7:E:11:VAL:HG11	7:E:22:VAL:HG13	2.02	0.41
1:0:2346:C:O3'	6:D:52:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:129:ARG:NH2	4:B:176:ASP:OD1	2.52	0.41
1:O:2779:G:H21	7:E:143:GLN:HE22	1.69	0.41
1:O:1878:G:H5''	36:O:9307:HOH:O	2.20	0.41
1:O:2241:C:H2'	1:O:2242:U:C6	2.56	0.41
13:K:104:ASP:O	13:K:105:TYR:HB3	2.21	0.41
1:O:40:C:O5'	1:O:40:C:H6	2.04	0.41
27:Y:42:CYS:SG	27:Y:44:PHE:HB2	2.61	0.41
1:O:2597:U:H2'	1:O:2598:U:H5'	2.03	0.41
1:O:412:C:H2'	1:O:413:G:O4'	2.21	0.41
19:Q:149:GLU:HA	19:Q:150:PRO:HD3	1.95	0.41
6:D:15:GLU:HA	6:D:16:PRO:HD3	1.87	0.41
10:H:85:ILE:HB	10:H:132:PHE:HE2	1.84	0.41
25:W:37:LEU:HD21	25:W:72:VAL:HG11	2.02	0.41
6:D:64:ARG:HG2	6:D:66:GLY:O	2.21	0.41
7:E:20:ILE:CD1	7:E:33:LEU:HD12	2.50	0.41
4:B:254:GLN:NE2	36:B:8595:HOH:O	2.51	0.41
14:L:138:HIS:C	14:L:139:PRO:O	2.54	0.41
19:Q:39:THR:CG2	19:Q:42:GLU:HG3	2.50	0.41
7:E:7:ILE:HA	7:E:8:PRO:HD3	1.89	0.41
1:O:2748:G:H5'	36:O:7073:HOH:O	2.21	0.41
28:Z:25:LYS:HD2	29:1:49:GLU:N	2.35	0.41
28:Z:17:THR:HA	29:1:49:GLU:HA	2.03	0.41
6:D:48:MET:HA	6:D:49:PRO:HD3	1.78	0.41
10:H:114:PRO:O	10:H:115:PHE:C	2.58	0.41
15:M:66:LEU:HA	15:M:66:LEU:HD12	1.95	0.41
1:O:1615:A:H4'	36:O:5402:HOH:O	2.20	0.41
1:O:625:U:H5''	1:O:1044:C:N4	2.35	0.41
1:O:1462:C:H2'	1:O:1463:A:H8	1.84	0.41
6:D:153:THR:O	6:D:156:ARG:HB2	2.20	0.41
12:J:101:ASN:O	12:J:102:GLU:CB	2.69	0.41
1:O:2413:A:N7	15:M:109:PRO:HB3	2.35	0.41
14:L:134:ILE:O	14:L:136:PRO:HD3	2.20	0.41
36:O:4589:HOH:O	4:B:216:LYS:HA	2.21	0.41
19:Q:47:LEU:O	19:Q:51:ILE:HG13	2.21	0.41
6:D:151:ILE:HA	6:D:152:PRO:HD3	1.93	0.41
4:B:223:ARG:HG3	4:B:232:TRP:O	2.21	0.41
25:W:51:ASP:O	25:W:53:SER:N	2.54	0.41
1:O:694:A:H2'	1:O:695:C:H5'	2.02	0.41
1:O:141:C:P	36:O:3373:HOH:O	2.79	0.41
5:C:95:GLU:HG3	36:C:8475:HOH:O	2.20	0.41
1:O:1339:G:C6	1:O:1340:G:N1	2.88	0.41
1:O:245:C:H2'	1:O:246:G:H5'	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.41
1:0:638:C:H2'	1:0:639:A:C8	2.56	0.41
1:0:1242:A:C5'	11:I:82:THR:HG23	2.30	0.41
5:C:115:LEU:HA	5:C:115:LEU:HD12	1.89	0.41
10:H:150:LYS:CB	10:H:157:ILE:HD12	2.46	0.41
1:0:2718:C:H5'	1:0:2718:C:C6	2.52	0.41
1:0:2506:A:H1'	36:0:5574:HOH:O	2.21	0.41
15:M:164:ASP:OD1	15:M:167:ASP:HA	2.19	0.41
30:2:65:THR:HG23	30:2:67:LEU:CG	2.45	0.41
1:0:1524:U:O2'	1:0:1525:G:P	2.78	0.41
6:D:18:ILE:HD13	6:D:84:LEU:HD12	2.03	0.41
17:O:131:PHE:CD1	17:O:137:LEU:HD13	2.55	0.41
22:T:49:LEU:CD1	36:T:3805:HOH:O	2.69	0.41
14:L:133:LEU:O	14:L:134:ILE:HD13	2.21	0.41
30:2:15:ASN:ND2	36:2:8547:HOH:O	2.53	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
4:B:88:GLU:HG3	4:B:88:GLU:O	2.20	0.41
6:D:103:ASN:ND2	6:D:133:ASN:HD22	2.18	0.40
1:0:157:G:H4'	14:L:95:LYS:HE3	2.04	0.40
24:V:4:LEU:HA	24:V:4:LEU:HD23	1.94	0.40
14:L:45:ARG:CZ	14:L:48:ARG:HG3	2.50	0.40
3:A:128:LEU:HD21	3:A:131:HIS:CE1	2.55	0.40
1:0:1377:C:H1'	36:0:6797:HOH:O	2.19	0.40
1:0:2909:G:H2'	1:0:2910:A:H8	1.86	0.40
1:0:1878:G:H5''	36:0:4675:HOH:O	2.20	0.40
4:B:82:VAL:CG1	4:B:82:VAL:O	2.67	0.40
27:Y:23:ARG:NH1	36:Y:8404:HOH:O	2.53	0.40
1:0:317:A:OP1	21:S:52:ARG:O	2.39	0.40
4:B:286:ASN:O	4:B:306:LYS:HE3	2.20	0.40
1:0:204:A:H2'	1:0:205:U:H5'	2.03	0.40
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.35	0.40
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.85	0.40
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.40
1:0:1393:A:H2'	1:0:1394:C:C6	2.57	0.40
1:0:1947:G:H2'	1:0:1948:G:C8	2.56	0.40
24:V:2:HIS:HD2	24:V:56:GLU:N	2.19	0.40
13:K:24:ALA:HB2	13:K:30:ARG:HD2	2.03	0.40
1:0:708:A:H2'	1:0:709:G:O4'	2.20	0.40
1:0:166:A:N7	13:K:25:GLY:HA2	2.36	0.40
1:0:2478:U:O2'	1:0:2479:A:H5'	2.21	0.40
1:0:377:C:H5	36:0:9820:HOH:O	2.04	0.40
1:0:2691:A:OP1	1:0:2691:A:H8	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:84:LEU:HD13	4:B:84:LEU:O	2.21	0.40
22:T:6:CYS:HA	22:T:13:ILE:HD11	2.03	0.40
9:G:64:ASN:O	9:G:68:GLU:HG3	2.21	0.40
6:D:59:GLY:O	6:D:61:PHE:N	2.42	0.40
1:O:1677:U:OP2	29:1:8:LYS:NZ	2.51	0.40
