



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:24 am BST

PDB ID : 1S72  
Title : REFINED CRYSTAL STRUCTURE OF THE HALOARCUA MARISMORTUI LARGE RIBOSOMAL SUBUNIT AT 2.4 ANGSTROM RESOLUTION  
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2004-01-28  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

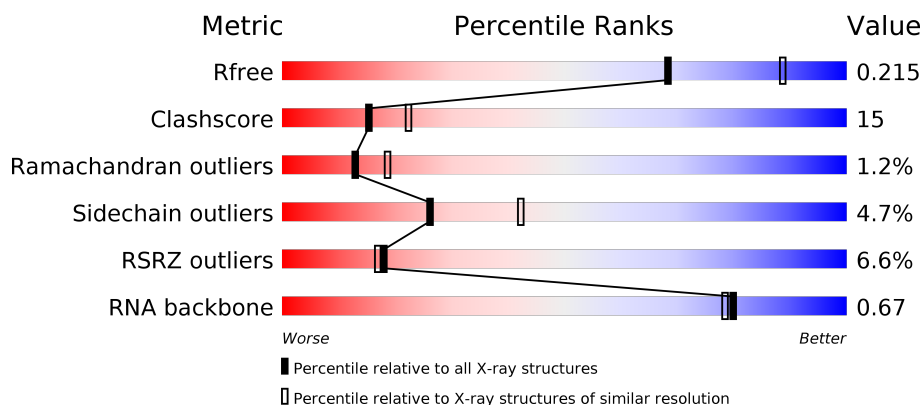
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>35%</div> <div>7%</div> <div></div> </div> </div>
3	A	240	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>6%</div> <div></div> </div> </div>
4	B	338	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	73	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	<div><div></div><div>12%</div><div>54%</div><div>36%</div><div>• 8%</div></div>
31	3	92	<div><div></div><div>3%</div><div>64%</div><div>33%</div><div>• •</div></div>

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

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

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 50S ribosomal protein L2P.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	ASP	CONFLICT	UNP P20276
A	160	ALA	GLY	CONFLICT	UNP P20276

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	CONFLICT	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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 50S ribosomal protein L6P.

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 50S ribosomal protein L7Ae.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	103	GLU	ALA	CONFLICT	UNP P12743
F	105	ASP	ALA	CONFLICT	UNP P12743
F	106	ALA	THR	CONFLICT	UNP P12743
F	107	ASP	VAL	CONFLICT	UNP P12743
F	108	VAL	LEU	CONFLICT	UNP P12743
F	110	ASP	GLU	CONFLICT	UNP P12743

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 11 is a protein called 50S ribosomal protein L11P.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.



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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			579	346	116	112	5			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	72	Total Na 72 72	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	2	Total Na 2 2	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total	Cl	0	0
			1	1		
35	3	1	Total	Cl	0	0
			1	1		
35	M	1	Total	Cl	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5893	Total	O	0	0
			5893	5893		
37	9	136	Total	O	0	0
			136	136		
37	A	127	Total	O	0	0
			127	127		
37	B	153	Total	O	0	0
			153	153		
37	C	172	Total	O	0	0
			172	172		
37	D	49	Total	O	0	0
			49	49		
37	E	44	Total	O	0	0
			44	44		
37	F	25	Total	O	0	0
			25	25		
37	G	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	71	Total 71	O 71	0	0
37	I	9	Total 9	O 9	0	0
37	J	55	Total 55	O 55	0	0
37	K	61	Total 61	O 61	0	0
37	L	85	Total 85	O 85	0	0
37	M	121	Total 121	O 121	0	0
37	N	64	Total 64	O 64	0	0
37	O	44	Total 44	O 44	0	0
37	P	65	Total 65	O 65	0	0
37	Q	52	Total 52	O 52	0	0
37	R	83	Total 83	O 83	0	0
37	S	33	Total 33	O 33	0	0
37	T	40	Total 40	O 40	0	0
37	U	25	Total 25	O 25	0	0
37	V	14	Total 14	O 14	0	0
37	W	67	Total 67	O 67	0	0
37	X	28	Total 28	O 28	0	0
37	Y	96	Total 96	O 96	0	0
37	Z	29	Total 29	O 29	0	0
37	1	51	Total 51	O 51	0	0
37	2	40	Total 40	O 40	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	71	Total	O	0	0
			71	71		



- Molecule 1: 23S ribosomal RNA

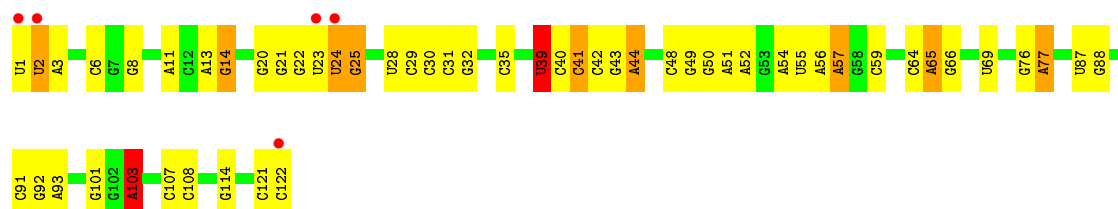




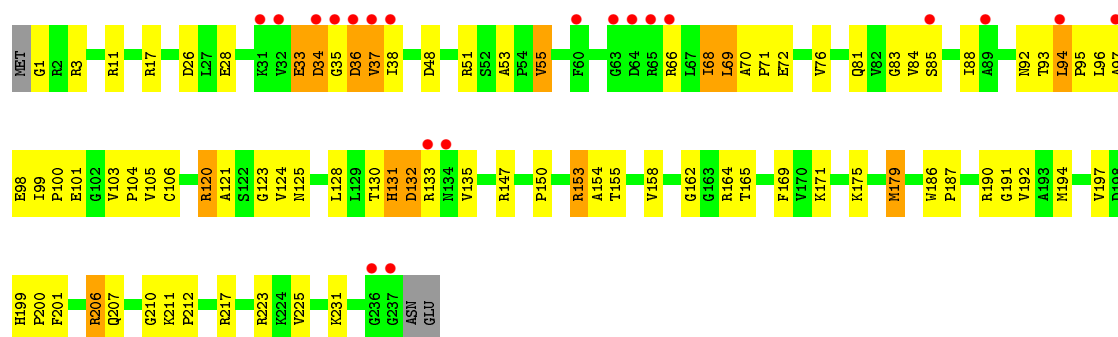




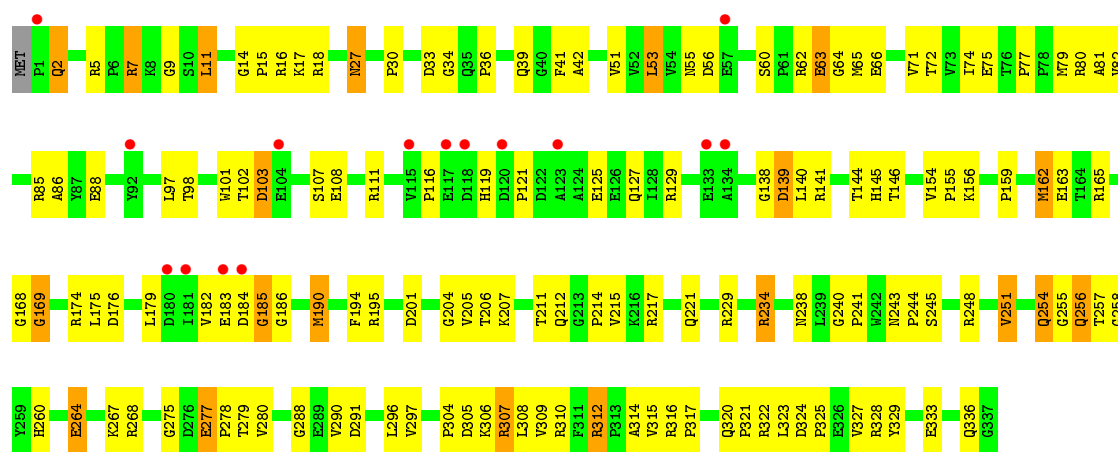
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

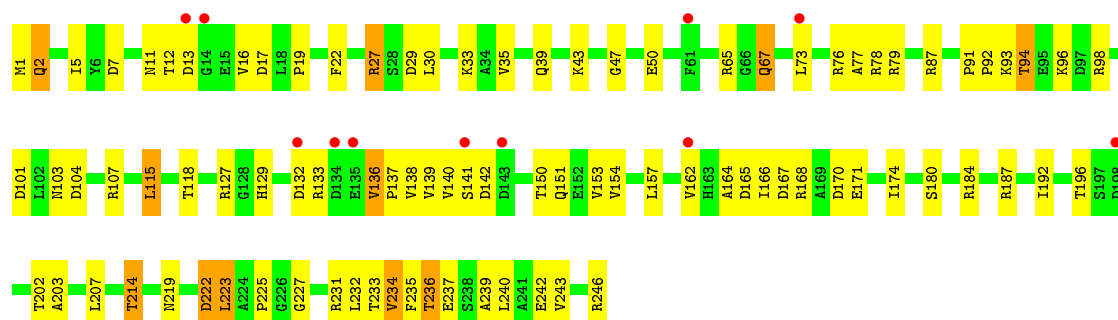


• Molecule 4: 50S ribosomal protein L3P

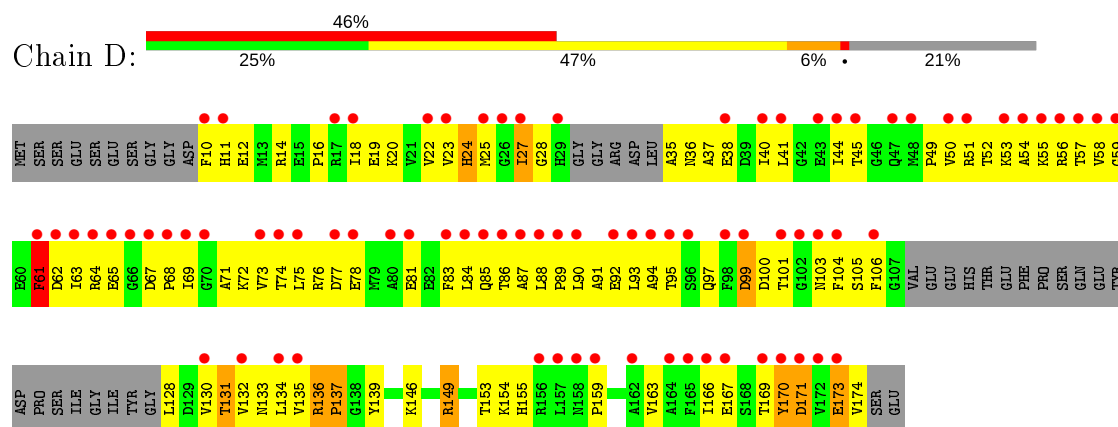


• Molecule 5: 50S ribosomal protein L4E

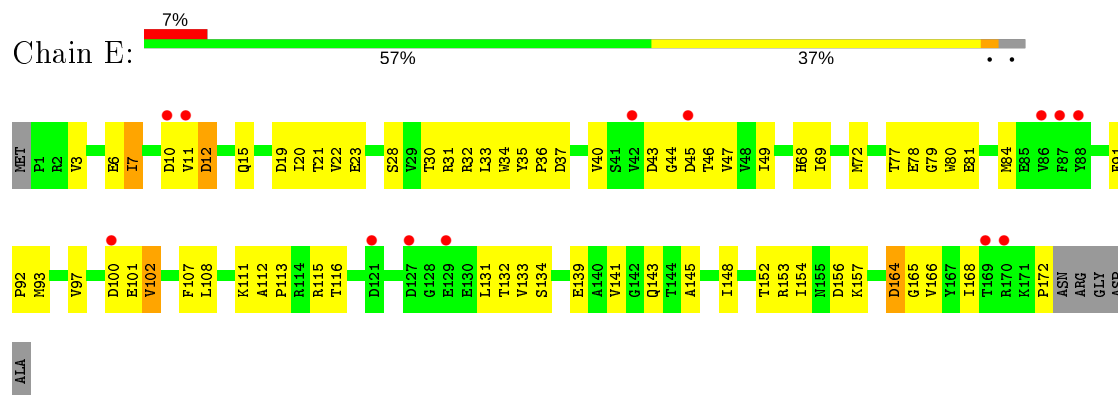




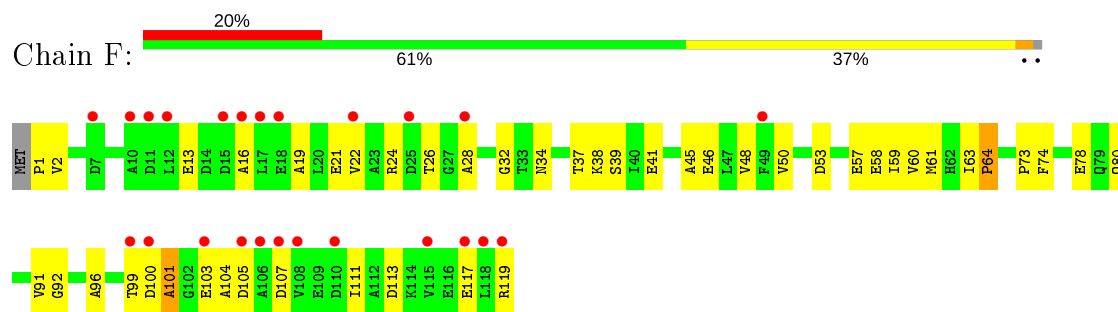
• Molecule 6: 50S ribosomal protein L5P



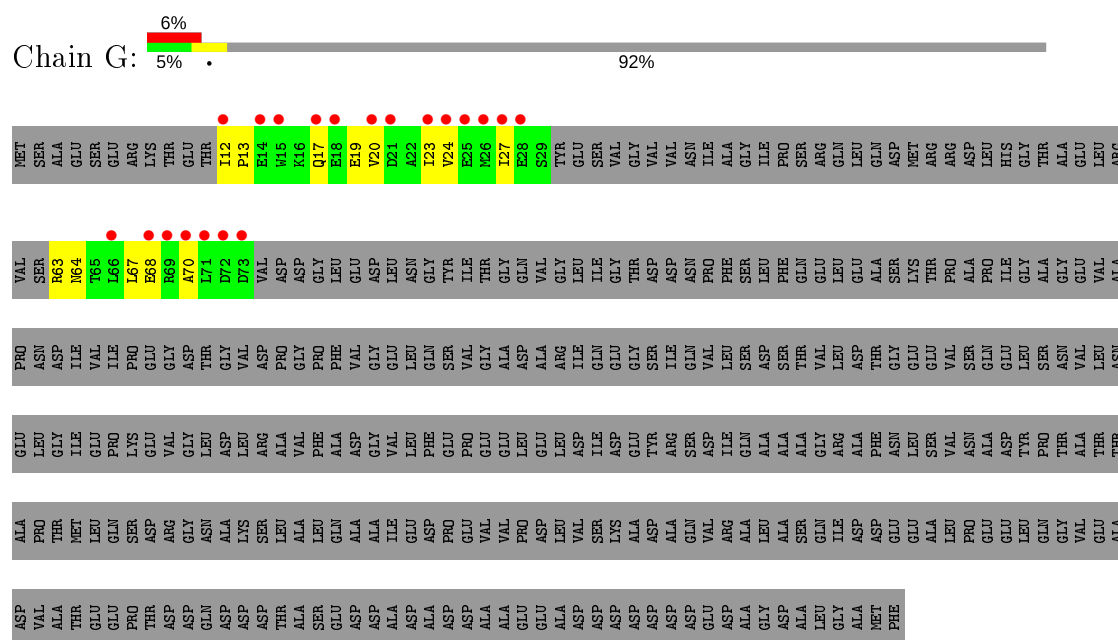
• Molecule 7: 50S ribosomal protein L6P



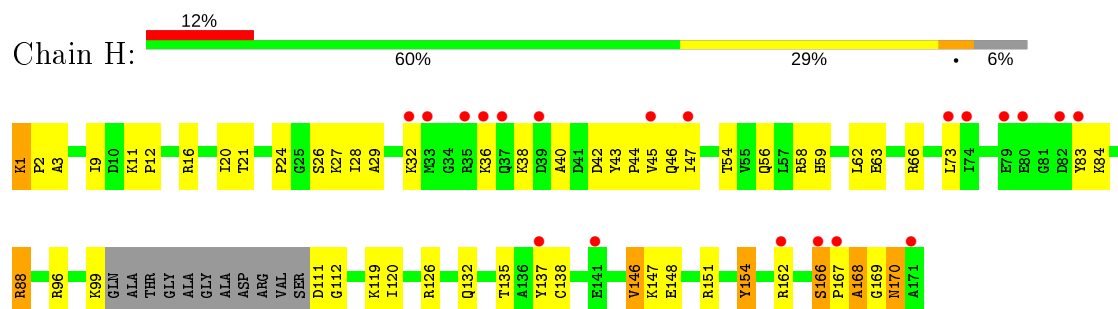
• Molecule 8: 50S ribosomal protein L7Ae