36:O:9057:HOH:O	14:L:84:LYS:HD3	2.21	0.40
1:O:2256:G:C2'	1:O:2257:G:H5'	2.51	0.40
7:E:156:ASP:OD2	7:E:157:LYS:HG3	2.19	0.40
1:O:1614:G:H2'	36:O:4136:HOH:O	2.21	0.40
12:J:118:ALA:C	12:J:120:ARG:H	2.24	0.40
5:C:196:THR:HG23	36:C:8400:HOH:O	2.22	0.40
30:2:11:CYS:HB2	30:2:20:HIS:CE1	2.57	0.40
1:O:2471:G:N3	1:O:2633:A:H2	2.18	0.40
6:D:99:ASP:HB2	6:D:103:ASN:CA	2.51	0.40
14:L:95:LYS:HG2	14:L:99:ARG:HB3	2.02	0.40
15:M:175:LEU:HA	15:M:175:LEU:HD12	1.86	0.40
1:O:1194:A:C5	1:O:1206:U:N3	2.90	0.40
11:I:46:ILE:HG12	11:I:53:ILE:HD13	2.03	0.40
30:2:74:CYS:N	36:2:8560:HOH:O	2.54	0.40
13:K:73:VAL:HG11	13:K:118:LEU:HD21	2.01	0.40
6:D:10:PHE:CE1	6:D:11:HIS:HB3	2.55	0.40
19:Q:61:GLN:NE2	36:Q:8538:HOH:O	2.53	0.40
17:O:16:VAL:CG1	17:O:20:ARG:HB2	2.52	0.40
19:Q:119:VAL:HG21	19:Q:142:ASP:CG	2.42	0.40
5:C:46:TYR:CE1	5:C:92:PRO:HB3	2.56	0.40
1:O:2089:A:O2'	1:O:2090:G:H5'	2.22	0.40
15:M:138:ASP:C	36:M:8572:HOH:O	2.60	0.40
1:O:419:A:H1'	1:O:1921:A:C2	2.57	0.40
1:O:151:A:H2'	1:O:152:A:O4'	2.22	0.40
1:O:934:C:H2'	1:O:935:G:C8	2.57	0.40
1:O:1166:A:N3	1:O:1166:A:H2'	2.37	0.40
3:A:192:VAL:O	3:A:207:GLN:HG2	2.22	0.40
14:L:87:MET:HG2	30:2:46:ILE:CG2	2.45	0.40
20:R:53:ASN:ND2	36:R:8320:HOH:O	2.55	0.40
3:A:35:GLY:O	3:A:36:ASP:CB	2.62	0.40
1:O:771:G:P	14:L:79:LYS:HG3	2.61	0.40
6:D:94:ALA:HB3	6:D:174:VAL:CA	2.52	0.40
24:V:13:MET:HE3	24:V:17:ILE:CG2	2.48	0.40
16:N:32:ARG:NE	36:N:3360:HOH:O	2.54	0.40
4:B:275:GLY:C	36:B:8656:HOH:O	2.59	0.40
1:O:1756:G:H1'	36:O:5783:HOH:O	2.21	0.40
1:O:398:U:H2'	1:O:399:C:C6	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:132:HIS:HB2	4:B:137:LEU:HD22	2.03	0.40
1:0:2289:G:N2	1:0:2291:A:H2	2.19	0.40
17:O:13:VAL:HG13	17:O:14:LEU:N	2.36	0.40
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.49	0.40
1:0:894:A:C2	5:C:87:ARG:NH2	2.90	0.40
2:9:92:G:H22	10:H:52:LYS:HZ1	1.68	0.40
1:0:370:G:O2'	1:0:371:U:H5'	2.22	0.40
14:L:23:LEU:O	14:L:26:HIS:HB2	2.21	0.40
4:B:215:VAL:HB	4:B:234:ARG:NH1	2.35	0.40
1:0:2255:A:H2'	1:0:2256:G:O4'	2.21	0.40
2:9:31:C:O2'	2:9:32:G:H5'	2.21	0.40
21:S:14:ALA:HA	21:S:15:PRO:HD3	1.93	0.40
1:0:517:U:H1'	36:0:7111:HOH:O	2.22	0.40
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.93	0.40
19:Q:82:GLU:HG3	19:Q:83:LYS:N	2.35	0.40
4:B:189:ALA:HB1	36:B:8568:HOH:O	2.21	0.40
1:0:2019:A:H5'	36:0:4048:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/239 (98%)	216 (92%)	14 (6%)	5 (2%)	11	12
4	B	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	11	12
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/176 (76%)	97 (72%)	28 (21%)	9 (7%)	2	1
7	E	170/177 (96%)	161 (95%)	8 (5%)	1 (1%)	33	47
8	F	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	14	17
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	6	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	I	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	11	12
12	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	27	39
13	K	141/164 (86%)	121 (86%)	19 (14%)	1 (1%)	30	43
14	L	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	38	53
15	M	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	5	4
16	N	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	O	141/148 (95%)	138 (98%)	3 (2%)	0	100	100
18	P	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
19	Q	148/154 (96%)	143 (97%)	4 (3%)	1 (1%)	30	43
20	R	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	S	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	6	5
24	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	30	43
25	W	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	9	8
26	X	140/240 (58%)	140 (100%)	0	0	100	100
27	Y	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	8	6
28	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	1	42/48 (88%)	42 (100%)	0	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	10	11
All	All	3633/4235 (86%)	3372 (93%)	209 (6%)	52 (1%)	16	22