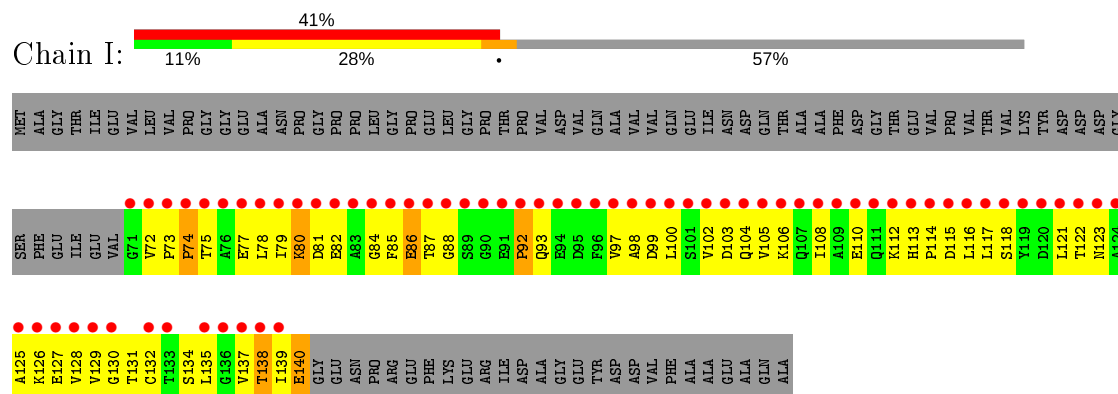
• Molecule 9: Acidic ribosomal protein P0 homolog



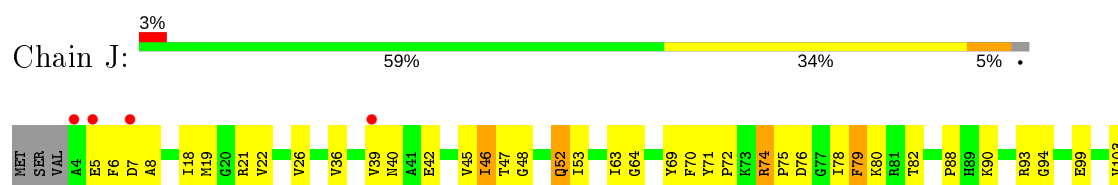
- Molecule 10: 50S ribosomal protein L10e



- Molecule 11: 50S ribosomal protein L11P

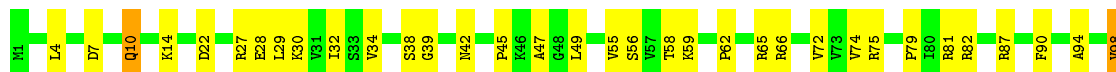


- Molecule 12: 50S ribosomal protein L13P

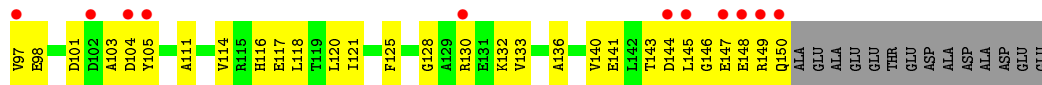




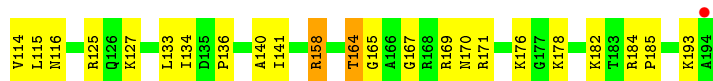
• Molecule 13: 50S ribosomal protein L14P



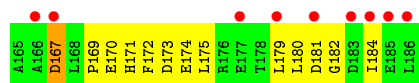
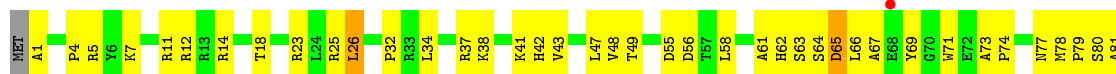
• Molecule 14: 50S ribosomal protein L15P



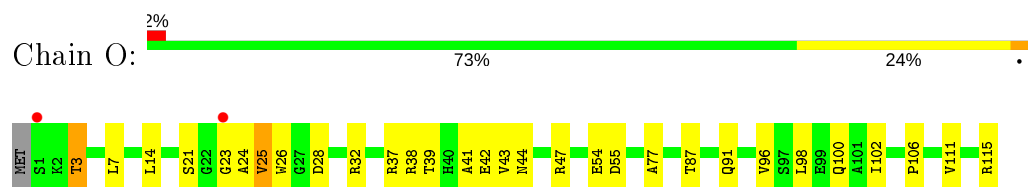
• Molecule 15: 50S ribosomal protein L15e



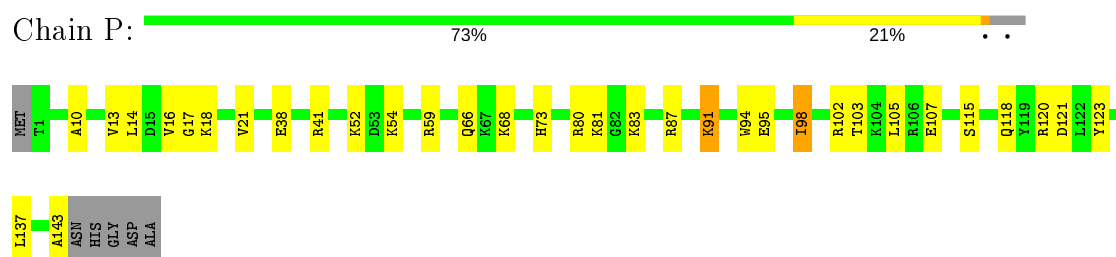
• Molecule 16: 50S ribosomal protein L18P



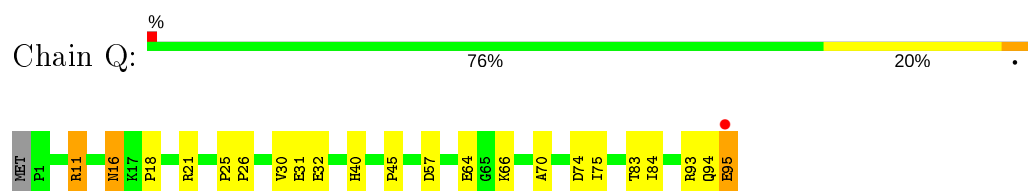
- Molecule 17: 50S ribosomal protein L18e



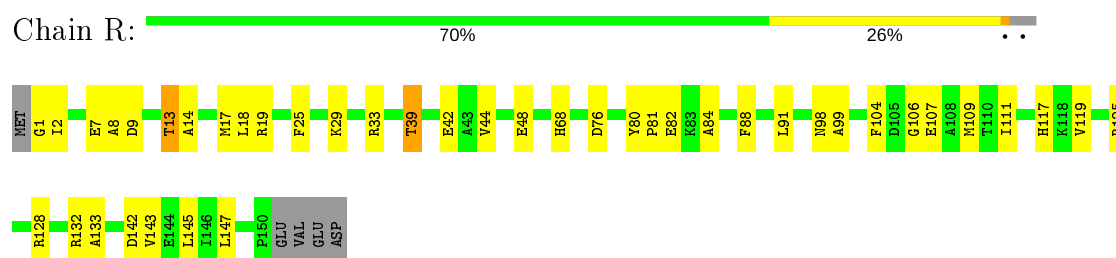
- Molecule 18: 50S ribosomal protein L19E



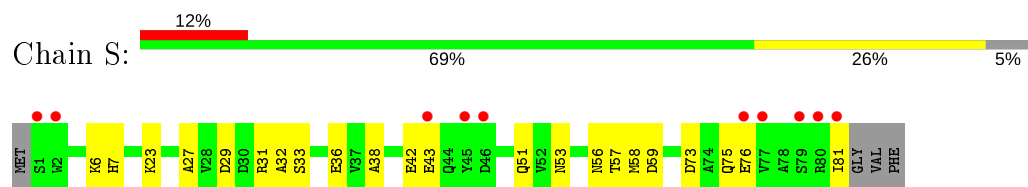
- Molecule 19: 50S ribosomal protein L21e



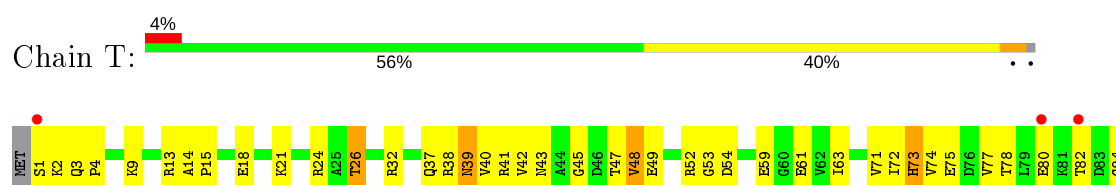
- Molecule 20: 50S ribosomal protein L22P



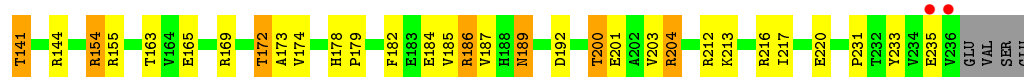
- Molecule 21: 50S ribosomal protein L23P



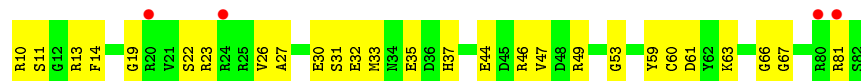
- Molecule 22: 50S ribosomal protein L24P



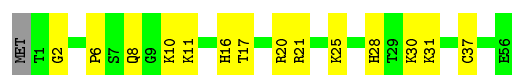




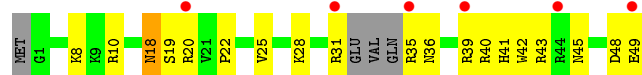
- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 90.6 (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, $R_{free}$	0.188 , 0.222 0.182 , 0.215	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
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> )	0.32 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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.

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



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.37	0/65959	0.70	27/102870 (0.0%)
2	9	0.35	0/2905	0.73	4/4528 (0.1%)
3	A	0.34	0/1786	0.67	0/2408
4	B	0.34	0/2690	0.65	0/3652
5	C	0.39	0/1884	0.67	0/2551
6	D	0.32	0/1111	0.57	0/1498
7	E	0.32	0/1382	0.57	0/1880
8	F	0.38	0/901	0.57	0/1224
9	G	0.28	0/241	0.48	0/324
10	H	0.33	0/1287	0.66	0/1725
11	I	0.36	0/526	0.56	0/716
12	J	0.34	0/1136	0.61	0/1530
13	K	0.34	0/1001	0.65	0/1347
14	L	0.34	0/1130	0.68	0/1509
15	M	0.36	0/1584	0.64	0/2119
16	N	0.37	0/1474	0.70	0/1999
17	O	0.33	0/874	0.61	0/1181
18	P	0.35	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.36	0/1172	0.66	0/1578
21	S	0.34	0/648	0.59	0/875
22	T	0.32	0/958	0.64	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.31	0/502	0.55	0/675
25	W	0.34	0/1219	0.63	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.35	0/1146	0.63	0/1536
28	Z	0.35	0/590	0.66	0/787
29	1	0.44	0/438	0.68	0/578
30	2	0.37	0/401	0.55	0/529
31	3	0.38	0/771	0.62	0/1024
All	All	0.36	0/98693	0.68	31/147577 (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	60
2	9	0	2
All	All	1	62

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.56	130.53	109.50
1	0	1942	A	C5'-C4'-C3'	9.41	131.06	116.00
1	0	871	G	C5'-C4'-O4'	-8.49	98.91	109.10
1	0	1942	A	C5'-C4'-O4'	7.87	118.55	109.10
1	0	1979	G	C2'-C3'-O3'	7.87	126.82	109.50
2	9	103	A	C5'-C4'-O4'	7.66	118.30	109.10
1	0	1819	G	C5'-C4'-C3'	7.37	127.80	116.00
2	9	39	U	N1-C1'-C2'	7.26	123.44	114.00
1	0	2316	G	C5'-C4'-C3'	-6.98	104.83	116.00
1	0	2467	A	C1'-O4'-C4'	-6.65	104.58	109.90
1	0	1504	A	C1'-O4'-C4'	-6.61	104.62	109.90
1	0	206	G	C5'-C4'-C3'	-6.39	105.77	116.00
1	0	1504	A	N9-C1'-C2'	6.21	122.07	114.00
1	0	2291	A	N9-C1'-C2'	6.12	121.95	114.00
1	0	1559	A	C2'-C3'-O3'	5.85	123.05	113.70
1	0	1942	A	C4'-C3'-C2'	-5.67	96.93	102.60
1	0	1942	A	C1'-O4'-C4'	-5.67	105.37	109.90
1	0	777	U	O4'-C1'-N1	5.60	112.68	108.20
1	0	1819	G	C4'-C3'-C2'	-5.47	97.13	102.60
1	0	1120	U	C5'-C4'-C3'	-5.45	107.28	116.00
1	0	1829	A	N9-C1'-C2'	-5.42	106.03	112.00
1	0	2313	C	C5'-C4'-O4'	5.32	115.48	109.10
1	0	841	A	C1'-O4'-C4'	-5.28	105.67	109.90
1	0	1878	G	N9-C1'-C2'	-5.26	106.21	112.00
1	0	1592	G	N9-C1'-C2'	5.23	120.80	114.00
2	9	103	A	C1'-O4'-C4'	-5.21	105.74	109.90
2	9	103	A	C4'-C3'-C2'	-5.15	97.45	102.60
1	0	1563	G	C4'-C3'-O3'	5.05	123.10	113.00
1	0	1819	G	C1'-O4'-C4'	-5.05	105.86	109.90
1	0	2726	U	N1-C1'-C2'	5.04	120.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2526	C	N1-C1'-C2'	5.03	120.54	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1292	G	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1794	G	Sidechain
1	0	1809	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	196	G	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	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2386	U	Sidechain
1	0	2395	A	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain