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO
6	D	173	GLU
10	H	162	SER
13	K	80	ASP
15	M	154	LEU
15	M	164	ASP
15	M	183	ASP

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Mol	Chain	Res	Type
23	U	43	PRO
3	A	34	ASP
3	A	37	VAL
3	A	132	ASP
4	B	34	GLY
4	B	169	GLY
6	D	11	HIS
6	D	20	LYS
8	F	101	ALA
10	H	164	ALA
11	I	7	ASP
11	I	143	LYS
15	M	162	ASP
30	2	56	PRO
30	2	57	GLY
4	B	184	ASP
6	D	171	ASP
10	H	40	PRO
10	H	138	PRO
11	I	5	GLU
14	L	140	ALA
15	M	167	ASP
15	M	181	ASP
24	V	77	ALA
25	W	77	PHE
27	Y	81	LYS
4	B	185	GLY
6	D	61	PHE
10	H	72	VAL
15	M	65	ASP
4	B	107	SER
8	F	64	PRO
6	D	96	SER
12	J	119	GLN
23	U	40	PRO
4	B	2	GLN
27	Y	41	VAL
7	E	44	GLY
19	Q	81	PRO
3	A	211	LYS
25	W	52	PRO
3	A	112	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	166 (93%)	13 (7%)	20	30
4	B	282/282 (100%)	264 (94%)	18 (6%)	25	37
5	C	193/193 (100%)	179 (93%)	14 (7%)	20	30
6	D	117/147 (80%)	106 (91%)	11 (9%)	13	18
7	E	152/155 (98%)	148 (97%)	4 (3%)	59	79
8	F	92/92 (100%)	91 (99%)	1 (1%)	84	94
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	122/122 (100%)	109 (89%)	13 (11%)	10	13
11	I	118/121 (98%)	109 (92%)	9 (8%)	19	28
12	J	106/106 (100%)	103 (97%)	3 (3%)	56	77
13	K	112/126 (89%)	108 (96%)	4 (4%)	47	68
14	L	166/166 (100%)	157 (95%)	9 (5%)	31	47
15	M	149/149 (100%)	143 (96%)	6 (4%)	42	63
16	N	93/93 (100%)	91 (98%)	2 (2%)	64	83
17	O	113/116 (97%)	111 (98%)	2 (2%)	71	88
18	P	79/79 (100%)	75 (95%)	4 (5%)	33	50
19	Q	117/121 (97%)	114 (97%)	3 (3%)	59	79
20	R	71/73 (97%)	71 (100%)	0	100	100
21	S	105/105 (100%)	101 (96%)	4 (4%)	44	65
22	T	44/52 (85%)	44 (100%)	0	100	100
23	U	51/56 (91%)	50 (98%)	1 (2%)	68	86
24	V	130/130 (100%)	122 (94%)	8 (6%)	26	39
25	W	66/73 (90%)	62 (94%)	4 (6%)	26	40
26	X	120/195 (62%)	110 (92%)	10 (8%)	16	24
27	Y	56/56 (100%)	52 (93%)	4 (7%)	21	32
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	61	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	2	79/79 (100%)	76 (96%)	3 (4%)	44 65
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	34 51

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

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	68	ILE
3	A	69	LEU
3	A	78	ASP
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	53	LEU
4	B	63	GLU
4	B	84	LEU
4	B	97	LEU
4	B	98	THR
4	B	103	ASP
4	B	162	MET
4	B	234	ARG
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	264	GLU
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	94	THR
5	C	101	ASP

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Mol	Chain	Res	Type
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS
6	D	50	VAL
6	D	61	PHE
6	D	95	THR
6	D	99	ASP
6	D	100	ASP
6	D	131	THR
6	D	133	ASN
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	54	ASP
7	E	102	VAL
7	E	164	ASP
8	F	1	PRO
10	H	1	LYS
10	H	59	ASN
10	H	61	LEU
10	H	72	VAL
10	H	73	GLN
10	H	82	LYS
10	H	85	ILE
10	H	86	ARG
10	H	118	PRO
10	H	129	ASN
10	H	142	VAL
10	H	150	LYS
10	H	166	ASN
11	I	46	ILE
11	I	52	GLN
11	I	74	ARG
11	I	79	PHE

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Mol	Chain	Res	Type
11	I	107	ASN
11	I	112	ASP
11	I	120	SER
11	I	125	SER
11	I	127	ILE
12	J	7	ASP
12	J	10	GLN
12	J	98	VAL
13	K	30	ARG
13	K	35	ARG
13	K	80	ASP
13	K	117	GLU
14	L	38	VAL
14	L	46	LEU
14	L	48	ARG
14	L	68	ARG
14	L	81	ARG
14	L	87	MET
14	L	93	ARG
14	L	99	ARG
14	L	164	THR
15	M	26	LEU
15	M	43	VAL
15	M	127	LEU
15	M	128	ASP
15	M	152	GLU
15	M	163	PHE
16	N	3	THR
16	N	28	ASP
17	O	91	LYS
17	O	98	ILE
18	P	11	ARG
18	P	16	ASN
18	P	57	ASP
18	P	95	GLU
19	Q	13	THR
19	Q	39	THR
19	Q	82	GLU
21	S	39	ASN
21	S	48	VAL
21	S	73	HIS
21	S	96	VAL

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Mol	Chain	Res	Type
23	U	43	PRO
24	V	4	LEU
24	V	35	VAL
24	V	52	VAL
24	V	73	LEU
24	V	122	ARG
24	V	142	ASP
24	V	146	ILE
24	V	154	ARG
25	W	15	ARG
25	W	27	ASP
25	W	49	ARG
25	W	72	VAL
26	X	141	THR
26	X	154	ARG
26	X	163	THR
26	X	172	THR
26	X	186	ARG
26	X	189	ASN
26	X	200	THR
26	X	203	VAL
26	X	204	ARG
26	X	231	PRO
27	Y	11	THR
27	Y	44	PHE
27	Y	49	ARG
27	Y	64	ILE
29	1	18	ASN
30	2	14	CYS
30	2	42	ARG
30	2	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	92	ASN
3	A	127	GLN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN

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Mol	Chain	Res	Type
4	B	256	GLN
4	B	260	HIS
4	B	318	ASN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
5	C	163	HIS
6	D	103	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	8	ASN
10	H	35	ASN
10	H	55	GLN
10	H	58	HIS
10	H	59	ASN
10	H	69	ASN
10	H	74	ASN
10	H	91	HIS
10	H	129	ASN
10	H	130	HIS
10	H	166	ASN
11	I	52	GLN
11	I	107	ASN
11	I	126	ASN
12	J	10	GLN
13	K	18	HIS
13	K	41	HIS
13	K	42	ASN
13	K	116	HIS
14	L	26	HIS
14	L	58	GLN
14	L	89	ASN
14	L	176	GLN
15	M	21	HIS
15	M	107	ASN
15	M	153	GLN
16	N	53	GLN
17	O	50	GLN

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Mol	Chain	Res	Type
17	O	66	GLN
17	O	73	HIS
17	O	118	GLN
18	P	16	ASN
18	P	40	HIS
19	Q	61	GLN
19	Q	94	ASN
19	Q	98	ASN
19	Q	113	HIS
19	Q	117	HIS
19	Q	122	GLN
20	R	53	ASN
21	S	39	ASN
21	S	73	HIS
22	T	39	ASN
23	U	60	GLN
24	V	27	HIS
24	V	87	HIS
24	V	110	GLN
24	V	119	HIS
24	V	125	HIS
24	V	141	HIS
25	W	23	HIS
26	X	133	HIS
26	X	134	HIS
26	X	149	GLN
26	X	189	ASN
27	Y	33	HIS
27	Y	70	GLN
28	Z	8	GLN
28	Z	16	HIS
28	Z	28	HIS
29	1	16	ASN
29	1	18	ASN
29	1	41	HIS
29	1	45	ASN
30	2	30	GLN
30	2	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	239 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	5 (4%)
All	All	2868/3044 (94%)	255 (8%)	40 (1%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G