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Mol	Chain	Res	Type	Group
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	2616	G	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
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	771	G	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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	712	0
2	9	2600	0	1326	54	0
3	A	1753	0	1766	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2625	0	2533	163	0
5	C	1859	0	1816	109	0
6	D	1094	0	1085	116	0
7	E	1357	0	1266	76	0
8	F	890	0	843	56	0
9	G	240	0	231	17	0
10	H	1266	0	1268	78	0
11	I	519	0	500	72	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	55	0
14	L	1118	0	1076	56	0
15	M	1560	0	1568	59	0
16	N	1445	0	1401	114	0
17	O	865	0	873	29	0
18	P	1136	0	1123	35	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	45	0
21	S	641	0	605	20	0
22	T	950	0	923	48	0
23	U	410	0	364	31	0
24	V	499	0	511	29	0
25	W	1196	0	1137	96	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	53	0
28	Z	579	0	539	27	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	29	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5893	0	0	145	0
37	1	51	0	0	1	0
37	2	40	0	0	5	0
37	3	71	0	0	9	0
37	9	136	0	0	8	0
37	A	127	0	0	18	0
37	B	153	0	0	28	0
37	C	172	0	0	28	0
37	D	49	0	0	20	0
37	E	44	0	0	11	0
37	F	25	0	0	7	0
37	G	20	0	0	3	0
37	H	71	0	0	16	0
37	I	9	0	0	9	0
37	J	55	0	0	5	0
37	K	61	0	0	13	0
37	L	85	0	0	18	0
37	M	121	0	0	10	0
37	N	64	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	O	44	0	0	6	0
37	P	65	0	0	3	0
37	Q	52	0	0	2	0
37	R	83	0	0	8	0
37	S	33	0	0	5	0
37	T	40	0	0	5	0
37	U	25	0	0	4	0
37	V	14	0	0	4	0
37	W	67	0	0	10	0
37	X	28	0	0	3	0
37	Y	96	0	0	15	0
37	Z	29	0	0	5	0
All	All	99039	0	59899	2245	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.11
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.09
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.09
1:0:960:G:H4'	37:0:6920:HOH:O	1.51	1.08
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.36	1.07
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.36	1.06
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.37	1.05
1:0:1242:A:H5'	12:J:82:THR:HG23	1.38	1.04
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.39	1.03
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.40	1.03
1:0:156:C:H5''	15:M:171:ARG:HD3	1.40	1.03
28:Z:10:ARG:HA	37:Z:8414:HOH:O	1.58	1.01
1:0:871:G:C8	1:0:871:G:H5'	1.94	1.01
2:9:6:C:H5''	16:N:37:ARG:NH1	1.76	1.00
2:9:76:G:H3'	2:9:77:A:H5''	1.44	1.00
15:M:164:THR:HG22	15:M:167:GLY:H	1.22	0.99
1:0:21:G:H5'	20:R:2:ILE:HA	1.45	0.99
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.42	0.99
1:0:1751:G:H2'	1:0:1752:G:H5''	1.43	0.98
2:9:56:A:H2'	2:9:57:A:H5''	1.46	0.98
4:B:140:LEU:HA	37:B:8583:HOH:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:115:SER:H	18:P:118:GLN:HE21	1.01	0.97
13:K:39:GLY:HA2	37:K:4183:HOH:O	1.62	0.97
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.46	0.97
13:K:10:GLN:H	13:K:10:GLN:NE2	1.61	0.96
2:9:6:C:H5"	16:N:37:ARG:HH12	1.30	0.96
1:0:870:G:H2'	1:0:871:G:H5"	1.45	0.96
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.12	0.96
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.47	0.95
6:D:154:LYS:HD2	6:D:154:LYS:H	1.31	0.94
25:W:88:THR:HB	37:W:6679:HOH:O	1.66	0.94
21:S:57:THR:HG22	21:S:59:ASP:H	1.32	0.94
1:0:968:G:H1'	10:H:32:LYS:NZ	1.80	0.94
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.48	0.94
1:0:871:G:H8	1:0:871:G:H5'	1.29	0.94
12:J:76:ASP:HA	37:J:5907:HOH:O	1.68	0.94
16:N:144:GLY:O	16:N:147:ILE:HG22	1.68	0.93
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.51	0.93
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.84	0.93
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.28	0.93
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.51	0.92
4:B:86:ALA:HA	37:B:8583:HOH:O	1.68	0.92
25:W:88:THR:HG22	25:W:89:ASP:H	1.32	0.91
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.52	0.91
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.49	0.90
5:C:236:THR:HG22	5:C:239:ALA:N	1.86	0.90
5:C:2:GLN:HB3	37:C:8334:HOH:O	1.70	0.90
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.20	0.90
1:0:1835:U:H5	1:0:1840:A:N7	1.70	0.90
1:0:1116:U:H3	1:0:1246:A:H62	1.19	0.90
13:K:10:GLN:N	13:K:10:GLN:HE21	1.69	0.89
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.71	0.89
11:I:110:GLU:HA	11:I:113:HIS:NE2	1.86	0.89
3:A:199:HIS:HD2	3:A:201:PHE:H	1.20	0.89
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.53	0.88
1:0:1701:A:H4'	1:0:1702:U:H5"	1.53	0.88
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.88
6:D:25:MET:HE2	6:D:41:LEU:HG	1.56	0.88
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.88
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.38	0.88
1:0:645:U:OP2	14:L:4:LYS:HE2	1.74	0.88
1:0:214:U:H5'	37:0:5641:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.18	0.87
24:V:42:ASN:HB3	37:V:7247:HOH:O	1.75	0.87
1:0:1184:C:H1'	37:0:6954:HOH:O	1.75	0.87
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.55	0.86
10:H:166:SER:HB2	10:H:167:PRO:CD	2.05	0.86
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.54	0.86
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.39	0.86
1:0:2716:G:H5''	4:B:206:THR:HG21	1.58	0.86
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.74	0.86
6:D:27:ILE:HG22	6:D:28:GLY:H	1.40	0.85
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.58	0.85
1:0:856:G:H2'	37:0:4928:HOH:O	1.75	0.85
6:D:95:THR:OG1	6:D:174:VAL:HG22	1.76	0.85
1:0:2717:C:H2'	1:0:2718:C:H5''	1.58	0.85
4:B:238:ASN:HD22	4:B:240:GLY:H	1.24	0.85
5:C:236:THR:CG2	5:C:239:ALA:H	1.88	0.85
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.91	0.85
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.58	0.85
30:2:41:HIS:H	30:2:45:ASN:HD22	1.25	0.85
1:0:381:G:H5''	37:0:3823:HOH:O	1.75	0.85
16:N:23:ARG:HD3	37:N:8545:HOH:O	1.77	0.85
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.92	0.84
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.84
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.57	0.84
7:E:97:VAL:HG12	37:E:4191:HOH:O	1.77	0.84
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.57	0.84
1:0:560:C:H42	1:0:597:A:H61	1.24	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.08	0.84
16:N:164:ASP:CG	16:N:167:ASP:HA	1.98	0.84
25:W:154:ARG:OXT	37:W:4276:HOH:O	1.95	0.84
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.74	0.84
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.42	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.88	0.83
16:N:163:PHE:O	16:N:164:ASP:CG	2.17	0.83
11:I:118:SER:HB2	11:I:123:ASN:HB2	1.57	0.83
1:0:962:C:H1'	16:N:5:ARG:NH1	1.93	0.83
10:H:29:ALA:HB3	10:H:66:ARG:HH12	1.43	0.83
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.58	0.83
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.59	0.82
9:G:12:ILE:HA	37:G:4499:HOH:O	1.77	0.82
5:C:214:THR:HG21	37:C:8402:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.82
4:B:321:PRO:HA	37:B:8664:HOH:O	1.79	0.82
10:H:99:LYS:HD3	10:H:119:LYS:HD3	1.60	0.82
16:N:113:SER:HB2	37:N:8557:HOH:O	1.79	0.82
14:L:133:VAL:HA	37:L:8573:HOH:O	1.80	0.82
1:0:541:C:H2'	1:0:542:A:H5''	1.61	0.82
1:0:870:G:C2'	1:0:871:G:H5''	2.10	0.82
17:O:42:GLU:HB2	37:O:2176:HOH:O	1.78	0.81
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.63	0.81
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.81	0.81
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.62	0.81
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.63	0.80
24:V:12:THR:HG22	24:V:15:GLU:CG	2.11	0.80
1:0:1667:A:H8	1:0:1667:A:H5'	1.46	0.80
1:0:2812:A:H2	1:0:2814:A:H62	1.23	0.80
3:A:191:GLY:HA2	3:A:194:MET:CE	2.11	0.80
1:0:1372:A:H3'	37:0:6680:HOH:O	1.80	0.80
6:D:105:SER:HB2	6:D:131:THR:HG23	1.63	0.80
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.63	0.80
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.62	0.80
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.80
5:C:236:THR:HG21	37:C:8373:HOH:O	1.81	0.80
31:3:62:THR:HB	37:3:8549:HOH:O	1.81	0.80
37:0:6368:HOH:O	15:M:178:LYS:HB2	1.81	0.79
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.64	0.79
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.10	0.79
1:0:1625:U:H4'	37:0:4167:HOH:O	1.83	0.79
14:L:79:ASP:HB3	37:L:8558:HOH:O	1.83	0.79
8:F:91:VAL:HG12	8:F:92:GLY:H	1.48	0.79
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.98	0.79
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.64	0.78
10:H:27:LYS:H	10:H:59:HIS:HD2	1.31	0.78
26:X:78:GLU:HG2	26:X:79:GLU:H	1.47	0.78
1:0:1160:G:H5'	1:0:1161:A:C5'	2.11	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.78
3:A:192:VAL:HB	37:A:8597:HOH:O	1.83	0.78
16:N:163:PHE:O	16:N:163:PHE:CG	2.35	0.78
1:0:1162:G:H1'	11:I:117:LEU:HD11	1.65	0.78
1:0:1701:A:H5'	37:0:5782:HOH:O	1.84	0.78
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.48	0.78
11:I:80:LYS:HD3	11:I:86:GLU:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2710:U:H1'	37:0:7113:HOH:O	1.84	0.78
1:0:559:U:H5'	1:0:559:U:H6	1.49	0.78
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.64	0.78
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.18	0.78
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.65	0.78
1:0:545:G:H8	1:0:545:G:H5'	1.46	0.78
37:0:6914:HOH:O	22:T:9:LYS:HB2	1.81	0.78
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.66	0.78
37:0:6266:HOH:O	16:N:4:PRO:HD2	1.83	0.78
37:0:5794:HOH:O	6:D:99:ASP:HA	1.84	0.78
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.32	0.78
24:V:1:THR:HG23	24:V:2:VAL:H	1.48	0.78
1:0:2506:A:O2'	1:0:2507:G:H8	1.65	0.78
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.66	0.77
1:0:506:G:H22	1:0:509:A:H5'	1.48	0.77
5:C:132:ASP:HB3	37:C:8362:HOH:O	1.83	0.77
2:9:14:G:H5'	2:9:14:G:H8	1.50	0.77
4:B:62:ARG:HA	4:B:65:MET:HE3	1.64	0.77
5:C:236:THR:HA	37:C:8450:HOH:O	1.84	0.77
11:I:110:GLU:HA	11:I:113:HIS:CD2	2.19	0.77
1:0:1119:G:H22	1:0:1246:A:H2	1.26	0.77
1:0:544:G:H2'	1:0:545:G:H5''	1.65	0.77
3:A:35:GLY:O	3:A:36:ASP:HB3	1.83	0.77
25:W:88:THR:HG22	25:W:89:ASP:N	1.99	0.77
1:0:346:U:H4'	37:0:6338:HOH:O	1.84	0.77
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.67	0.77
1:0:1182:C:H1'	1:0:1192:A:H8	1.47	0.77
37:0:9208:HOH:O	4:B:254:GLN:HG3	1.85	0.77
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.65	0.77
30:2:39:ARG:HG2	37:2:3143:HOH:O	1.85	0.76
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.67	0.76
1:0:2768:A:H2'	1:0:2769:C:O4'	1.85	0.76
11:I:132:CYS:HB3	11:I:137:VAL:HB	1.67	0.76
1:0:2291:A:C8	1:0:2309:C:H5'	2.20	0.76
11:I:99:ASP:O	11:I:100:LEU:HD23	1.85	0.76
1:0:1160:G:C5'	1:0:1161:A:H5'	2.10	0.76
2:9:39:U:H1'	2:9:44:A:H61	1.51	0.76
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.50	0.76
8:F:96:ALA:HA	37:F:3111:HOH:O	1.83	0.76
1:0:541:C:C2'	1:0:542:A:H5''	2.16	0.76
37:0:4336:HOH:O	12:J:47:THR:HB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1130:U:H5'	37:0:7165:HOH:O	1.86	0.76
1:0:1751:G:C2'	1:0:1752:G:H5''	2.15	0.76
20:R:9:ASP:O	20:R:13:THR:HB	1.86	0.76
16:N:164:ASP:OD2	16:N:167:ASP:HA	1.87	0.75
1:0:1166:A:H1'	1:0:1192:A:C2	2.21	0.75
1:0:1634:G:H3'	37:0:3396:HOH:O	1.85	0.75
2:9:56:A:C2'	2:9:57:A:H5''	2.16	0.75
11:I:75:THR:HA	11:I:112:LYS:HZ1	1.51	0.75
10:H:166:SER:CB	10:H:167:PRO:HD3	2.16	0.75
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.50	0.75
21:S:57:THR:HG22	21:S:59:ASP:N	2.01	0.75
10:H:169:GLY:HA3	37:H:8391:HOH:O	1.86	0.75
11:I:78:LEU:HD12	11:I:112:LYS:HE3	1.68	0.75
11:I:113:HIS:N	11:I:114:PRO:HD2	2.01	0.75
10:H:162:ARG:HD2	37:H:8383:HOH:O	1.86	0.75
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.49	0.75
18:P:115:SER:H	18:P:118:GLN:NE2	1.82	0.75
25:W:149:LEU:HG	25:W:153:MET:HE2	1.69	0.74
37:0:9741:HOH:O	11:I:92:PRO:HD2	1.87	0.74
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.68	0.74
8:F:91:VAL:HG12	8:F:92:GLY:N	2.03	0.74
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.50	0.74
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.74
1:0:288:A:H61	1:0:364:C:H42	1.35	0.74
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.52	0.74
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.23	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.67	0.74
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.67	0.74
1:0:2637:A:H5'	37:0:8785:HOH:O	1.87	0.74
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.70	0.74
6:D:57:THR:HG23	6:D:63:ILE:HA	1.70	0.74
14:L:143:THR:HG22	14:L:144:ASP:N	2.03	0.73
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.69	0.73
31:3:70:ARG:HD3	37:3:8538:HOH:O	1.86	0.73
3:A:131:HIS:O	3:A:132:ASP:HB2	1.88	0.73
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.19	0.73
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.19	0.73
1:0:2054:A:N3	20:R:128:ARG:NH2	2.37	0.73
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.88	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.87	0.73