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Mol	Chain	Res	Type
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	898	G
1	0	905	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1161	A
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G
1	0	1177	A
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1380	U

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Mol	Chain	Res	Type
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1904	A
1	0	1919	A
1	0	1942	A

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Mol	Chain	Res	Type
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1982	C
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2346	C
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G

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Mol	Chain	Res	Type
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2914	A
2	9	2	U
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	26	C

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Mol	Chain	Res	Type
2	9	41	C
2	9	43	G
2	9	44	A
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	699	C
1	0	716	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1164	U
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C

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Mol	Chain	Res	Type
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
2	9	2	U
2	9	23	U
2	9	24	U
2	9	65	A
2	9	103	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	0	2754/2922 (94%)	-0.14	58 (2%) 60 58	17, 36, 79, 127	0
2	9	122/122 (100%)	-0.07	6 (4%) 28 26	31, 54, 78, 136	0
3	A	237/239 (99%)	0.24	18 (7%) 14 12	19, 38, 71, 92	0
4	B	337/337 (100%)	0.28	11 (3%) 44 42	21, 45, 71, 82	0
5	C	246/246 (100%)	0.14	6 (2%) 56 54	15, 35, 58, 70	0
6	D	140/176 (79%)	2.20	73 (52%) 0 0	43, 86, 105, 108	0
7	E	172/177 (97%)	0.58	8 (4%) 30 28	37, 59, 77, 81	0
8	F	119/119 (100%)	0.71	15 (12%) 4 4	37, 58, 83, 88	0
9	G	29/348 (8%)	2.33	18 (62%) 0 0	64, 79, 86, 91	0
10	H	156/167 (93%)	0.63	18 (11%) 5 5	30, 47, 75, 79	0
11	I	142/145 (97%)	0.29	5 (3%) 42 40	29, 42, 63, 84	0
12	J	132/132 (100%)	0.09	3 (2%) 57 55	27, 42, 61, 71	0
13	K	145/164 (88%)	0.58	14 (9%) 8 7	18, 54, 90, 102	0
14	L	194/194 (100%)	-0.03	6 (3%) 47 44	19, 32, 50, 62	0
15	M	186/186 (100%)	0.54	20 (10%) 6 6	31, 50, 91, 103	0
16	N	115/115 (100%)	0.02	2 (1%) 67 65	27, 44, 60, 69	0
17	O	143/148 (96%)	0.15	1 (0%) 84 84	30, 44, 57, 64	0
18	P	95/95 (100%)	0.07	2 (2%) 60 58	25, 34, 50, 61	0
19	Q	150/154 (97%)	-0.13	0 100 100	23, 36, 54, 63	0
20	R	81/84 (96%)	0.51	11 (13%) 4 3	31, 47, 68, 72	0
21	S	119/119 (100%)	0.40	2 (1%) 67 65	28, 45, 69, 81	0
22	T	53/66 (80%)	0.08	1 (1%) 64 61	33, 47, 63, 71	0
23	U	65/70 (92%)	1.42	9 (13%) 4 3	39, 59, 97, 101	0
24	V	154/154 (100%)	0.26	5 (3%) 45 43	27, 40, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	82/91 (90%)	0.46	6 (7%) 15 13	35, 48, 73, 91	0
26	X	142/240 (59%)	-0.05	4 (2%) 50 48	22, 35, 59, 74	0
27	Y	73/73 (100%)	0.47	7 (9%) 8 8	36, 49, 63, 77	0
28	Z	56/56 (100%)	-0.13	0 100 100	17, 24, 32, 35	0
29	1	46/48 (95%)	0.48	6 (13%) 4 4	27, 49, 77, 86	0
30	2	92/92 (100%)	0.09	2 (2%) 59 57	23, 44, 59, 72	0
All	All	6577/7279 (90%)	0.15	337 (5%) 28 25	15, 41, 80, 136	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	1	THR	12.5
23	U	39	ALA	9.7
6	D	63	ILE	9.2
6	D	57	THR	7.5
23	U	40	PRO	7.4
1	0	1172	G	6.6
20	R	81	ILE	6.6
6	D	18	ILE	6.3
25	W	88	GLU	6.1
23	U	38	GLY	5.9
4	B	1	PRO	5.9
2	9	25	G	5.8
1	0	282	C	5.8
2	9	1	U	5.7
6	D	66	GLY	5.6
3	A	37	VAL	5.4
25	W	80	GLU	5.3
1	0	960	G	5.3
15	M	166	ALA	5.2
6	D	10	PHE	5.2
15	M	186	LEU	5.0
3	A	237	GLY	5.0
6	D	170	TYR	4.9
9	G	12	ILE	4.9
15	M	162	ASP	4.9
8	F	106	THR	4.7
1	0	284	C	4.6
6	D	165	PHE	4.6
6	D	44	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	0	1200	A	4.5
9	G	23	ILE	4.5
23	U	43	PRO	4.5
9	G	26	MET	4.5
1	0	1198	U	4.4
6	D	166	ILE	4.4
1	0	1171	A	4.4
1	0	1951	G	4.4
1	0	1177	A	4.4
1	0	1173	A	4.4
27	Y	22	ILE	4.4
6	D	61	PHE	4.3
6	D	85	GLN	4.3
6	D	172	VAL	4.3
6	D	58	VAL	4.3
1	0	1199	A	4.3
6	D	88	LEU	4.1
6	D	69	ILE	4.1
13	K	80	ASP	4.1
2	9	23	U	4.1
6	D	27	ILE	4.1
1	0	2237	G	4.1
1	0	1169	U	4.0
23	U	41	GLU	4.0
1	0	1196	C	4.0
6	D	75	LEU	4.0
6	D	92	GLU	4.0
6	D	62	ASP	4.0
6	D	64	ARG	3.9
6	D	94	ALA	3.9
26	X	235	GLU	3.9
3	A	36	ASP	3.9
1	0	1950	G	3.8
1	0	1202	A	3.8
6	D	56	ARG	3.7
1	0	1181	A	3.7
6	D	40	ILE	3.7
1	0	1203	G	3.7
7	E	45	ASP	3.7
13	K	81	VAL	3.7
1	0	1525	G	3.7
15	M	152	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
7	E	87	PHE	3.6
10	H	146	TRP	3.6
21	S	1	SER	3.6
3	A	85	ASP	3.6
20	R	2	TRP	3.5
12	J	119	GLN	3.5
10	H	83	PHE	3.5
5	C	132	ASP	3.5
6	D	50	VAL	3.5
6	D	67	ASP	3.4
26	X	108	ASP	3.4
11	I	4	ALA	3.4
1	0	2637	A	3.4
1	0	1170	U	3.4
5	C	135	GLU	3.4
15	M	154	LEU	3.4
13	K	148	GLU	3.4
13	K	104	ASP	3.3
13	K	150	GLN	3.3
1	0	1168	C	3.3
2	9	2	U	3.3
13	K	145	LEU	3.3
13	K	147	GLU	3.3
9	G	27	ILE	3.3
1	0	970	U	3.3
1	0	1192	A	3.2
6	D	22	VAL	3.2
8	F	119	ARG	3.2
29	1	24	TRP	3.2
6	D	171	ASP	3.2
13	K	102	ASP	3.2
25	W	85	VAL	3.2
1	0	10	U	3.2
27	Y	11	THR	3.2
1	0	999	C	3.2
9	G	24	VAL	3.2
1	0	1195	G	3.2
26	X	95	THR	3.2
6	D	106	PHE	3.1
6	D	17	ARG	3.1
29	1	35	ARG	3.1
15	M	138	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	0	1279	U	3.1
1	0	1174	A	3.1
27	Y	80	MET	3.1
6	D	134	LEU	3.1
9	G	72	ASP	3.1
12	J	132	VAL	3.1
4	B	92	TYR	3.0
6	D	74	THR	3.0
2	9	24	U	3.0
6	D	95	THR	3.0
1	0	1201	C	3.0
3	A	35	GLY	3.0
6	D	23	VAL	3.0
1	0	1197	G	3.0
9	G	15	TRP	3.0
3	A	236	GLY	3.0
9	G	69	ARG	3.0
13	K	105	TYR	3.0
1	0	1948	G	2.9
6	D	65	GLU	2.9
7	E	10	ASP	2.9
16	N	23	GLY	2.9
8	F	108	LEU	2.9
23	U	2	VAL	2.9
25	W	71	ARG	2.9
1	0	1178	G	2.9
6	D	173	GLU	2.9
7	E	100	ASP	2.9
9	G	14	GLU	2.9
3	A	64	ASP	2.9
10	H	72	VAL	2.9
6	D	84	LEU	2.8
14	L	152	ARG	2.8
15	M	181	ASP	2.8
4	B	104	GLU	2.8
6	D	104	PHE	2.8
6	D	96	SER	2.8
3	A	32	VAL	2.8
1	0	128	A	2.8
15	M	157	PRO	2.8
23	U	37	GLY	2.8
13	K	60	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	89	PRO	2.8
9	G	73	ASP	2.8
20	R	46	ASP	2.8
22	T	47	ARG	2.8
27	Y	38	LYS	2.8
24	V	93	ILE	2.8
15	M	163	PHE	2.8
6	D	93	LEU	2.7
15	M	184	ILE	2.7
24	V	86	GLU	2.7
6	D	55	LYS	2.7
10	H	79	ALA	2.7
4	B	57	GLU	2.7
6	D	81	GLU	2.7
1	0	1165	G	2.7
14	L	87	MET	2.7
6	D	26	GLY	2.7
8	F	17	LEU	2.7
10	H	81	TYR	2.7
6	D	25	MET	2.7
6	D	101	THR	2.6
1	0	1180	U	2.6
20	R	45	TYR	2.6
6	D	68	PRO	2.6
6	D	102	GLY	2.6
6	D	73	VAL	2.6
1	0	2825	C	2.6
10	H	41	THR	2.6
13	K	149	ARG	2.6
14	L	194	ALA	2.6
6	D	11	HIS	2.6
15	M	155	GLU	2.6
8	F	118	LEU	2.6
30	2	56	PRO	2.6
10	H	157	ILE	2.6
6	D	132	VAL	2.6
8	F	115	VAL	2.6
20	R	1	SER	2.6
12	J	108	GLU	2.6
1	0	1179	C	2.6
1	0	2250	G	2.6
1	0	2508	C	2.6

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Mol	Chain	Res	Type	RSRZ
27	Y	21	LYS	2.6
6	D	139	TYR	2.6
9	G	21	ASP	2.6
20	R	77	VAL	2.6
6	D	45	THR	2.6
1	0	735	C	2.6
29	1	49	GLU	2.6
7	E	88	TYR	2.5
11	I	5	GLU	2.5
11	I	7	ASP	2.5
1	0	2238	A	2.5
9	G	20	VAL	2.5
29	1	39	ARG	2.5
3	A	38	ILE	2.5
6	D	157	LEU	2.5
2	9	122	C	2.5
14	L	63	VAL	2.5
8	F	99	THR	2.5
10	H	66	VAL	2.5
6	D	133	ASN	2.5
30	2	92	GLU	2.5
1	0	1204	C	2.5
4	B	181	ILE	2.5
15	M	147	ILE	2.5
1	0	2004	U	2.5
25	W	10	VAL	2.5
18	P	92	ARG	2.4
9	G	71	LEU	2.4
29	1	20	ARG	2.4
10	H	139	ASP	2.4
9	G	25	GLU	2.4
6	D	59	GLY	2.4
20	R	20	PHE	2.4
1	0	1182	C	2.4
7	E	169	THR	2.4
20	R	43	GLU	2.4
5	C	134	ASP	2.4
6	D	98	PHE	2.4
10	H	32	ASP	2.4
9	G	28	GLU	2.4
15	M	159	TYR	2.4
10	H	135	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	31	LYS	2.4
1	0	1163	G	2.4
27	Y	44	PHE	2.4
6	D	51	ARG	2.4
16	N	1	SER	2.4
4	B	117	GLU	2.4
8	F	28	ALA	2.4
9	G	65	THR	2.4
15	M	68	GLU	2.4
1	0	1167	G	2.4
6	D	47	GLN	2.4
9	G	70	ALA	2.4
13	K	61	ALA	2.3
7	E	129	GLU	2.3
6	D	154	LYS	2.3
15	M	158	LEU	2.3
3	A	63	GLY	2.3
10	H	128	ALA	2.3
1	0	1162	G	2.3
7	E	126	ILE	2.3
6	D	90	LEU	2.3
10	H	80	ASN	2.3
5	C	198	ASP	2.3
1	0	1000	C	2.3
8	F	117	GLU	2.3
3	A	65	ARG	2.3
3	A	82	VAL	2.3
3	A	60	PHE	2.3
6	D	87	ALA	2.3
8	F	107	VAL	2.3
1	0	280	C	2.3
6	D	167	GLU	2.3
6	D	103	ASN	2.2
24	V	96	LEU	2.2
6	D	80	ALA	2.2
8	F	22	VAL	2.2
4	B	180	ASP	2.2
8	F	20	LEU	2.2
8	F	100	ASP	2.2
1	0	138	U	2.2
1	0	281	U	2.2
4	B	105	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
5	C	61	PHE	2.2
3	A	68	ILE	2.2
3	A	89	ALA	2.2
4	B	115	VAL	2.2
14	L	165	SER	2.2
18	P	95	GLU	2.2
9	G	66	LEU	2.2
5	C	162	VAL	2.2
17	O	76	GLY	2.2
10	H	163	PRO	2.2
14	L	140	ALA	2.2
20	R	76	GLU	2.2
1	0	1949	G	2.2
6	D	86	THR	2.2
24	V	61	THR	2.2
6	D	43	GLU	2.2
23	U	28	LEU	2.1
3	A	133	ARG	2.1
13	K	130	ARG	2.1
10	H	59	ASN	2.1
10	H	158	ASN	2.1
26	X	236	VAL	2.1
8	F	16	ALA	2.1
4	B	109	LEU	2.1
8	F	98	VAL	2.1
6	D	156	ARG	2.1
4	B	118	ASP	2.1
15	M	150	TYR	2.1
1	0	1206	U	2.1
1	0	1176	C	2.1
21	S	63	ILE	2.1
3	A	66	ARG	2.1
10	H	70	ARG	2.1
1	0	1967	U	2.1
6	D	135	VAL	2.1
15	M	149	GLU	2.1
20	R	80	ARG	2.1
15	M	139	TRP	2.1
11	I	47	THR	2.1
27	Y	25	ARG	2.1
1	0	1175	G	2.1
1	0	2344	G	2.1