25:W:65:VAL:HA	25:W:68:THR:HG22	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:G:H22	1:0:363:A:H2	1.37	0.73
1:0:968:G:H1'	10:H:32:LYS:HZ2	1.54	0.73
18:P:115:SER:OG	18:P:118:GLN:HG3	1.88	0.73
1:0:21:G:C5'	20:R:2:ILE:HA	2.18	0.73
20:R:39:THR:HB	20:R:42:GLU:HG3	1.69	0.73
1:0:2586:U:H3	1:0:2592:G:H22	1.34	0.73
1:0:1666:C:H2'	1:0:1667:A:H5'	1.71	0.73
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.71	0.73
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.18	0.73
37:0:5779:HOH:O	28:Z:49:ARG:HD2	1.87	0.73
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.37	0.72
14:L:136:ALA:HB3	37:L:8573:HOH:O	1.88	0.72
18:P:115:SER:N	18:P:118:GLN:HE21	1.84	0.72
30:2:41:HIS:N	30:2:45:ASN:HD22	1.87	0.72
1:0:1594:C:OP2	18:P:120:ARG:HD2	1.88	0.72
1:0:1118:A:H3'	1:0:1118:A:C8	2.24	0.72
1:0:968:G:H1'	10:H:32:LYS:HZ1	1.53	0.72
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.72
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.02	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.90	0.72
1:0:272:A:H3'	37:0:7018:HOH:O	1.88	0.72
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.87	0.72
1:0:657:G:OP1	5:C:27:ARG:NH2	2.20	0.72
3:A:199:HIS:CD2	3:A:201:PHE:H	2.07	0.72
14:L:148:GLU:HA	37:L:8572:HOH:O	1.90	0.72
22:T:9:LYS:HE3	22:T:13:ARG:NH1	2.05	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.54	0.71
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.71
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.23	0.71
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.71	0.71
24:V:39:ALA:N	24:V:40:PRO:HD2	2.05	0.71
1:0:1116:U:O2'	1:0:1118:A:H2	1.67	0.71
37:0:6942:HOH:O	4:B:211:THR:HG21	1.90	0.71
5:C:242:GLU:HG3	37:C:8381:HOH:O	1.89	0.71
15:M:164:THR:HG22	15:M:167:GLY:N	2.03	0.71
20:R:39:THR:HG22	20:R:42:GLU:H	1.56	0.71
1:0:1450:C:H4'	1:0:1451:C:OP2	1.89	0.71
1:0:1559:A:H1'	37:0:5365:HOH:O	1.91	0.71
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.21	0.71
2:9:6:C:OP1	16:N:37:ARG:NH1	2.24	0.71
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.72	0.71
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.73	0.70
12:J:45:VAL:HG23	12:J:130:VAL:O	1.90	0.70
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.56	0.70
1:0:1119:G:H8	12:J:52:GLN:HE22	1.38	0.70
5:C:246:ARG:NE	37:C:8423:HOH:O	2.23	0.70
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.74	0.70
9:G:12:ILE:N	9:G:13:PRO:HD3	2.06	0.70
1:0:1163:G:H5'	11:I:115:ASP:O	1.92	0.70
1:0:236:A:H4'	1:0:237:G:H5'	1.74	0.70
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.22	0.70
1:0:2896:A:H5''	37:0:5599:HOH:O	1.90	0.70
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.70
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.21	0.70
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.70
1:0:284:C:H4'	1:0:285:A:O5'	1.92	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.90	0.70
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.74	0.70
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.73	0.70
11:I:106:LYS:O	11:I:110:GLU:HG3	1.91	0.70
11:I:110:GLU:HA	11:I:113:HIS:CE1	2.26	0.70
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.72	0.70
10:H:146:VAL:HG13	37:H:8379:HOH:O	1.92	0.70
23:U:14:GLU:O	23:U:17:THR:HB	1.92	0.70
1:0:2908:A:H2'	1:0:2909:G:O4'	1.92	0.69
2:9:49:G:H5''	37:9:8464:HOH:O	1.92	0.69
37:C:8357:HOH:O	17:O:3:THR:HG21	1.91	0.69
12:J:107:ASN:ND2	12:J:109:TYR:H	1.89	0.69
1:0:2426:G:H1'	37:0:5592:HOH:O	1.91	0.69
2:9:29:C:H2'	2:9:30:C:H5'	1.75	0.69
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.22	0.69
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.39	0.69
30:2:18:ASN:HD21	30:2:40:ARG:H	1.41	0.69
4:B:103:ASP:HB2	37:B:8597:HOH:O	1.92	0.69
1:0:396:U:H1'	37:0:7121:HOH:O	1.93	0.69
1:0:1505:U:H6	1:0:1505:U:H5'	1.57	0.69
37:9:8464:HOH:O	16:N:147:ILE:HB	1.92	0.69
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.07	0.69
7:E:68:HIS:O	7:E:72:MET:HG3	1.93	0.69
31:3:65:THR:HG23	31:3:67:LEU:HG	1.74	0.69
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.74	0.69
4:B:16:ARG:NH1	37:B:8621:HOH:O	2.25	0.69
5:C:1:MET:HG2	5:C:2:GLN:H	1.56	0.69
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.20	0.69
1:O:182:G:H5'	37:O:4653:HOH:O	1.93	0.69
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.26	0.69
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.23	0.69
1:O:2468:A:H61	31:3:48:ASN:HD21	1.38	0.68
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.23	0.68
1:O:1701:A:H4'	1:O:1702:U:C5'	2.23	0.68
5:C:236:THR:H	5:C:239:ALA:HB3	1.59	0.68
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.76	0.68
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.74	0.68
5:C:140:VAL:HB	37:C:8450:HOH:O	1.93	0.68
25:W:13:MET:CE	25:W:17:ILE:HG22	2.23	0.68
5:C:139:VAL:HG13	37:C:8447:HOH:O	1.93	0.68
16:N:80:SER:HB2	37:N:8534:HOH:O	1.92	0.68
1:O:542:A:H5'	1:O:542:A:C8	2.26	0.68
1:O:1973:A:H5'	1:O:1973:A:H8	1.59	0.68
1:O:1165:G:H4'	1:O:1174:A:O2'	1.93	0.68
1:O:1474:C:C6	1:O:1474:C:H5'	2.29	0.68
1:O:2878:U:H2'	1:O:2879:A:O4'	1.94	0.68
31:3:73:GLU:HB3	37:3:8559:HOH:O	1.93	0.68
3:A:210:GLY:HA3	37:A:8589:HOH:O	1.93	0.68
4:B:141:ARG:HD2	4:B:163:GLU:OE2	1.94	0.68
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.57	0.68
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.23	0.68
1:O:2840:A:OP1	4:B:211:THR:HG23	1.94	0.68
3:A:192:VAL:HG13	37:A:8558:HOH:O	1.92	0.67
1:O:20:G:H21	20:R:117:HIS:HD2	1.43	0.67
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.73	0.67
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.59	0.67
29:1:25:LYS:HE2	37:2:7213:HOH:O	1.93	0.67
4:B:185:GLY:HA2	37:B:8639:HOH:O	1.93	0.67
10:H:9:ILE:HD12	10:H:54:THR:HG22	1.77	0.67
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.60	0.67
14:L:72:ASN:HB2	37:L:8583:HOH:O	1.93	0.67
1:O:962:C:H1'	16:N:5:ARG:HH12	1.58	0.67
6:D:135:VAL:HG22	6:D:136:ARG:H	1.59	0.67
7:E:100:ASP:HB2	37:E:2789:HOH:O	1.94	0.67
5:C:115:LEU:O	5:C:118:THR:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:41:HIS:H	30:2:45:ASN:ND2	1.92	0.67
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.07	0.67
22:T:47:THR:HB	22:T:100:ASP:HB3	1.77	0.67
27:Y:141:THR:HG23	37:Y:8589:HOH:O	1.93	0.67
1:0:1329:A:H2	37:0:4183:HOH:O	1.76	0.67
2:9:51:A:H5'	16:N:160:SER:HB3	1.77	0.67
1:0:1377:C:H6	1:0:1377:C:H5'	1.60	0.67
1:0:541:C:H2'	1:0:542:A:C5'	2.25	0.67
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.76	0.67
4:B:62:ARG:HA	4:B:65:MET:CE	2.24	0.67
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.76	0.67
1:0:1080:C:H4'	1:0:1081:A:OP1	1.94	0.67
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.25	0.67
15:M:169:ARG:HD2	37:M:8590:HOH:O	1.95	0.67
1:0:1206:U:H6	1:0:1206:U:H5'	1.58	0.67
2:9:14:G:H5'	2:9:14:G:C8	2.28	0.67
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.76	0.67
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.10	0.66
1:0:2346:C:O2'	6:D:52:THR:HG21	1.94	0.66
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.76	0.66
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.76	0.66
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.24	0.66
1:0:2508:C:H2'	37:0:6248:HOH:O	1.95	0.66
8:F:99:THR:HA	37:F:3461:HOH:O	1.95	0.66
15:M:80:GLY:O	15:M:81:ARG:HD3	1.95	0.66
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.26	0.66
22:T:53:GLY:HA3	37:T:6384:HOH:O	1.94	0.66
1:0:1701:A:H5''	1:0:1702:U:H3'	1.78	0.66
1:0:31:C:H2'	37:0:7180:HOH:O	1.96	0.66
4:B:307:ARG:HB2	4:B:307:ARG:HH11	1.61	0.66
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.60	0.66
1:0:1118:A:H62	1:0:1244:U:H3	1.44	0.66
1:0:2533:C:H5'	1:0:2533:C:H6	1.61	0.66
10:H:59:HIS:HA	10:H:62:LEU:HD23	1.78	0.66
22:T:61:GLU:HG3	37:T:3851:HOH:O	1.93	0.66
25:W:122:ARG:NH2	25:W:154:ARG:OXT	2.28	0.66
1:0:1603:A:H5'	1:0:1605:G:O4'	1.96	0.65
1:0:2635:A:O2'	1:0:2636:C:H5'	1.97	0.65
1:0:299:U:H5'	37:0:6826:HOH:O	1.96	0.65
2:9:39:U:H1'	2:9:44:A:N6	2.11	0.65
2:9:6:C:C5'	16:N:37:ARG:NH1	2.57	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.76	0.65
10:H:9:ILE:O	10:H:9:ILE:HG22	1.95	0.65
7:E:11:VAL:HG12	7:E:12:ASP:N	2.11	0.65
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.10	0.65
14:L:68:GLU:HA	37:L:8542:HOH:O	1.97	0.65
1:0:1058:A:H2'	1:0:1060:C:H5''	1.77	0.65
1:0:1766:U:O2	1:0:1778:A:H5'	1.96	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
1:0:1172:G:H1'	37:0:4474:HOH:O	1.96	0.65
1:0:1778:A:H2'	1:0:1779:A:H5'	1.78	0.65
1:0:259:G:H21	15:M:58:GLN:NE2	1.95	0.65
25:W:4:LEU:O	25:W:32:CYS:HA	1.97	0.65
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.78	0.65
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.65
1:0:2748:G:H2'	37:0:7030:HOH:O	1.96	0.65
1:0:2756:U:H3	1:0:2896:A:H2	1.39	0.65
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.96	0.65
5:C:27:ARG:HG3	5:C:29:ASP:OD1	1.97	0.65
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.78	0.65
17:O:32:ARG:HD3	17:O:32:ARG:O	1.95	0.65
27:Y:133:HIS:HD2	37:Y:8582:HOH:O	1.78	0.65
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.65
7:E:132:THR:HB	37:E:2227:HOH:O	1.97	0.65
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.79	0.65
25:W:149:LEU:HG	25:W:153:MET:CE	2.27	0.65
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.79	0.65
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.97	0.65
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.09	0.65
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.62	0.65
1:0:1730:G:H5'	1:0:1731:C:C5	2.32	0.65
3:A:55:VAL:HG22	3:A:68:ILE:O	1.97	0.65
1:0:474:C:O3'	5:C:73:LEU:HD21	1.96	0.65
10:H:47:ILE:HD12	37:H:8379:HOH:O	1.97	0.65
1:0:558:C:O2'	1:0:559:U:H5''	1.97	0.65
6:D:25:MET:CE	6:D:37:ALA:HB1	2.27	0.65
11:I:72:VAL:HG13	11:I:73:PRO:HD2	1.79	0.65
4:B:125:GLU:O	4:B:129:ARG:HG3	1.97	0.64
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.62	0.64
4:B:51:VAL:HG23	4:B:329:TYR:O	1.96	0.64
7:E:69:ILE:HA	7:E:72:MET:CE	2.28	0.64
13:K:22:ASP:HB2	37:K:5264:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:37:ARG:NE	37:N:8532:HOH:O	2.30	0.64
18:P:18:LYS:O	18:P:21:VAL:HG22	1.97	0.64
1:0:553:G:P	27:Y:204:ARG:HH22	2.20	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.97	0.64
1:0:69:A:H5'	1:0:69:A:C8	2.33	0.64
10:H:9:ILE:HG23	10:H:126:ARG:CZ	2.28	0.64
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.78	0.64
1:0:1209:C:H2'	1:0:1210:G:H8	1.61	0.64
5:C:107:ARG:NE	37:C:8457:HOH:O	2.22	0.64
7:E:101:GLU:HB2	7:E:116:THR:O	1.98	0.64
20:R:39:THR:HG23	20:R:107:GLU:O	1.98	0.64
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.80	0.64
1:0:1120:U:H5''	1:0:1120:U:C6	2.33	0.64
1:0:1666:C:O2'	1:0:1667:A:H5''	1.98	0.64
1:0:603:A:H5''	1:0:604:G:OP1	1.97	0.64
2:9:13:A:O2'	2:9:14:G:H5''	1.97	0.64
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.78	0.64
6:D:65:GLU:HG3	37:D:6752:HOH:O	1.96	0.64
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.63	0.64
1:0:2505:G:O2'	1:0:2506:A:H5'	1.98	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
1:0:558:C:C2'	1:0:559:U:H5''	2.28	0.63
3:A:33:GLU:O	3:A:34:ASP:HB2	1.97	0.63
4:B:36:PRO:HA	4:B:168:GLY:CA	2.28	0.63
6:D:99:ASP:HB3	6:D:103:ASN:H	1.63	0.63
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.28	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.97	0.63
16:N:73:ALA:HB2	16:N:163:PHE:CZ	2.33	0.63
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.27	0.63
4:B:248:ARG:O	4:B:251:VAL:HG13	1.98	0.63
1:0:2783:A:H3'	37:O:4728:HOH:O	1.97	0.63
2:9:69:U:OP1	16:N:4:PRO:HG3	1.99	0.63
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.81	0.63
1:0:902:G:N7	14:L:18:HIS:HD2	1.97	0.63
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.28	0.63
37:O:6896:HOH:O	22:T:2:LYS:HE2	1.99	0.63
4:B:307:ARG:CG	4:B:307:ARG:HH11	2.11	0.63
37:O:3483:HOH:O	31:3:57:GLY:HA2	1.98	0.63
1:0:1008:C:H5''	10:H:16:ARG:HH12	1.63	0.63
1:0:2414:A:H2'	1:0:2415:A:C8	2.33	0.63
17:O:87:THR:O	17:O:91:GLN:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:38:THR:HG22	37:W:3580:HOH:O	1.99	0.63
6:D:55:LYS:O	6:D:56:ARG:HB2	1.98	0.63
7:E:15:GLN:HG2	7:E:19:ASP:O	1.97	0.62
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.81	0.62
27:Y:220:GLU:HG2	37:Y:8549:HOH:O	1.98	0.62
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.80	0.62
11:I:78:LEU:HD12	11:I:112:LYS:CE	2.29	0.62
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.29	0.62
5:C:162:VAL:HG13	5:C:232:LEU:HD21	1.81	0.62
37:9:8438:HOH:O	16:N:41:LYS:HD3	1.99	0.62
7:E:7:ILE:HD11	7:E:11:VAL:C	2.19	0.62
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.33	0.62
9:G:23:ILE:O	9:G:27:ILE:HG13	2.00	0.62
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.81	0.62
20:R:44:VAL:O	20:R:48:GLU:HG3	1.99	0.62
24:V:44:GLY:O	24:V:48:GLU:HG2	2.00	0.62
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.11	0.62
10:H:170:ASN:HD22	10:H:170:ASN:N	1.96	0.62
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.64	0.62
11:I:108:ILE:HG21	11:I:128:VAL:HG11	1.82	0.62
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.62
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.33	0.62
1:0:2570:G:H5''	37:0:4412:HOH:O	2.00	0.62