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Mol	Chain	Res	Type	RSRZ
15	M	177	GLU	2.1
25	W	7	GLU	2.1
20	R	71	ASP	2.1
6	D	15	GLU	2.0
6	D	158	ASN	2.0
29	1	27	LEU	2.0
13	K	97	VAL	2.0
24	V	85	ALA	2.0
6	D	77	ASP	2.0
6	D	128	LEU	2.0
15	M	179	LEU	2.0
11	I	39	VAL	2.0
6	D	54	ALA	2.0
10	H	162	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	0	8370	1/1	0.40	74.46	61,61,61,61	0
31	MG	0	8087	1/1	0.26	34.54	72,72,72,72	0
31	MG	0	8101	1/1	0.27	30.69	48,48,48,48	0
33	NA	0	8358	1/1	0.31	22.79	74,74,74,74	0
33	NA	0	8379	1/1	0.32	20.33	48,48,48,48	0
33	NA	0	8366	1/1	0.26	19.42	54,54,54,54	0
33	NA	0	8350	1/1	0.28	18.59	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	0	8371	1/1	0.26	17.92	49,49,49,49	0
33	NA	0	8320	1/1	0.21	17.75	38,38,38,38	0
33	NA	0	8363	1/1	0.24	17.44	52,52,52,52	0
31	MG	0	8103	1/1	0.23	15.15	54,54,54,54	0
33	NA	0	8372	1/1	0.29	13.11	54,54,54,54	0
31	MG	0	8082	1/1	0.18	12.67	56,56,56,56	0
33	NA	0	8385	1/1	0.32	12.36	48,48,48,48	0
33	NA	0	8327	1/1	0.22	12.32	38,38,38,38	0
33	NA	0	8340	1/1	0.19	10.84	47,47,47,47	0
33	NA	0	8367	1/1	0.22	10.16	45,45,45,45	0
33	NA	Q	8386	1/1	0.36	9.60	74,74,74,74	0
33	NA	0	8326	1/1	0.19	8.43	37,37,37,37	0
33	NA	K	8380	1/1	0.27	7.73	42,42,42,42	0
33	NA	0	8373	1/1	0.15	7.34	43,43,43,43	0
34	CL	0	8522	1/1	0.17	7.16	44,44,44,44	0
33	NA	0	8364	1/1	0.20	6.98	38,38,38,38	0
33	NA	0	8314	1/1	0.25	6.97	40,40,40,40	0
31	MG	0	8042	1/1	0.13	6.17	29,29,29,29	0
33	NA	0	8376	1/1	0.21	6.08	39,39,39,39	0
33	NA	0	8362	1/1	0.23	6.06	51,51,51,51	0
33	NA	0	8302	1/1	0.18	5.40	44,44,44,44	0
31	MG	0	8066	1/1	0.39	5.20	85,85,85,85	0
33	NA	0	8318	1/1	0.18	5.11	49,49,49,49	0
33	NA	0	8359	1/1	0.22	4.57	39,39,39,39	0
33	NA	0	8329	1/1	0.14	4.20	48,48,48,48	0
33	NA	0	8331	1/1	0.20	4.11	39,39,39,39	0
31	MG	0	8090	1/1	0.23	3.95	53,53,53,53	0
33	NA	0	8384	1/1	0.14	3.61	52,52,52,52	0
33	NA	0	8374	1/1	0.14	3.22	44,44,44,44	0
33	NA	0	8369	1/1	0.19	3.05	40,40,40,40	0
33	NA	0	8377	1/1	0.16	3.03	50,50,50,50	0
33	NA	9	8383	1/1	0.21	2.91	43,43,43,43	0
33	NA	0	8307	1/1	0.15	2.83	42,42,42,42	0
31	MG	0	8099	1/1	0.20	2.67	44,44,44,44	0
31	MG	0	8012	1/1	0.14	2.67	32,32,32,32	0
33	NA	0	8360	1/1	0.17	2.59	41,41,41,41	0
31	MG	0	8060	1/1	0.19	2.54	31,31,31,31	0
33	NA	0	8361	1/1	0.18	2.53	38,38,38,38	0
31	MG	0	8007	1/1	0.19	2.48	21,21,21,21	0
33	NA	0	8355	1/1	0.33	2.42	47,47,47,47	0
31	MG	0	8117	1/1	0.17	2.41	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	0	8325	1/1	0.18	2.03	47,47,47,47	0
33	NA	0	8382	1/1	0.14	1.93	64,64,64,64	0
33	NA	0	8365	1/1	0.28	1.84	28,28,28,28	0
33	NA	0	8308	1/1	0.15	1.72	42,42,42,42	0
33	NA	0	8321	1/1	0.19	1.02	40,40,40,40	0
33	NA	0	8328	1/1	0.13	0.89	28,28,28,28	0
33	NA	H	8322	1/1	0.17	0.58	52,52,52,52	0
31	MG	0	8015	1/1	0.17	0.50	26,26,26,26	0
31	MG	0	8041	1/1	0.12	0.32	33,33,33,33	0
34	CL	0	8514	1/1	0.15	0.28	36,36,36,36	0
34	CL	0	8516	1/1	0.13	0.20	42,42,42,42	0
34	CL	0	8503	1/1	0.13	0.07	40,40,40,40	0
33	NA	0	8356	1/1	0.15	0.02	37,37,37,37	0
33	NA	0	8315	1/1	0.17	-0.18	30,30,30,30	0
33	NA	0	8324	1/1	0.12	-0.22	48,48,48,48	0
31	MG	0	8010	1/1	0.14	-0.35	24,24,24,24	0
31	MG	0	8026	1/1	0.15	-0.36	26,26,26,26	0
33	NA	0	8375	1/1	0.17	-0.50	39,39,39,39	0
31	MG	0	8067	1/1	0.12	-0.56	34,34,34,34	0
31	MG	9	8095	1/1	0.14	-0.57	69,69,69,69	0
31	MG	J	8069	1/1	0.12	-0.59	46,46,46,46	0
35	CD	Y	8403	1/1	0.13	-0.65	49,49,49,49	0
33	NA	C	8304	1/1	0.12	-0.66	30,30,30,30	0
31	MG	0	8013	1/1	0.13	-0.77	22,22,22,22	0
31	MG	0	8049	1/1	0.11	-0.92	56,56,56,56	0
35	CD	T	8401	1/1	0.10	-0.92	49,49,49,49	0
31	MG	0	8086	1/1	0.07	-0.94	33,33,33,33	0
34	CL	L	8518	1/1	0.12	-1.05	32,32,32,32	0
34	CL	A	8509	1/1	0.11	-1.11	50,50,50,50	0
31	MG	0	8061	1/1	0.13	-1.17	32,32,32,32	0
33	NA	0	8378	1/1	0.14	-1.18	39,39,39,39	0
33	NA	L	8347	1/1	0.11	-1.20	18,18,18,18	0
31	MG	A	8105	1/1	0.12	-1.22	27,27,27,27	0
33	NA	0	8368	1/1	0.10	-1.24	48,48,48,48	0
33	NA	0	8342	1/1	0.15	-1.26	33,33,33,33	0
34	CL	X	8520	1/1	0.10	-1.26	38,38,38,38	0
34	CL	I	8521	1/1	0.12	-1.31	47,47,47,47	0
31	MG	0	8079	1/1	0.15	-1.44	19,19,19,19	0
31	MG	0	8106	1/1	0.11	-1.63	42,42,42,42	0
35	CD	2	8404	1/1	0.08	-1.66	47,47,47,47	0
31	MG	0	8038	1/1	0.11	-1.69	22,22,22,22	0
33	NA	0	8311	1/1	0.11	-1.70	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8102	1/1	0.10	-1.73	51,51,51,51	0
31	MG	0	8054	1/1	0.14	-1.87	18,18,18,18	0
33	NA	H	8309	1/1	0.06	-1.89	28,28,28,28	0
33	NA	9	8351	1/1	0.11	-1.90	42,42,42,42	0
34	CL	I	8502	1/1	0.07	-1.92	53,53,53,53	0
31	MG	0	8104	1/1	0.12	-2.02	45,45,45,45	0
34	CL	0	8511	1/1	0.08	-2.05	37,37,37,37	0
31	MG	0	8064	1/1	0.11	-2.08	26,26,26,26	0
33	NA	I	8346	1/1	0.07	-2.15	34,34,34,34	0
33	NA	0	8319	1/1	0.10	-2.17	29,29,29,29	0
31	MG	0	8023	1/1	0.13	-2.21	30,30,30,30	0
31	MG	0	8077	1/1	0.14	-2.21	23,23,23,23	0
31	MG	0	8093	1/1	0.12	-2.22	35,35,35,35	0
33	NA	0	8305	1/1	0.12	-2.23	32,32,32,32	0
33	NA	0	8344	1/1	0.08	-2.28	24,24,24,24	0
34	CL	I	8501	1/1	0.07	-2.36	44,44,44,44	0
35	CD	N	8405	1/1	0.07	-2.38	71,71,71,71	0
34	CL	K	8510	1/1	0.06	-2.39	36,36,36,36	0
33	NA	0	8317	1/1	0.09	-2.40	27,27,27,27	0
31	MG	0	8003	1/1	0.10	-2.52	21,21,21,21	0
31	MG	0	8091	1/1	0.09	-2.53	41,41,41,41	0
33	NA	0	8316	1/1	0.15	-2.57	35,35,35,35	0
33	NA	P	8348	1/1	0.06	-2.57	32,32,32,32	0
34	CL	N	8508	1/1	0.06	-2.61	52,52,52,52	0
31	MG	S	8073	1/1	0.04	-2.62	39,39,39,39	0
33	NA	0	8339	1/1	0.11	-2.63	20,20,20,20	0
31	MG	0	8074	1/1	0.05	-2.63	36,36,36,36	0
33	NA	0	8349	1/1	0.13	-2.68	37,37,37,37	0
31	MG	0	8027	1/1	0.04	-2.68	37,37,37,37	0
31	MG	0	8108	1/1	0.09	-2.76	62,62,62,62	0
34	CL	B	8519	1/1	0.10	-2.81	33,33,33,33	0
34	CL	M	8507	1/1	0.06	-2.82	45,45,45,45	0
33	NA	S	8343	1/1	0.05	-2.85	29,29,29,29	0
31	MG	0	8001	1/1	0.12	-2.92	25,25,25,25	0
33	NA	0	8334	1/1	0.06	-2.96	33,33,33,33	0
34	CL	0	8515	1/1	0.09	-2.98	48,48,48,48	0
34	CL	0	8512	1/1	0.07	-3.04	34,34,34,34	0
34	CL	Q	8506	1/1	0.09	-3.04	40,40,40,40	0
33	NA	A	8345	1/1	0.08	-3.05	46,46,46,46	0
31	MG	0	8070	1/1	0.14	-3.08	40,40,40,40	0
33	NA	0	8306	1/1	0.11	-3.10	28,28,28,28	0
31	MG	B	8055	1/1	0.08	-3.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8004	1/1	0.12	-3.12	21,21,21,21	0
31	MG	0	8081	1/1	0.09	-3.20	39,39,39,39	0
31	MG	0	8047	1/1	0.09	-3.21	54,54,54,54	0
33	NA	0	8332	1/1	0.09	-3.21	33,33,33,33	0
31	MG	0	8024	1/1	0.08	-3.25	22,22,22,22	0
31	MG	0	8020	1/1	0.10	-3.26	24,24,24,24	0
33	NA	0	8335	1/1	0.10	-3.30	31,31,31,31	0
31	MG	0	8009	1/1	0.13	-3.34	24,24,24,24	0
31	MG	0	8107	1/1	0.03	-3.49	30,30,30,30	0
33	NA	0	8310	1/1	0.07	-3.56	27,27,27,27	0
34	CL	0	8505	1/1	0.08	-3.57	41,41,41,41	0
31	MG	0	8046	1/1	0.05	-3.60	38,38,38,38	0
31	MG	0	8005	1/1	0.14	-3.60	24,24,24,24	0
31	MG	0	8080	1/1	0.07	-3.61	41,41,41,41	0
33	NA	0	8333	1/1	0.06	-3.61	23,23,23,23	0
31	MG	0	8016	1/1	0.09	-3.64	32,32,32,32	0
31	MG	0	8096	1/1	0.08	-3.64	37,37,37,37	0
33	NA	0	8341	1/1	0.09	-3.68	37,37,37,37	0
31	MG	2	8078	1/1	0.08	-3.85	39,39,39,39	0
31	MG	0	8033	1/1	0.08	-3.93	20,20,20,20	0
31	MG	0	8050	1/1	0.13	-3.94	56,56,56,56	0