1:0:417:G:P	37:0:6908:HOH:O	2.57	0.62
29:1:17:THR:HG22	30:2:49:GLU:OXT	1.99	0.62
37:0:6519:HOH:O	3:A:211:LYS:HG2	1.99	0.62
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.30	0.62
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.82	0.62
4:B:7:ARG:CG	4:B:7:ARG:HH11	2.10	0.62
14:L:143:THR:HG22	14:L:144:ASP:H	1.65	0.62
27:Y:144:ARG:NH1	37:Y:8576:HOH:O	2.33	0.62
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.14	0.62
20:R:39:THR:HB	20:R:42:GLU:CG	2.29	0.62
23:U:9:CYS:HA	23:U:52:THR:HG23	1.80	0.62
1:0:1189:A:H3'	37:0:7173:HOH:O	1.99	0.62
1:0:2769:C:H2'	1:0:2770:G:O4'	2.00	0.62
4:B:238:ASN:HD22	4:B:240:GLY:N	1.97	0.62
13:K:55:VAL:HG12	13:K:56:SER:N	2.15	0.62
21:S:43:GLU:HB3	37:S:8342:HOH:O	1.99	0.62
1:0:2830:U:H3'	37:0:4724:HOH:O	2.00	0.62
8:F:101:ALA:HB3	8:F:105:ASP:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:23:ARG:NH1	37:N:8545:HOH:O	2.33	0.62
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.80	0.61
1:O:282:C:O2'	1:O:283:U:H5'	2.00	0.61
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.15	0.61
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.30	0.61
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.81	0.61
5:C:237:GLU:HB2	37:C:8429:HOH:O	2.00	0.61
10:H:27:LYS:N	10:H:59:HIS:HD2	1.98	0.61
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.81	0.61
1:O:69:A:H5'	1:O:69:A:H8	1.65	0.61
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.82	0.61
7:E:6:GLU:HA	7:E:46:THR:HG22	1.83	0.61
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.98	0.61
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.98	0.61
1:O:2346:C:O5'	1:O:2346:C:H6	1.83	0.61
6:D:23:VAL:O	6:D:23:VAL:HG23	2.01	0.61
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.30	0.61
11:I:134:SER:O	11:I:135:LEU:HD23	2.01	0.61
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.00	0.61
27:Y:144:ARG:CZ	37:Y:8612:HOH:O	2.47	0.61
1:O:1189:A:O2'	1:O:1208:C:H2'	2.01	0.61
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.61
12:J:131:THR:HG22	12:J:134:GLU:H	1.64	0.61
1:O:2851:G:O2'	1:O:2852:A:H5'	2.00	0.61
1:O:470:U:O2'	29:1:16:HIS:HD2	1.82	0.61
5:C:76:ARG:HD3	37:C:8366:HOH:O	1.99	0.61
27:Y:186:ARG:HH11	27:Y:186:ARG:HG2	1.66	0.61
1:O:545:G:C8	1:O:545:G:H5'	2.32	0.61
5:C:16:VAL:HG12	5:C:17:ASP:N	2.16	0.61
12:J:103:VAL:HG12	37:J:5907:HOH:O	2.00	0.61
1:O:1189:A:H1'	1:O:1209:C:O4'	2.00	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.04	0.61
2:9:48:C:H4'	16:N:141:ARG:HH21	1.66	0.61
6:D:99:ASP:CB	6:D:103:ASN:H	2.14	0.61
7:E:81:GLU:HG2	7:E:134:SER:CB	2.31	0.61
13:K:75:ARG:CZ	37:K:4172:HOH:O	2.48	0.61
26:X:75:ALA:O	26:X:83:ALA:HA	2.00	0.61
1:O:1159:G:H21	1:O:1189:A:H8	1.48	0.60
8:F:107:ASP:O	8:F:111:ILE:HG13	2.00	0.60
1:O:338:C:H4'	5:C:174:ILE:CD1	2.31	0.60
6:D:166:ILE:HD12	37:D:6326:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:105:VAL:HG11	11:I:129:VAL:HG23	1.83	0.60
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.84	0.60
1:O:1528:A:H2'	1:O:1529:G:O4'	2.01	0.60
1:O:1667:A:C8	1:O:1667:A:H5'	2.34	0.60
1:O:1862:C:H1'	37:O:6711:HOH:O	2.00	0.60
1:O:2638:G:H5'	37:O:4429:HOH:O	2.00	0.60
6:D:149:ARG:NH1	37:D:3066:HOH:O	2.24	0.60
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.84	0.60
27:Y:185:VAL:HG12	37:Y:8570:HOH:O	2.01	0.60
27:Y:187:VAL:HB	37:Y:8570:HOH:O	2.01	0.60
1:O:1741:U:H5'	1:O:1742:A:OP1	2.02	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.60
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.29	0.60
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.31	0.60
1:O:1120:U:H6	1:O:1120:U:H5''	1.67	0.60
4:B:307:ARG:CB	4:B:307:ARG:HH11	2.15	0.60
1:O:2548:C:OP2	4:B:5:ARG:NH2	2.35	0.60
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.84	0.60
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.67	0.60
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.31	0.60
1:O:1641:A:H2'	1:O:1642:A:H5'	1.82	0.60
5:C:98:ARG:NH1	37:C:8355:HOH:O	2.33	0.60
37:O:3349:HOH:O	10:H:11:LYS:HE2	2.01	0.60
1:O:1244:U:OP1	12:J:18:ILE:HD13	2.01	0.60
37:O:3491:HOH:O	22:T:82:THR:HA	2.01	0.60
1:O:1679:C:H5'	37:O:8834:HOH:O	2.02	0.60
29:I:21:ARG:HD2	29:I:37:CYS:SG	2.41	0.60
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.84	0.60
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.83	0.60
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.83	0.60
14:L:73:VAL:HG23	14:L:74:THR:H	1.66	0.60
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.99	0.60
4:B:179:LEU:O	4:B:183:GLU:HG2	2.01	0.60
6:D:37:ALA:O	6:D:40:ILE:HG12	2.02	0.60
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.70	0.60
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.37	0.60
25:W:88:THR:CG2	25:W:89:ASP:H	2.10	0.60
8:F:26:THR:HG21	8:F:103:GLU:CG	2.32	0.59
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.17	0.59
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.02	0.59
1:O:1187:U:O2'	1:O:1189:A:H2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:43:VAL:HG11	16:N:81:ALA:HA	1.84	0.59
26:X:25:ARG:HG2	37:X:5356:HOH:O	2.01	0.59
1:0:2438:G:H5'	37:0:5671:HOH:O	2.01	0.59
14:L:114:VAL:HG11	37:L:8573:HOH:O	2.02	0.59
21:S:81:ILE:HG23	37:S:8335:HOH:O	2.02	0.59
1:0:191:A:OP1	15:M:176:LYS:HE3	2.03	0.59
1:0:2779:G:H21	7:E:143:GLN:NE2	2.00	0.59
3:A:121:ALA:O	3:A:124:VAL:HG22	2.02	0.59
4:B:7:ARG:CD	4:B:9:GLY:O	2.50	0.59
5:C:12:THR:HB	37:C:8440:HOH:O	2.01	0.59
10:H:21:THR:O	10:H:120:ILE:HD12	2.01	0.59
15:M:64:ARG:HD2	37:M:8585:HOH:O	2.02	0.59
37:K:408:HOH:O	23:U:37:GLU:HB3	2.01	0.59
1:0:2630:G:O6	3:A:206:ARG:NH2	2.36	0.59
4:B:204:GLY:HA3	37:B:8660:HOH:O	2.03	0.59
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.38	0.59
1:0:2241:C:O2'	1:0:2242:U:H5'	2.02	0.59
1:0:289:G:N2	1:0:363:A:H2	2.01	0.59
2:9:41:C:O4'	6:D:50:VAL:HG23	2.03	0.59
6:D:136:ARG:HD2	6:D:155:HIS:O	2.02	0.59
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.66	0.59
9:G:63:ARG:O	9:G:67:LEU:HG	2.02	0.59
12:J:131:THR:HG22	12:J:133:GLY:N	2.18	0.59
14:L:149:ARG:O	14:L:150:GLN:HB2	2.03	0.59
1:0:2578:G:H5'	1:0:2578:G:H8	1.67	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
37:0:4451:HOH:O	2:9:103:A:H4'	2.01	0.59
3:A:223:ARG:HG3	37:A:8605:HOH:O	2.02	0.59
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.83	0.59
7:E:172:PRO:HB3	37:E:6931:HOH:O	2.02	0.59
8:F:26:THR:HG21	8:F:103:GLU:HG3	1.84	0.59
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.82	0.59
21:S:81:ILE:HG12	37:S:8335:HOH:O	2.02	0.59
25:W:80:ASP:O	25:W:84:VAL:HG23	2.02	0.59
1:0:328:U:O4'	5:C:202:THR:HG22	2.02	0.59
2:9:76:G:C3'	2:9:77:A:H5''	2.27	0.59
1:0:1162:G:H1'	11:I:117:LEU:CD1	2.32	0.59
1:0:710:G:OP1	17:O:24:ALA:HB3	2.03	0.59
1:0:1299:G:O6	14:L:6:ARG:HD3	2.03	0.59
4:B:145:HIS:HD2	4:B:146:THR:O	1.86	0.59
22:T:80:GLU:OE2	22:T:84:GLY:HA2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.02	0.59
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.21	0.58
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.84	0.58
23:U:31:PHE:CG	23:U:37:GLU:HG2	2.38	0.58
1:0:567:U:H5''	37:W:5817:HOH:O	2.03	0.58
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.85	0.58
19:Q:11:ARG:HD3	37:Q:5620:HOH:O	2.01	0.58
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.03	0.58
4:B:162:MET:HG3	4:B:310:ARG:NH1	2.18	0.58
5:C:79:ARG:O	5:C:87:ARG:HG2	2.03	0.58
7:E:31:ARG:NH1	37:E:5919:HOH:O	2.36	0.58
11:I:129:VAL:HG13	11:I:139:ILE:HD11	1.85	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
1:0:1182:C:H1'	1:0:1192:A:C8	2.34	0.58
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.67	0.58
1:0:558:C:H5'	37:0:4756:HOH:O	2.01	0.58
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.04	0.58
6:D:69:ILE:O	6:D:69:ILE:HG22	2.02	0.58
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.68	0.58
9:G:64:ASN:N	9:G:64:ASN:HD22	2.00	0.58
11:I:98:ALA:O	11:I:137:VAL:HA	2.03	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.84	0.58
1:0:1086:A:C6	25:W:11:VAL:HG11	2.38	0.58
4:B:175:LEU:C	4:B:175:LEU:HD23	2.24	0.58
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.04	0.58
15:M:61:ILE:HG13	37:M:8618:HOH:O	2.02	0.58
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.38	0.58
1:0:1525:G:H5'	1:0:1526:A:OP2	2.04	0.58
3:A:164:ARG:NE	37:A:8590:HOH:O	2.36	0.58
10:H:148:GLU:HA	10:H:148:GLU:OE1	2.04	0.58
12:J:130:VAL:HG12	12:J:131:THR:N	2.18	0.58
23:U:52:THR:HG22	23:U:54:THR:N	2.17	0.58
1:0:1119:G:N2	1:0:1246:A:H2	1.99	0.58
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.03	0.58
1:0:485:A:N3	1:0:487:G:H5''	2.18	0.58
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.30	0.58
4:B:42:ALA:HB1	4:B:308:LEU:HD11	1.85	0.58
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.85	0.58
27:Y:235:GLU:H	27:Y:235:GLU:CD	2.06	0.58
1:0:1441:G:O2'	1:0:1442:A:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2004:U:H4'	37:0:4805:HOH:O	2.03	0.58
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.85	0.58
3:A:88:ILE:HG22	3:A:88:ILE:O	2.02	0.58
10:H:147:LYS:HG3	37:H:8379:HOH:O	2.02	0.58
13:K:30:LYS:O	13:K:55:VAL:HG13	2.03	0.58
14:L:104:ASP:HB3	37:L:8563:HOH:O	2.04	0.58
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.58
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.03	0.58
1:0:1130:U:H2'	1:0:1131:G:O4'	2.04	0.58
25:W:81:ASP:OD1	25:W:92:ASP:HB2	2.03	0.58
1:0:2064:U:H5'	1:0:2652:U:O3'	2.04	0.58
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.04	0.58
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.18	0.58
10:H:99:LYS:CD	10:H:119:LYS:HD3	2.33	0.58
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.03	0.58
14:L:145:LEU:O	14:L:148:GLU:HG3	2.04	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.04	0.57
26:X:25:ARG:HD2	37:X:3861:HOH:O	2.04	0.57
26:X:31:ILE:O	26:X:35:GLU:HG3	2.04	0.57
1:0:31:C:H4'	37:0:6914:HOH:O	2.03	0.57
5:C:118:THR:O	5:C:136:VAL:HG13	2.04	0.57
7:E:23:GLU:HG2	7:E:28:SER:CB	2.34	0.57
10:H:73:LEU:HD21	10:H:146:VAL:HA	1.85	0.57
16:N:154:LEU:O	16:N:155:GLU:HB3	2.05	0.57
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.87	0.57
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.86	0.57
6:D:62:ASP:HA	37:D:4233:HOH:O	2.04	0.57
4:B:267:LYS:HD3	37:B:8528:HOH:O	2.04	0.57
6:D:35:ALA:N	37:D:5576:HOH:O	2.37	0.57
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.33	0.57
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.57
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.99	0.57
30:2:35:ARG:HB2	37:2:2691:HOH:O	2.04	0.57
2:9:44:A:O4'	6:D:76:ARG:NE	2.38	0.57
8:F:117:GLU:C	8:F:119:ARG:H	2.08	0.57
1:0:285:A:H2'	1:0:286:U:O4'	2.05	0.57
1:0:536:A:H3'	37:0:4546:HOH:O	2.03	0.57
7:E:7:ILE:HG22	7:E:45:ASP:O	2.04	0.57
8:F:37:THR:O	8:F:41:GLU:HG3	2.04	0.57
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.86	0.57
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:129:VAL:HG13	11:I:139:ILE:CD1	2.35	0.57
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.20	0.57
16:N:155:GLU:O	16:N:156:GLU:HG3	2.05	0.57
1:O:2420:G:O2'	1:O:2421:G:H5'	2.04	0.57
1:O:57:C:H5''	37:O:6253:HOH:O	2.05	0.57
6:D:170:TYR:O	6:D:171:ASP:HB3	2.05	0.57
10:H:27:LYS:H	10:H:59:HIS:CD2	2.17	0.57
27:Y:212:ARG:HD2	37:Y:8602:HOH:O	2.05	0.57
27:Y:216:ARG:HD3	37:Y:8569:HOH:O	2.04	0.57
1:O:2533:C:C6	1:O:2533:C:H5'	2.39	0.57
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.69	0.57
1:O:506:G:H22	1:O:509:A:H5''	1.67	0.57
1:O:111:C:O2'	29:1:20:ARG:HG2	2.04	0.57
30:2:31:ARG:CZ	37:2:7177:HOH:O	2.52	0.57
10:H:9:ILE:HG23	10:H:126:ARG:NE	2.20	0.57
11:I:75:THR:HA	11:I:112:LYS:NZ	2.18	0.57
1:O:797:A:C4'	28:Z:10:ARG:N	2.68	0.57
22:T:111:ARG:HB3	22:T:119:ALA:HB2	1.87	0.56
26:X:78:GLU:CG	26:X:79:GLU:H	2.17	0.56
27:Y:155:ARG:NH1	37:Y:8557:HOH:O	2.38	0.56
1:O:2456:A:H5'	37:O:5194:HOH:O	2.05	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.03	0.56
4:B:62:ARG:CA	4:B:65:MET:HE3	2.33	0.56
1:O:1377:C:H5'	1:O:1377:C:C6	2.40	0.56
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.56
1:O:316:A:H5'	22:T:54:ASP:OD2	2.04	0.56
1:O:500:G:H21	20:R:98:ASN:HD21	1.53	0.56
16:N:110:THR:HB	16:N:113:SER:OG	2.04	0.56
16:N:64:SER:C	16:N:66:LEU:H	2.09	0.56
1:O:1189:A:H1'	1:O:1209:C:C1'	2.35	0.56
1:O:1878:G:H1'	37:O:5621:HOH:O	2.04	0.56
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.20	0.56
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.19	0.56
25:W:139:GLY:O	25:W:141:HIS:HD2	1.88	0.56
4:B:85:ARG:NH1	37:B:8640:HOH:O	2.39	0.56
14:L:143:THR:CG2	14:L:144:ASP:N	2.68	0.56
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.52	0.56
1:O:2815:G:OP2	12:J:99:GLU:HG2	2.06	0.56
1:O:449:A:N7	5:C:43:LYS:HG2	2.20	0.56
10:H:170:ASN:N	10:H:170:ASN:ND2	2.53	0.56
20:R:132:ARG:NH1	37:R:8582:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:O:7046:HOH:O	31:3:60:LYS:HG3	2.05	0.56
16:N:151:ASP:O	16:N:154:LEU:HB2	2.06	0.56
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.06	0.56
23:U:52:THR:CG2	23:U:54:THR:HB	2.36	0.56
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.05	0.56
1:O:1667:A:H2'	1:O:1668:U:C6	2.40	0.56
1:O:558:C:H2'	1:O:559:U:H5'	1.88	0.56
1:O:738:G:H3'	37:O:6540:HOH:O	2.06	0.56
1:O:1119:G:H2'	12:J:52:GLN:NE2	2.21	0.56
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.56
25:W:41:TYR:HA	25:W:44:MET:HE3	1.88	0.56
1:O:1119:G:H8	12:J:52:GLN:NE2	2.03	0.56
1:O:2690:U:O2'	7:E:111:LYS:HE3	2.06	0.56
12:J:107:ASN:HD22	12:J:109:TYR:H	1.52	0.56
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.86	0.56
1:O:1116:U:O2'	1:O:1118:A:C2	2.50	0.56
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.88	0.56
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.87	0.56
10:H:38:LYS:HE2	10:H:42:ASP:CB	2.36	0.56
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.20	0.56
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.21	0.56
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.06	0.56
1:O:1919:A:H4'	37:O:4350:HOH:O	2.06	0.56
2:9:49:G:H2'	2:9:50:G:O4'	2.06	0.56
3:A:105:VAL:HG12	3:A:106:CYS:N	2.21	0.56
3:A:179:MET:HG2	3:A:186:TRP:CB	2.36	0.56
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.56
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.34	0.56
18:P:121:ASP:HB2	37:P:195:HOH:O	2.05	0.56
21:S:23:LYS:HE2	37:S:8330:HOH:O	2.04	0.56
1:O:1615:A:H5'	37:O:3687:HOH:O	2.06	0.55
1:O:711:G:H1'	37:O:6586:HOH:O	2.05	0.55
2:9:54:A:O2'	2:9:55:U:H5'	2.06	0.55
6:D:99:ASP:HB2	6:D:103:ASN:HB2	1.87	0.55
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.05	0.55
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.21	0.55
1:O:1118:A:H8	1:O:1119:G:H5''	1.69	0.55
1:O:2862:G:H4'	4:B:336:GLN:O	2.05	0.55
4:B:82:VAL:HG12	4:B:82:VAL:O	2.06	0.55
7:E:15:GLN:NE2	7:E:40:VAL:O	2.38	0.55
1:O:244:C:OP2	8:F:38:LYS:HE3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:77:ALA:HB3	37:L:8529:HOH:O	2.04	0.55
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.88	0.55
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.06	0.55
1:O:1299:G:N2	37:O:4183:HOH:O	2.38	0.55
1:O:2837:U:H2'	37:O:6334:HOH:O	2.05	0.55
3:A:100:PRO:HG2	3:A:103:VAL:CG2	2.33	0.55
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.21	0.55
10:H:147:LYS:N	37:H:8379:HOH:O	2.40	0.55
10:H:63:GLU:HA	37:H:8382:HOH:O	2.06	0.55
16:N:157:PRO:HA	37:N:8525:HOH:O	2.05	0.55
1:O:280:C:H2'	1:O:281:U:O4'	2.07	0.55
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.72	0.55
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.87	0.55
37:O:9044:HOH:O	18:P:81:LYS:HG2	2.05	0.55
20:R:29:LYS:HB3	37:R:8532:HOH:O	2.06	0.55
21:S:38:ALA:O	21:S:42:GLU:HG3	2.06	0.55
24:V:4:HIS:HB3	37:V:6622:HOH:O	2.07	0.55
1:O:1044:C:H5''	37:O:8542:HOH:O	2.06	0.55
4:B:41:PHE:CD2	4:B:190:MET:HE3	2.42	0.55
11:I:72:VAL:CG1	11:I:73:PRO:HD2	2.36	0.55
1:O:1123:A:C6	1:O:1238:C:H5'	2.42	0.55
1:O:1306:U:OP1	5:C:184:ARG:HD2	2.07	0.55
1:O:1878:G:O2'	1:O:1879:U:C6	2.57	0.55
1:O:2604:A:H5'	37:O:5291:HOH:O	2.07	0.55
1:O:282:C:H1'	1:O:368:C:H42	1.72	0.55
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.41	0.55
3:A:53:ALA:HB3	37:A:8609:HOH:O	2.06	0.55
4:B:119:HIS:O	4:B:121:PRO:HD3	2.07	0.55
4:B:140:LEU:HD23	37:B:8583:HOH:O	2.06	0.55
4:B:258:GLY:H	4:B:260:HIS:CE1	2.25	0.55
13:K:115:ARG:HG3	13:K:116:GLU:N	2.21	0.55
16:N:179:LEU:HA	16:N:184:ILE:HD12	1.89	0.55
27:Y:144:ARG:NE	37:Y:8612:HOH:O	2.39	0.55
3:A:212:PRO:HB2	37:A:8562:HOH:O	2.06	0.55
3:A:34:ASP:OD1	3:A:35:GLY:N	2.35	0.55
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.88	0.55
20:R:33:ARG:NH1	37:R:8543:HOH:O	2.37	0.55
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.88	0.55
1:O:263:U:O4'	8:F:59:ILE:HD13	2.06	0.55
1:O:2717:C:O2'	1:O:2718:C:H5''	2.06	0.55
3:A:175:LYS:HE2	37:A:8578:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:VAL:HG22	37:A:8600:HOH:O	2.06	0.55
4:B:297:VAL:HB	37:B:8610:HOH:O	2.07	0.55
14:L:133:VAL:HB	37:L:8557:HOH:O	2.06	0.55
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.37	0.55
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.60	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.72	0.55
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.55
1:0:775:G:OP1	29:1:16:HIS:HE1	1.90	0.55
30:2:19:SER:HB3	37:2:4479:HOH:O	2.07	0.55
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.88	0.55
1:0:2898:G:H4'	4:B:288:GLY:HA2	1.88	0.55
6:D:93:LEU:O	6:D:174:VAL:O	2.25	0.55
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.42	0.55
1:0:2815:G:N7	12:J:80:LYS:NZ	2.54	0.55
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.89	0.55
15:M:61:ILE:HA	37:M:8618:HOH:O	2.07	0.55
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.36	0.55
1:0:1299:G:H5'	37:0:3576:HOH:O	2.07	0.55
4:B:16:ARG:NE	37:B:8557:HOH:O	2.26	0.55
6:D:94:ALA:HB3	6:D:97:GLN:HG3	1.89	0.55
14:L:73:VAL:HG23	14:L:74:THR:N	2.22	0.55
16:N:38:LYS:HD2	16:N:114:LYS:HE3	1.89	0.55
16:N:154:LEU:HG	16:N:155:GLU:H	1.71	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.54
1:0:2064:U:H5'	1:0:2652:U:H4'	1.89	0.54
6:D:36:ASN:HA	37:D:7500:HOH:O	2.06	0.54
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.07	0.54
25:W:38:THR:HG22	25:W:39:ASP:H	1.73	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.21	0.54
7:E:11:VAL:HG13	7:E:23:GLU:O	2.06	0.54
10:H:28:ILE:HA	10:H:63:GLU:OE1	2.07	0.54
21:S:33:SER:OG	21:S:36:GLU:HG3	2.07	0.54
26:X:30:MET:HE1	26:X:55:ASN:HA	1.89	0.54
1:0:1209:C:H4'	37:0:4778:HOH:O	2.06	0.54
1:0:2502:C:H2'	1:0:2503:A:H5'	1.88	0.54
8:F:101:ALA:HA	37:F:5413:HOH:O	2.07	0.54
16:N:11:ARG:NH2	37:N:8519:HOH:O	2.40	0.54
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.43	0.54
1:0:138:U:H5''	1:0:139:C:OP2	2.08	0.54
1:0:1477:C:H5'	1:0:1868:G:C5'	2.37	0.54
1:0:1669:A:H2'	1:0:1670:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:154:LYS:H	6:D:154:LYS:CD	2.09	0.54
6:D:51:ARG:HD3	37:D:7636:HOH:O	2.06	0.54
15:M:60:VAL:C	15:M:61:ILE:HD12	2.27	0.54
28:Z:13:ARG:NH1	37:Z:8419:HOH:O	2.39	0.54
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.54
1:0:1191:A:H3'	1:0:1192:A:H5''	1.88	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.06	0.54
1:0:602:A:O2'	1:0:605:C:H4'	2.08	0.54
1:0:951:A:C2'	1:0:952:G:H5'	2.37	0.54
7:E:69:ILE:HA	7:E:72:MET:HE3	1.88	0.54
11:I:79:ILE:HA	11:I:108:ILE:HD11	1.88	0.54
24:V:58:THR:O	24:V:62:GLU:HG3	2.08	0.54
25:W:125:HIS:CD2	25:W:127:GLY:H	2.25	0.54
1:0:1181:A:H2'	1:0:1182:C:O4'	2.08	0.54
1:0:1441:G:H1'	37:0:7256:HOH:O	2.05	0.54
1:0:2289:G:H21	1:0:2291:A:H2	1.54	0.54
1:0:2361:A:H5''	37:0:8523:HOH:O	2.08	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.34	0.54
1:0:272:A:H5'	1:0:273:G:OP2	2.06	0.54
1:0:899:C:H5'	37:0:9708:HOH:O	2.07	0.54
31:3:17:HIS:O	31:3:18:GLN:HG3	2.08	0.54
37:0:8593:HOH:O	4:B:214:PRO:HD2	2.07	0.54
4:B:162:MET:CE	4:B:308:LEU:HD21	2.38	0.54
4:B:7:ARG:HG2	4:B:7:ARG:NH1	2.16	0.54
5:C:214:THR:HG23	37:C:8436:HOH:O	2.07	0.54
8:F:99:THR:O	8:F:100:ASP:HB2	2.07	0.54
11:I:118:SER:CB	11:I:123:ASN:HB2	2.35	0.54
12:J:107:ASN:C	12:J:107:ASN:HD22	2.11	0.54
15:M:30:GLU:O	15:M:34:GLU:HG3	2.07	0.54
1:0:21:G:H5''	20:R:1:GLY:O	2.07	0.54
6:D:91:ALA:HB1	37:D:5198:HOH:O	2.08	0.54
15:M:57:LYS:HE2	15:M:140:ALA:O	2.08	0.54
20:R:119:VAL:HG12	20:R:119:VAL:O	2.07	0.54
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.10	0.54
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.33	0.54
1:0:200:U:H2'	37:0:9953:HOH:O	2.06	0.54
37:9:8515:HOH:O	16:N:107:ASN:HB3	2.08	0.54
23:U:52:THR:HG22	23:U:54:THR:H	1.73	0.54
16:N:163:PHE:CD2	16:N:163:PHE:O	2.61	0.54
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.06	0.54
24:V:49:LEU:O	24:V:53:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.89	0.54
1:0:703:G:O2'	1:0:704:C:H5'	2.08	0.54
2:9:1:U:H5'	2:9:121:C:O2	2.08	0.54
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.36	0.54
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.89	0.54
11:I:113:HIS:N	11:I:114:PRO:CD	2.69	0.54
25:W:84:VAL:HG12	37:W:6679:HOH:O	2.08	0.54
1:0:2787:C:H5	37:0:4133:HOH:O	1.91	0.53
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.38	0.53
6:D:57:THR:HG23	6:D:63:ILE:CA	2.37	0.53
9:G:12:ILE:HG22	9:G:12:ILE:O	2.08	0.53
10:H:45:VAL:HA	10:H:167:PRO:O	2.07	0.53
14:L:143:THR:CG2	14:L:144:ASP:H	2.20	0.53
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.36	0.53
17:O:38:ARG:NH1	37:O:7674:HOH:O	2.41	0.53
37:0:9459:HOH:O	26:X:23:HIS:HD2	1.91	0.53
1:0:1333:U:H2'	1:0:1334:C:C6	2.44	0.53
1:0:2591:C:H2'	1:0:2592:G:O4'	2.09	0.53
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.53
1:0:2821:C:H4'	4:B:116:PRO:HB3	1.91	0.53
1:0:2756:U:N3	1:0:2896:A:H2	2.06	0.53
1:0:542:A:H2'	1:0:543:G:O4'	2.08	0.53
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.92	0.53
12:J:133:GLY:O	12:J:137:GLU:HG3	2.09	0.53
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.91	0.53
18:P:91:LYS:O	18:P:95:GLU:HG3	2.07	0.53
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.42	0.53
1:0:317:A:H5''	22:T:52:ARG:HD2	1.91	0.53
1:0:371:U:H2'	1:0:372:A:H8	1.74	0.53
14:L:61:ALA:HA	37:L:8563:HOH:O	2.09	0.53
25:W:122:ARG:CZ	37:W:5817:HOH:O	2.55	0.53
25:W:122:ARG:NH1	25:W:122:ARG:HG2	2.18	0.53
2:9:42:C:O2	6:D:76:ARG:NH1	2.41	0.53
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.90	0.53
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.53
17:O:39:THR:O	17:O:115:ARG:NH2	2.42	0.53
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.53
1:0:65:C:O2'	1:0:66:G:H5'	2.09	0.53
1:0:681:G:N3	1:0:681:G:H5'	2.24	0.53
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.33	0.53
4:B:168:GLY:O	4:B:169:GLY:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1:MET:HG2	5:C:2:GLN:N	2.22	0.53
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.38	0.53
6:D:27:ILE:HG22	6:D:28:GLY:N	2.17	0.53
9:G:12:ILE:N	9:G:13:PRO:CD	2.71	0.53
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.55	0.53
24:V:38:GLY:C	24:V:40:PRO:HD2	2.29	0.53
25:W:122:ARG:HH21	25:W:154:ARG:HD2	1.73	0.53
26:X:30:MET:CE	26:X:58:ALA:HB3	2.39	0.53
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.91	0.53
1:0:1209:C:H2'	1:0:1210:G:C8	2.42	0.53
1:0:2094:G:H4'	4:B:245:SER:HB3	1.90	0.53
1:0:2419:U:H5''	1:0:2420:G:H5'	1.91	0.53
2:9:24:U:H3'	2:9:25:G:H5'	1.90	0.53
4:B:305:ASP:O	4:B:306:LYS:HB2	2.09	0.53
4:B:310:ARG:NH2	37:B:8560:HOH:O	2.41	0.53
6:D:163:VAL:HA	37:D:6326:HOH:O	2.09	0.53
7:E:7:ILE:HD11	7:E:11:VAL:O	2.08	0.53
22:T:41:ARG:NH1	22:T:42:VAL:O	2.42	0.53
1:0:1044:C:H3'	1:0:1045:G:H5''	1.91	0.53
1:0:1353:C:P	37:0:4179:HOH:O	2.67	0.53
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.44	0.53
11:I:108:ILE:CG2	11:I:128:VAL:HG11	2.39	0.53
20:R:29:LYS:HD3	37:R:8532:HOH:O	2.08	0.53
1:0:338:C:H5''	37:C:8420:HOH:O	2.09	0.53
3:A:164:ARG:CZ	37:A:8590:HOH:O	2.57	0.53
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.91	0.53
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.37	0.53
23:U:33:SER:O	23:U:37:GLU:HG3	2.09	0.53
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.53
1:0:1500:U:P	18:P:41:ARG:HH22	2.32	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.40	0.52
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.52
4:B:2:GLN:HA	37:B:8626:HOH:O	2.08	0.52
5:C:246:ARG:NH2	37:C:8423:HOH:O	2.41	0.52
5:C:76:ARG:HG2	5:C:78:ARG:HH12	1.73	0.52
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.45	0.52
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.23	0.52
1:0:1205:U:H2'	1:0:1206:U:C5'	2.39	0.52
1:0:1527:A:H1'	1:0:1528:A:C8	2.44	0.52
1:0:1834:C:H2'	1:0:1840:A:N6	2.24	0.52
2:9:55:U:H4'	2:9:56:A:C8	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:ARG:NH1	4:B:11:LEU:HD22	2.24	0.52
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.45	0.52
11:I:128:VAL:HA	37:I:5331:HOH:O	2.09	0.52
2:9:6:C:C5'	16:N:37:ARG:HH12	2.12	0.52
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.91	0.52
1:0:1972:U:H2'	1:0:1973:A:H5'	1.92	0.52
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.74	0.52
6:D:135:VAL:HG22	6:D:136:ARG:N	2.24	0.52
23:U:47:ARG:HG3	37:U:4381:HOH:O	2.08	0.52
25:W:122:ARG:NH2	25:W:154:ARG:HD2	2.25	0.52
1:0:2812:A:N7	37:0:7006:HOH:O	2.34	0.52
1:0:920:C:H5''	1:0:921:G:O5'	2.10	0.52
7:E:69:ILE:HA	7:E:72:MET:HE2	1.91	0.52
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.08	0.52
12:J:99:GLU:HA	37:J:7377:HOH:O	2.09	0.52
13:K:87:ARG:CZ	37:K:4854:HOH:O	2.57	0.52
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.39	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.24	0.52
26:X:43:VAL:HG12	26:X:44:ASP:N	2.24	0.52
1:0:2265:U:H2'	1:0:2266:A:C8	2.45	0.52
1:0:281:U:H3'	37:0:6698:HOH:O	2.09	0.52
3:A:153:ARG:HD3	37:A:8531:HOH:O	2.09	0.52
1:0:1137:G:H1'	37:0:3380:HOH:O	2.09	0.52
1:0:2301:A:H5''	1:0:2302:A:H5'	1.91	0.52
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.52
10:H:58:ARG:O	10:H:62:LEU:HD22	2.10	0.52
11:I:75:THR:N	11:I:112:LYS:HE2	2.24	0.52
25:W:122:ARG:NH2	37:W:5817:HOH:O	2.43	0.52
26:X:41:PHE:O	26:X:43:VAL:HG23	2.08	0.52
1:0:2768:A:O2'	1:0:2769:C:H5'	2.09	0.52
2:9:29:C:C2'	2:9:30:C:H5'	2.39	0.52
4:B:156:LYS:HE3	37:B:8636:HOH:O	2.09	0.52
4:B:333:GLU:HB2	23:U:14:GLU:OE2	2.09	0.52
1:0:2256:G:H2'	1:0:2257:G:C5'	2.40	0.52
1:0:2256:G:H2'	1:0:2257:G:H5'	1.92	0.52
1:0:2506:A:O2'	1:0:2507:G:O5'	2.27	0.52
21:S:56:ASN:O	30:2:8:LYS:HE2	2.10	0.52