31	MG	0	8053	1/1	0.09	-3.95	28,28,28,28	0
31	MG	0	8008	1/1	0.08	-3.98	22,22,22,22	0
31	MG	X	8109	1/1	0.07	-3.99	25,25,25,25	0
31	MG	0	8045	1/1	0.05	-4.09	51,51,51,51	0
31	MG	0	8030	1/1	0.07	-4.10	22,22,22,22	0
33	NA	Q	8337	1/1	0.06	-4.17	33,33,33,33	0
35	CD	Z	8402	1/1	0.03	-4.19	37,37,37,37	0
31	MG	0	8051	1/1	0.07	-4.32	56,56,56,56	0
31	MG	0	8116	1/1	0.08	-4.34	42,42,42,42	0
31	MG	0	8025	1/1	0.07	-4.36	36,36,36,36	0
31	MG	0	8068	1/1	0.04	-4.37	44,44,44,44	0
31	MG	0	8011	1/1	0.10	-4.51	23,23,23,23	0
31	MG	0	8058	1/1	0.07	-4.60	27,27,27,27	0
34	CL	2	8504	1/1	0.05	-4.66	45,45,45,45	0
31	MG	0	8075	1/1	0.07	-4.68	28,28,28,28	0
31	MG	0	8034	1/1	0.10	-4.69	31,31,31,31	0
34	CL	0	8517	1/1	0.08	-4.71	50,50,50,50	0
31	MG	0	8056	1/1	0.06	-4.72	31,31,31,31	0
31	MG	0	8022	1/1	0.13	-4.89	32,32,32,32	0
31	MG	0	8037	1/1	0.06	-4.91	35,35,35,35	0
31	MG	0	8114	1/1	0.06	-4.92	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	A	8065	1/1	0.06	-4.92	24,24,24,24	0
34	CL	0	8513	1/1	0.07	-4.97	44,44,44,44	0
31	MG	0	8040	1/1	0.10	-5.18	38,38,38,38	0
31	MG	0	8084	1/1	0.05	-5.28	39,39,39,39	0
33	NA	0	8338	1/1	0.05	-5.36	36,36,36,36	0
31	MG	0	8035	1/1	0.07	-5.37	36,36,36,36	0
31	MG	0	8088	1/1	0.06	-5.50	20,20,20,20	0
31	MG	0	8112	1/1	0.06	-5.52	23,23,23,23	0
31	MG	0	8057	1/1	0.10	-5.53	35,35,35,35	0
31	MG	0	8094	1/1	0.08	-5.59	59,59,59,59	0
31	MG	0	8072	1/1	0.09	-5.60	47,47,47,47	0
31	MG	0	8036	1/1	0.08	-5.65	35,35,35,35	0
31	MG	0	8098	1/1	0.08	-5.66	27,27,27,27	0
33	NA	0	8353	1/1	0.08	-5.68	18,18,18,18	0
31	MG	0	8017	1/1	0.12	-6.20	12,12,12,12	0
33	NA	0	8357	1/1	0.06	-6.23	39,39,39,39	0
33	NA	0	8330	1/1	0.05	-6.46	39,39,39,39	0
33	NA	0	8354	1/1	0.13	-6.56	25,25,25,25	0
31	MG	0	8031	1/1	0.10	-6.68	24,24,24,24	0
31	MG	0	8021	1/1	0.08	-6.68	24,24,24,24	0
31	MG	0	8044	1/1	0.07	-6.69	32,32,32,32	0
31	MG	0	8110	1/1	0.07	-6.77	24,24,24,24	0
33	NA	R	8312	1/1	0.07	-6.91	26,26,26,26	0
31	MG	0	8063	1/1	0.07	-7.17	62,62,62,62	0
31	MG	0	8085	1/1	0.07	-7.25	35,35,35,35	0
33	NA	0	8323	1/1	0.07	-7.48	31,31,31,31	0
33	NA	0	8313	1/1	0.06	-7.68	48,48,48,48	0
31	MG	0	8113	1/1	0.10	-7.71	36,36,36,36	0
31	MG	0	8029	1/1	0.09	-7.78	35,35,35,35	0
31	MG	0	8059	1/1	0.06	-7.99	25,25,25,25	0
33	NA	0	8381	1/1	0.05	-8.03	41,41,41,41	0
31	MG	0	8062	1/1	0.07	-8.07	41,41,41,41	0
32	K	0	8201	1/1	0.08	-8.08	62,62,62,62	0
31	MG	0	8039	1/1	0.07	-8.12	32,32,32,32	0
31	MG	0	8019	1/1	0.04	-8.31	23,23,23,23	0
31	MG	0	8071	1/1	0.05	-8.45	62,62,62,62	0
33	NA	0	8301	1/1	0.07	-8.58	33,33,33,33	0
33	NA	0	8303	1/1	0.10	-8.64	32,32,32,32	0
31	MG	0	8032	1/1	0.04	-8.76	23,23,23,23	0
31	MG	0	8018	1/1	0.05	-8.97	27,27,27,27	0
31	MG	0	8006	1/1	0.07	-9.10	27,27,27,27	0
31	MG	0	8076	1/1	0.04	-9.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8052	1/1	0.06	-9.76	45,45,45,45	0
31	MG	0	8083	1/1	0.06	-10.16	30,30,30,30	0
33	NA	0	8352	1/1	0.07	-10.16	40,40,40,40	0
32	K	0	8202	1/1	0.06	-10.17	37,37,37,37	0
31	MG	0	8100	1/1	0.07	-10.35	64,64,64,64	0
31	MG	0	8111	1/1	0.06	-10.79	32,32,32,32	0
31	MG	0	8092	1/1	0.07	-11.28	66,66,66,66	0
31	MG	0	8028	1/1	0.04	-11.71	25,25,25,25	0
31	MG	0	8002	1/1	0.06	-12.28	26,26,26,26	0
31	MG	0	8014	1/1	0.07	-12.39	25,25,25,25	0
31	MG	0	8043	1/1	0.05	-12.84	33,33,33,33	0
31	MG	0	8048	1/1	0.05	-13.00	39,39,39,39	0
31	MG	0	8089	1/1	0.06	-17.58	51,51,51,51	0
33	NA	0	8336	1/1	0.04	-17.64	37,37,37,37	0
31	MG	0	8115	1/1	0.07	-23.50	36,36,36,36	0
31	MG	0	8097	1/1	0.06	-26.68	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.