2:9:64:C:H2'	2:9:65:A:H5'	1.92	0.52
4:B:215:VAL:HB	4:B:234:ARG:HH12	1.75	0.52
4:B:307:ARG:HD3	37:B:8524:HOH:O	2.10	0.52
5:C:233:THR:HG22	5:C:234:VAL:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:86:THR:O	6:D:90:LEU:HG	2.10	0.52
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.92	0.52
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.25	0.52
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.10	0.52
25:W:119:HIS:HD2	25:W:120:PRO:O	1.93	0.52
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.40	0.52
1:0:2004:U:H2'	1:0:2004:U:O2	2.08	0.52
1:0:2526:C:O2'	1:0:2527:U:H5'	2.10	0.52
1:0:2638:G:H1'	37:0:7250:HOH:O	2.09	0.52
1:0:2768:A:H5''	37:0:3931:HOH:O	2.09	0.52
2:9:49:G:O2'	2:9:50:G:H5'	2.10	0.52
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.91	0.52
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.90	0.52
1:0:1384:C:H5'	26:X:30:MET:HG2	1.92	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
1:0:2090:G:H2'	1:0:2091:G:C8	2.44	0.52
1:0:2300:A:H4'	1:0:2301:A:O5'	2.11	0.52
1:0:2316:G:H4'	37:0:5592:HOH:O	2.09	0.52
37:0:5631:HOH:O	30:2:20:ARG:HB3	2.10	0.52
2:9:35:C:H5''	37:9:8453:HOH:O	2.10	0.52
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.25	0.52
8:F:19:ALA:O	8:F:22:VAL:HG22	2.10	0.52
11:I:134:SER:N	37:I:7330:HOH:O	2.43	0.52
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.25	0.52
20:R:39:THR:HB	20:R:42:GLU:CD	2.31	0.52
37:K:1387:HOH:O	23:U:20:MET:HE3	2.10	0.52
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.75	0.52
1:0:644:G:N3	1:0:644:G:H5'	2.24	0.51
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.40	0.51
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.71	0.51
10:H:56:GLN:HE21	10:H:126:ARG:NE	1.98	0.51
1:0:1185:U:OP1	11:I:126:LYS:HD3	2.10	0.51
14:L:57:VAL:HG12	14:L:57:VAL:O	2.10	0.51
20:R:68:HIS:CD2	20:R:76:ASP:HB2	2.45	0.51
24:V:56:ILE:O	24:V:60:GLN:HG3	2.09	0.51
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.08	0.51
1:0:1450:C:C4'	1:0:1451:C:OP2	2.57	0.51
1:0:1730:G:H5'	1:0:1731:C:C6	2.45	0.51
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.08	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.39	0.51
1:0:1266:U:H4'	27:Y:115:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:NH2	37:Y:8612:HOH:O	2.44	0.51
11:I:82:GLU:OE1	11:I:108:ILE:HG13	2.10	0.51
7:E:36:PRO:HD3	12:J:127:ILE:HD12	1.91	0.51
16:N:154:LEU:HG	16:N:155:GLU:N	2.24	0.51
26:X:74:ALA:HB1	26:X:85:VAL:HG22	1.91	0.51
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.31	0.51
1:O:2488:A:H61	1:O:2534:C:H42	1.58	0.51
10:H:162:ARG:HD3	37:H:8384:HOH:O	2.10	0.51
13:K:87:ARG:NE	37:K:4854:HOH:O	2.43	0.51
1:O:2363:G:O3'	19:Q:11:ARG:NH1	2.44	0.51
1:O:485:A:HO2'	1:O:487:G:H8	1.58	0.51
1:O:2434:A:O3'	31:3:28:GLY:HA3	2.11	0.51
6:D:10:PHE:CE1	6:D:11:HIS:HB3	2.45	0.51
6:D:58:VAL:HG12	6:D:59:GLY:N	2.25	0.51
7:E:31:ARG:HH12	7:E:68:HIS:CE1	2.29	0.51
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.92	0.51
8:F:46:GLU:N	37:F:3461:HOH:O	2.43	0.51
17:O:96:VAL:HA	37:O:4258:HOH:O	2.10	0.51
1:O:1173:A:H2'	37:O:3853:HOH:O	2.09	0.51
1:O:1878:G:H4'	37:O:3621:HOH:O	2.11	0.51
2:9:20:G:H3'	37:9:8433:HOH:O	2.10	0.51
6:D:65:GLU:HA	37:D:6752:HOH:O	2.10	0.51
8:F:99:THR:HG23	8:F:99:THR:O	2.10	0.51
10:H:38:LYS:HE2	10:H:42:ASP:HB2	1.93	0.51
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.57	0.51
16:N:169:PRO:O	16:N:172:PHE:HB3	2.11	0.51
16:N:171:HIS:CE1	37:N:8565:HOH:O	2.64	0.51
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.92	0.51
20:R:132:ARG:CZ	37:R:8582:HOH:O	2.58	0.51
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.45	0.51
1:O:1562:C:H42	1:O:2738:G:H1	1.58	0.51
1:O:2769:C:O2'	1:O:2770:G:H5'	2.10	0.51
14:L:62:ALA:HB2	14:L:103:ALA:CB	2.41	0.51
16:N:37:ARG:NH2	37:N:8532:HOH:O	2.44	0.51
18:P:16:VAL:HG12	18:P:17:GLY:N	2.26	0.51
22:T:49:GLU:HB3	22:T:59:GLU:CG	2.40	0.51
1:O:1497:G:H4'	1:O:1627:G:O2'	2.11	0.51
1:O:2251:G:H2'	1:O:2252:A:C8	2.46	0.51
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.10	0.51
29:1:10:LYS:HG3	37:1:8429:HOH:O	2.10	0.51
31:3:56:PRO:N	37:3:8548:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:138:GLY:O	4:B:139:ASP:O	2.28	0.51
4:B:14:GLY:HA2	4:B:15:PRO:C	2.31	0.51
5:C:27:ARG:HG2	5:C:30:LEU:HG	1.92	0.51
6:D:81:GLU:O	6:D:85:GLN:HG3	2.11	0.51
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.93	0.51
1:O:2896:A:OP1	26:X:15:ARG:NH1	2.44	0.51
2:9:91:C:H2'	2:9:92:G:O4'	2.10	0.51
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.51
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.93	0.51
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.26	0.51
37:O:4070:HOH:O	5:C:50:GLU:HG2	2.09	0.51
6:D:153:THR:HG22	37:D:5234:HOH:O	2.11	0.51
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.10	0.51
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.29	0.51
7:E:43:ASP:HA	37:E:5864:HOH:O	2.11	0.51
1:O:1503:U:H2'	1:O:1504:A:O4'	2.11	0.51
1:O:1592:G:O2'	1:O:1593:C:O4'	2.27	0.51
1:O:656:G:OP2	17:O:37:ARG:HD2	2.11	0.51
1:O:88:G:H5'	1:O:88:G:H8	1.76	0.51
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.76	0.51
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.46	0.51
5:C:246:ARG:CZ	37:C:8423:HOH:O	2.56	0.51
6:D:128:LEU:N	37:D:6007:HOH:O	2.44	0.51
6:D:99:ASP:O	6:D:159:PRO:HG3	2.10	0.51
10:H:167:PRO:O	10:H:168:ALA:HB2	2.11	0.51
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.93	0.51
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.92	0.51
1:O:2415:A:C2	16:N:25:ARG:HB3	2.46	0.51
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.41	0.51
25:W:31:HIS:HB3	37:W:5420:HOH:O	2.10	0.51
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.41	0.51
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.46	0.51
1:O:1236:A:H2'	1:O:1237:U:O4'	2.11	0.50
1:O:538:C:H5''	1:O:539:G:C8	2.45	0.50
1:O:558:C:C2'	1:O:559:U:C5'	2.89	0.50
2:9:2:U:OP2	2:9:2:U:H4'	2.11	0.50
18:P:103:THR:O	18:P:107:GLU:HG3	2.11	0.50
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.73	0.50
1:O:2507:G:H2'	1:O:2510:C:H42	1.76	0.50
37:O:6954:HOH:O	11:I:127:GLU:HG2	2.11	0.50
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:40:HIS:CE1	19:Q:94:GLN:HA	2.47	0.50
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.50
25:W:5:VAL:O	25:W:52:VAL:HG22	2.11	0.50
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.44	0.50
2:9:20:G:O2'	2:9:21:G:H5'	2.11	0.50
3:A:132:ASP:OD1	3:A:133:ARG:N	2.44	0.50
4:B:17:LYS:O	4:B:260:HIS:HD2	1.94	0.50
8:F:91:VAL:CG1	8:F:92:GLY:H	2.21	0.50
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.46	0.50
20:R:132:ARG:HG2	20:R:133:ALA:N	2.26	0.50
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.95	0.50
1:0:1234:U:N3	4:B:244:PRO:HB3	2.27	0.50
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.26	0.50
1:0:447:A:OP1	22:T:2:LYS:HG2	2.12	0.50
1:0:797:A:H4'	28:Z:10:ARG:N	2.26	0.50
1:0:960:G:H2'	1:0:960:G:N3	2.26	0.50
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.95	0.50
7:E:22:VAL:O	7:E:28:SER:HA	2.12	0.50
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.10	0.50
1:0:710:G:P	17:O:24:ALA:HB3	2.52	0.50
1:0:941:G:O2'	1:0:942:U:H5'	2.11	0.50
3:A:130:THR:HG22	3:A:131:HIS:O	2.10	0.50
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.26	0.50
5:C:16:VAL:HG12	5:C:17:ASP:H	1.74	0.50
2:9:41:C:C6	6:D:50:VAL:HG21	2.46	0.50
11:I:100:LEU:HD22	11:I:104:GLN:OE1	2.12	0.50
11:I:92:PRO:HG3	11:I:134:SER:O	2.10	0.50
1:0:1205:U:C2'	1:0:1206:U:H5''	2.42	0.50
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.50
1:0:2842:G:H2'	1:0:2843:A:H5'	1.92	0.50
31:3:87:ARG:NH1	37:3:8525:HOH:O	2.45	0.50
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.42	0.50
11:I:132:CYS:N	37:I:5371:HOH:O	2.43	0.50
12:J:88:PRO:O	12:J:94:GLY:HA3	2.11	0.50
23:U:52:THR:HG22	23:U:54:THR:HB	1.94	0.50
25:W:13:MET:HE1	25:W:18:GLN:HA	1.94	0.50
28:Z:44:GLU:HG3	28:Z:46:ARG:HG3	1.94	0.50
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.94	0.50
1:0:2320:U:H4'	1:0:2321:A:O4'	2.12	0.50
3:A:36:ASP:O	3:A:38:ILE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:102:THR:HG21	4:B:182:VAL:O	2.11	0.50
5:C:150:THR:HA	5:C:203:ALA:O	2.12	0.50
5:C:77:ALA:O	5:C:78:ARG:HG3	2.11	0.50
6:D:10:PHE:CD1	6:D:11:HIS:N	2.80	0.50
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.94	0.50
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.12	0.50
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.50
5:C:219:ASN:O	5:C:222:ASP:OD1	2.30	0.50
7:E:11:VAL:CG1	7:E:12:ASP:N	2.74	0.50
12:J:45:VAL:HG22	12:J:46:ILE:N	2.26	0.50
25:W:41:TYR:O	25:W:45:VAL:HG13	2.11	0.50
1:0:1185:U:H5'	37:0:6954:HOH:O	2.12	0.50
1:0:2524:G:H21	1:0:2526:C:N4	2.10	0.50
2:9:55:U:H4'	2:9:56:A:H8	1.74	0.50
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.94	0.50
7:E:21:THR:HG23	7:E:30:THR:OG1	2.12	0.50
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.50
1:0:1462:C:H2'	1:0:1463:A:C8	2.47	0.49
1:0:2329:C:O2'	1:0:2330:U:H5'	2.12	0.49
1:0:281:U:O2'	1:0:282:C:H5'	2.12	0.49
4:B:162:MET:CE	4:B:310:ARG:HD3	2.42	0.49
5:C:162:VAL:CG1	5:C:192:ILE:HD11	2.42	0.49
8:F:91:VAL:CG1	8:F:92:GLY:N	2.73	0.49
12:J:46:ILE:HA	37:J:1123:HOH:O	2.11	0.49
13:K:106:GLY:HA3	37:K:5264:HOH:O	2.12	0.49
16:N:7:LYS:HE2	37:N:8513:HOH:O	2.10	0.49
17:O:7:LEU:HD22	37:O:5650:HOH:O	2.12	0.49
18:P:143:ALA:HA	37:P:190:HOH:O	2.11	0.49
22:T:38:ARG:NH1	37:T:6217:HOH:O	2.44	0.49
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.12	0.49
3:A:94:LEU:N	3:A:94:LEU:HD23	2.26	0.49
6:D:10:PHE:CG	6:D:11:HIS:N	2.80	0.49
26:X:76:ARG:O	26:X:77:PHE:HB3	2.12	0.49
1:0:797:A:O4'	28:Z:10:ARG:N	2.45	0.49
1:0:1060:C:H6	1:0:1060:C:H5'	1.78	0.49
1:0:1183:C:N4	1:0:1184:C:H41	2.10	0.49
1:0:1699:C:H4'	37:0:5939:HOH:O	2.13	0.49
1:0:656:G:H5'	17:O:3:THR:CG2	2.42	0.49
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.93	0.49
11:I:88:GLY:C	37:I:5128:HOH:O	2.50	0.49
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:126:ASP:HB3	25:W:135:GLY:O	2.12	0.49
1:0:2403:C:H3'	37:0:4708:HOH:O	2.12	0.49
1:0:2756:U:N3	1:0:2896:A:C2	2.70	0.49
1:0:291:C:H2'	1:0:292:G:O4'	2.12	0.49
1:0:470:U:O2'	29:1:16:HIS:CD2	2.64	0.49
37:0:3568:HOH:O	4:B:27:ASN:HB2	2.11	0.49
4:B:27:ASN:H	4:B:27:ASN:HD22	1.60	0.49
12:J:74:ARG:O	12:J:78:ILE:HG12	2.12	0.49
14:L:143:THR:HG22	14:L:145:LEU:H	1.77	0.49
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.95	0.49
23:U:44:ARG:HB3	37:U:3805:HOH:O	2.11	0.49
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.48	0.49
1:0:1164:U:H4'	1:0:1165:G:OP1	2.12	0.49
1:0:189:A:OP1	15:M:171:ARG:NH2	2.44	0.49
1:0:1940:C:H4'	37:0:6837:HOH:O	2.11	0.49
3:A:194:MET:CE	3:A:199:HIS:HB2	2.43	0.49
5:C:180:SER:HB2	37:C:8444:HOH:O	2.11	0.49
6:D:56:ARG:N	37:D:6752:HOH:O	2.43	0.49
7:E:10:ASP:HA	37:E:3707:HOH:O	2.11	0.49
7:E:166:VAL:HG12	37:E:3134:HOH:O	2.12	0.49
11:I:110:GLU:HG2	11:I:113:HIS:NE2	2.28	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.49
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.27	0.49
1:0:1118:A:C8	1:0:1119:G:H5''	2.47	0.49
1:0:1197:G:N2	37:0:5734:HOH:O	2.45	0.49
1:0:1996:U:O2'	1:0:1997:A:H5'	2.13	0.49
1:0:2563:U:H2'	1:0:2565:C:O5'	2.12	0.49
2:9:31:C:H2'	2:9:32:G:O4'	2.13	0.49
4:B:241:PRO:HD2	37:B:8662:HOH:O	2.11	0.49
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.12	0.49
5:C:151:GLN:O	5:C:154:VAL:HB	2.13	0.49
14:L:97:VAL:HG12	14:L:98:GLU:O	2.13	0.49
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.49
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.29	0.49
1:0:1168:C:C5'	37:I:5128:HOH:O	2.61	0.49
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.49
5:C:236:THR:HG22	5:C:239:ALA:CB	2.43	0.49
1:0:2672:C:O2'	1:0:2673:U:H5'	2.13	0.49
16:N:58:LEU:N	16:N:58:LEU:HD12	2.28	0.49
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.13	0.49
25:W:130:HIS:O	25:W:136:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2912:C:H2'	1:0:2913:A:O4'	2.13	0.49
1:0:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.43	0.49
4:B:63:GLU:HG3	4:B:63:GLU:O	2.12	0.49
13:K:79:PRO:HB2	37:K:782:HOH:O	2.12	0.49
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.94	0.49
23:U:49:LEU:HD11	37:U:3805:HOH:O	2.13	0.49
27:Y:122:ARG:NH2	37:Y:8535:HOH:O	2.46	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.49
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.96	0.49
1:0:407:A:H5'	37:0:5526:HOH:O	2.12	0.49
4:B:248:ARG:HG2	37:B:8578:HOH:O	2.12	0.49
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.95	0.49
22:T:18:GLU:O	22:T:21:LYS:HG2	2.13	0.49
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.95	0.48
1:0:1789:G:O6	18:P:73:HIS:HE1	1.96	0.48
1:0:447:A:O2'	1:0:448:G:H5'	2.14	0.48
1:0:95:A:H5''	1:0:97:G:O4'	2.12	0.48
31:3:48:ASN:ND2	31:3:50:GLY:H	2.11	0.48
4:B:16:ARG:NH2	37:B:8557:HOH:O	2.40	0.48
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.47	0.48
4:B:80:ARG:HD3	37:B:8611:HOH:O	2.13	0.48
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.48	0.48
11:I:108:ILE:HG21	11:I:128:VAL:CG1	2.43	0.48
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.33	0.48
16:N:37:ARG:CZ	37:N:8532:HOH:O	2.61	0.48
21:S:73:ASP:OD1	21:S:75:GLN:HB2	2.13	0.48
27:Y:115:ARG:NE	37:Y:8555:HOH:O	2.45	0.48
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.46	0.48
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.96	0.48
1:0:584:U:H3'	37:0:5595:HOH:O	2.12	0.48
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.48	0.48
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.42	0.48
1:0:654:A:OP2	17:O:38:ARG:HD3	2.13	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.48
1:0:1484:G:H2'	37:0:8618:HOH:O	2.13	0.48
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.95	0.48
10:H:3:ALA:CA	10:H:58:ARG:HH12	2.25	0.48
12:J:19:MET:CE	12:J:132:LEU:HD11	2.43	0.48
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.09	0.48
23:U:17:THR:HG22	23:U:18:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:474:C:O3'	5:C:73:LEU:CD2	2.62	0.48
1:O:475:G:OP1	5:C:73:LEU:HD22	2.13	0.48
6:D:25:MET:CE	6:D:41:LEU:HG	2.38	0.48
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.43	0.48
7:E:77:THR:OG1	7:E:78:GLU:N	2.45	0.48
1:O:2521:A:OP2	10:H:3:ALA:HB3	2.13	0.48
16:N:86:LEU:O	16:N:90:LEU:HG	2.13	0.48
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.47	0.48
1:O:450:C:OP1	5:C:184:ARG:NH2	2.29	0.48
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.95	0.48
10:H:111:ASP:HB2	37:H:8349:HOH:O	2.13	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.48
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.94	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.48
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.95	0.48
37:O:6914:HOH:O	22:T:9:LYS:HD2	2.12	0.48
1:O:1878:G:O2'	1:O:1879:U:P	2.72	0.48
1:O:1909:A:N1	1:O:2128:G:H1'	2.28	0.48
31:3:3:MET:O	31:3:90:PHE:HA	2.13	0.48
2:9:92:G:H2'	2:9:93:A:C8	2.49	0.48
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.95	0.48
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.96	0.48
8:F:22:VAL:HG21	8:F:104:ALA:HB2	1.96	0.48
8:F:28:ALA:CB	8:F:99:THR:HG23	2.43	0.48
10:H:146:VAL:HG22	37:H:8379:HOH:O	2.12	0.48
1:O:1163:G:H5''	11:I:115:ASP:HB3	1.95	0.48
15:M:164:THR:HB	37:M:8519:HOH:O	2.13	0.48
15:M:84:LYS:HE2	37:M:8574:HOH:O	2.13	0.48
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.78	0.48
23:U:9:CYS:CA	23:U:52:THR:HG23	2.43	0.48
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.27	0.48
1:O:1730:G:C5'	1:O:1731:C:C6	2.96	0.48
1:O:920:C:H5'	1:O:921:G:C4	2.49	0.48
11:I:74:PRO:HG2	11:I:77:GLU:CD	2.34	0.48
16:N:79:PRO:HG3	16:N:142:THR:O	2.14	0.48
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.78	0.48
27:Y:172:THR:HG22	27:Y:173:ALA:N	2.29	0.48
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.95	0.48
28:Z:59:TYR:HA	37:Z:8432:HOH:O	2.14	0.48
1:O:1014:A:H2'	1:O:1015:C:H5'	1.95	0.48
1:O:396:U:OP2	31:3:38:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:12:ILE:HD12	37:G:692:HOH:O	2.14	0.48
9:G:19:GLU:O	9:G:23:ILE:HG13	2.14	0.48
12:J:52:GLN:HG3	12:J:53:ILE:N	2.29	0.48
22:T:49:GLU:HB3	22:T:59:GLU:HG3	1.96	0.48
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.61	0.48
11:I:105:VAL:HG11	11:I:129:VAL:CG2	2.44	0.48
12:J:42:GLU:O	12:J:131:THR:HG23	2.13	0.48
13:K:75:ARG:HE	13:K:94:ALA:HB3	1.78	0.48
20:R:106:GLY:HA2	20:R:109:MET:CE	2.44	0.48
27:Y:165:GLU:HB3	37:Y:8594:HOH:O	2.13	0.48
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.14	0.48
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.79	0.48
30:2:48:ASP:O	30:2:49:GLU:HB2	2.14	0.48
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.48
11:I:80:LYS:HB3	11:I:85:PHE:O	2.12	0.48
8:F:2:VAL:HG11	15:M:23:LEU:HD23	1.94	0.48
37:0:5031:HOH:O	15:M:58:GLN:HG3	2.14	0.48
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.36	0.48
1:0:121:U:OP2	30:2:10:ARG:NH2	2.39	0.47
1:0:1741:U:O2'	1:0:2723:G:H4'	2.14	0.47
1:0:344:C:H2'	1:0:345:G:O4'	2.13	0.47
1:0:432:G:O2'	1:0:433:C:H5'	2.14	0.47
16:N:170:GLU:O	16:N:174:GLU:HG3	2.14	0.47
1:0:2791:U:H1'	1:0:2792:A:H5"	1.95	0.47
1:0:564:G:H1'	37:0:5809:HOH:O	2.14	0.47
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.97	0.47
3:A:93:THR:HG23	3:A:154:ALA:O	2.14	0.47
4:B:175:LEU:O	4:B:175:LEU:HD23	2.14	0.47
4:B:79:MET:HE3	4:B:144:THR:HG21	1.96	0.47
5:C:13:ASP:OD1	5:C:13:ASP:O	2.32	0.47
6:D:101:THR:HG22	37:D:7400:HOH:O	2.13	0.47
1:0:2083:A:N6	12:J:90:LYS:HE2	2.28	0.47
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.58	0.47
25:W:3:ALA:O	25:W:54:PHE:HA	2.14	0.47
1:0:1505:U:C6	1:0:1505:U:H5'	2.46	0.47
1:0:2472:C:O2'	1:0:2634:G:H4'	2.14	0.47
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.13	0.47
8:F:38:LYS:NZ	15:M:3:SER:HA	2.29	0.47
23:U:47:ARG:CG	37:U:4381:HOH:O	2.61	0.47
25:W:108:ARG:HE	25:W:114:PRO:CG	2.27	0.47
1:0:1289:C:O2'	1:0:1290:G:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1439:C:OP1	30:2:41:HIS:HE1	1.97	0.47
1:0:1666:C:C2'	1:0:1667:A:C5'	2.92	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.33	0.47
1:0:2326:U:H4'	1:0:2412:G:H4'	1.96	0.47
1:0:2748:G:H5'	37:0:7030:HOH:O	2.14	0.47
1:0:420:U:H2'	1:0:421:C:C6	2.50	0.47
3:A:211:LYS:HD3	37:A:8614:HOH:O	2.13	0.47
4:B:51:VAL:HG22	4:B:53:LEU:HD13	1.97	0.47
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.97	0.47
14:L:21:ARG:N	37:L:8530:HOH:O	2.47	0.47
1:0:1667:A:H2'	1:0:1668:U:H6	1.78	0.47
1:0:1733:A:H4'	4:B:212:GLN:HA	1.95	0.47
1:0:820:G:C5	3:A:171:LYS:HB2	2.50	0.47
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.96	0.47
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.42	0.47
4:B:207:LYS:HG2	4:B:304:PRO:HB3	1.95	0.47
4:B:75:GLU:C	4:B:77:PRO:HD3	2.34	0.47
7:E:37:ASP:OD1	12:J:125:SER:HB3	2.15	0.47
10:H:9:ILE:HG12	10:H:56:GLN:HG2	1.96	0.47
16:N:181:ASP:OD1	16:N:182:GLY:N	2.47	0.47
20:R:104:PHE:HB2	20:R:109:MET:HE1	1.96	0.47
1:0:119:A:H2'	1:0:120:A:H5''	1.95	0.47
1:0:2415:A:H2'	1:0:2416:G:H5'	1.96	0.47
37:0:8728:HOH:O	3:A:11:ARG:HD3	2.15	0.47
5:C:140:VAL:HG12	5:C:141:SER:N	2.29	0.47
8:F:100:ASP:HB3	37:F:5691:HOH:O	2.15	0.47
8:F:60:VAL:HG12	8:F:60:VAL:O	2.15	0.47
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.43	0.47
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.22	0.47
15:M:24:GLN:HE21	15:M:27:ARG:HH11	1.62	0.47
1:0:1205:U:H2'	1:0:1206:U:H5''	1.97	0.47
1:0:1250:C:O2'	1:0:1251:C:H5'	2.14	0.47
1:0:2768:A:H3'	37:0:3931:HOH:O	2.13	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.30	0.47
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.15	0.47
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.30	0.47
5:C:246:ARG:NH1	37:C:8369:HOH:O	2.47	0.47
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.30	0.47
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.44	0.47
16:N:163:PHE:O	16:N:164:ASP:CB	2.62	0.47
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1164:U:H3	1:0:1192:A:H2	1.63	0.47
1:0:1409:G:H5'	37:0:3232:HOH:O	2.14	0.47
1:0:2073:G:OP2	1:0:2490:A:H5'	2.15	0.47
1:0:2724:U:H2'	1:0:2725:G:O4'	2.14	0.47
1:0:2769:C:H2'	1:0:2770:G:C5'	2.44	0.47
30:2:18:ASN:ND2	30:2:40:ARG:H	2.08	0.47
3:A:128:LEU:HG	37:A:8576:HOH:O	2.13	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.15	0.47
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.96	0.47
37:0:8627:HOH:O	5:C:103:ASN:HB3	2.13	0.47
6:D:11:HIS:O	6:D:14:ARG:N	2.46	0.47
12:J:47:THR:HG22	12:J:48:GLY:N	2.30	0.47
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.80	0.47
28:Z:46:ARG:NH1	37:Z:8432:HOH:O	2.47	0.47
1:0:1119:G:C8	12:J:52:GLN:NE2	2.83	0.47
1:0:2670:G:O2'	1:0:2671:U:H5'	2.15	0.47
1:0:926:A:O2'	14:L:41:HIS:HD2	1.98	0.47
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.30	0.47
3:A:105:VAL:HG13	3:A:155:THR:O	2.15	0.47
4:B:320:GLN:HE21	4:B:321:PRO:CD	2.26	0.47
6:D:38:GLU:HB3	6:D:49:PRO:HG2	1.97	0.47
8:F:117:GLU:C	8:F:119:ARG:N	2.67	0.47
10:H:66:ARG:HD3	37:H:8382:HOH:O	2.14	0.47
15:M:164:THR:HG23	15:M:165:GLY:N	2.30	0.47
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.42	0.47
25:W:65:VAL:CA	25:W:68:THR:HG22	2.44	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.47
1:0:1477:C:H5'	1:0:1868:G:H5''	1.96	0.47
1:0:776:A:OP1	29:1:28:HIS:HE1	1.98	0.47
7:E:108:LEU:HB3	37:E:1306:HOH:O	2.15	0.47
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.96	0.47
14:L:53:ARG:HH22	14:L:57:VAL:HG12	1.80	0.47
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.80	0.47
22:T:74:VAL:HB	22:T:77:VAL:HG21	1.97	0.47
25:W:125:HIS:HD2	25:W:127:GLY:H	1.62	0.47
2:9:64:C:C2'	2:9:65:A:H5'	2.45	0.47
6:D:10:PHE:N	37:D:1492:HOH:O	2.48	0.47
6:D:11:HIS:CG	6:D:12:GLU:N	2.83	0.47
6:D:99:ASP:CB	6:D:103:ASN:HB2	2.45	0.47
11:I:130:GLY:C	37:I:5371:HOH:O	2.52	0.47
14:L:145:LEU:HD23	14:L:145:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:70:ASP:OD1	14:L:116:HIS:HD2	1.97	0.47
1:0:1666:C:C2'	1:0:1667:A:H5'	2.42	0.46
1:0:558:C:H2'	1:0:559:U:H5''	1.95	0.46
31:3:73:GLU:HB2	37:3:8526:HOH:O	2.15	0.46
7:E:92:PRO:HB2	37:E:4917:HOH:O	2.14	0.46
9:G:20:VAL:O	9:G:24:VAL:HG23	2.15	0.46
13:K:98:VAL:HG22	13:K:102:GLU:C	2.35	0.46
13:K:10:GLN:N	13:K:10:GLN:NE2	2.43	0.46
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.15	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.98	0.46
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.97	0.46
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.80	0.46
5:C:107:ARG:NH2	37:C:8457:HOH:O	2.40	0.46
5:C:65:ARG:HG3	5:C:67:GLN:HB2	1.97	0.46
37:0:5819:HOH:O	6:D:55:LYS:HB2	2.16	0.46
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.44	0.46
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.44	0.46
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.45	0.46
1:0:1086:A:N6	25:W:11:VAL:HG11	2.31	0.46
1:0:371:U:H2'	1:0:372:A:C8	2.49	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
13:K:45:PRO:HB2	37:K:7169:HOH:O	2.15	0.46
1:0:1189:A:H1'	1:0:1209:C:H1'	1.97	0.46
1:0:204:A:C2'	1:0:205:U:H5'	2.45	0.46
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.40	0.46
7:E:93:MET:HE1	7:E:165:GLY:N	2.31	0.46
8:F:39:SER:CB	8:F:45:ALA:HB2	2.41	0.46
6:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.62	0.46
17:O:25:VAL:HG23	17:O:26:TRP:H	1.81	0.46
22:T:41:ARG:O	22:T:43:ASN:ND2	2.48	0.46
1:0:1684:A:O2'	1:0:1685:A:H5''	2.15	0.46
29:1:28:HIS:HD2	29:1:30:LYS:H	1.62	0.46
3:A:179:MET:HA	3:A:179:MET:CE	2.46	0.46
3:A:223:ARG:NH1	37:A:8518:HOH:O	2.48	0.46
7:E:32:ARG:O	7:E:33:LEU:HD23	2.15	0.46
12:J:90:LYS:HB2	35:J:8502:CL:CL	2.52	0.46
1:0:2601:A:N1	13:K:38:SER:HB2	2.31	0.46
14:L:101:ASP:C	14:L:103:ALA:H	2.18	0.46
1:0:2642:G:H2'	1:0:2643:G:O4'	2.15	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.45	0.46
25:W:38:THR:O	25:W:42:ARG:HB2	2.15	0.46
1:0:1735:C:O2'	1:0:1736:A:H5'	2.15	0.46
1:0:2010:A:H2'	37:0:5460:HOH:O	2.16	0.46
1:0:2383:G:H1'	37:0:6198:HOH:O	2.15	0.46
1:0:2781:U:H2'	1:0:2782:G:H5'	1.98	0.46
5:C:33:LYS:HD2	37:C:8459:HOH:O	2.15	0.46
8:F:34:ASN:HA	15:M:4:ALA:HB2	1.98	0.46
8:F:58:GLU:HA	8:F:61:MET:HG3	1.98	0.46
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.96	0.46
20:R:25:PHE:CE2	20:R:29:LYS:CE	2.98	0.46
1:0:1218:U:H2'	1:0:1219:U:C6	2.50	0.46
1:0:1657:A:H2'	1:0:1658:A:C8	2.51	0.46
1:0:1878:G:O2'	1:0:1879:U:H6	1.99	0.46
1:0:656:G:H5'	17:O:3:THR:HG22	1.98	0.46
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.16	0.46
3:A:36:ASP:HB2	3:A:83:GLY:HA3	1.98	0.46
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.51	0.46
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.34	0.46
16:N:71:TRP:N	37:N:8537:HOH:O	2.48	0.46
18:P:16:VAL:CG1	18:P:17:GLY:N	2.79	0.46
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.51	0.46
1:0:1249:U:H2'	1:0:1250:C:C6	2.51	0.46
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.46
31:3:7:PHE:HE2	31:3:22:VAL:HG21	1.81	0.46
4:B:144:THR:HG22	4:B:145:HIS:N	2.30	0.46
6:D:173:GLU:HG3	6:D:174:VAL:N	2.31	0.46
11:I:102:VAL:HG23	11:I:140:GLU:O	2.16	0.46
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.46
1:0:185:G:H4'	1:0:186:A:H4'	1.98	0.46
1:0:2361:A:H5'	1:0:2361:A:H8	1.81	0.46
1:0:514:G:OP1	1:0:514:G:H2'	2.15	0.46
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.15	0.46
7:E:3:VAL:CG2	7:E:49:ILE:HB	2.46	0.46
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.16	0.46
25:W:26:ILE:O	25:W:26:ILE:HG13	2.15	0.46
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.98	0.46
1:0:1132:A:N6	1:0:1229:C:H2'	2.32	0.45
1:0:2467:A:O2'	1:0:2468:A:H2'	2.16	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.45
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.78	0.45
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.44	0.45
37:0:4472:HOH:O	10:H:58:ARG:HG3	2.16	0.45
11:I:82:GLU:CD	11:I:108:ILE:HG13	2.36	0.45
11:I:97:VAL:HG12	11:I:97:VAL:O	2.15	0.45
1:0:2453:G:H5''	37:L:8540:HOH:O	2.15	0.45
1:0:2456:A:H2'	1:0:2457:U:C6	2.51	0.45
1:0:2781:U:C2'	1:0:2782:G:H5'	2.46	0.45
1:0:2883:A:H2'	1:0:2884:G:O4'	2.17	0.45
1:0:2896:A:N3	1:0:2896:A:H2'	2.31	0.45
1:0:820:G:C6	3:A:171:LYS:HB2	2.51	0.45
3:A:223:ARG:NE	37:A:8575:HOH:O	2.50	0.45
4:B:7:ARG:HD2	4:B:9:GLY:O	2.16	0.45
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.46	0.45
17:O:21:SER:OG	17:O:106:PRO:HB2	2.17	0.45
1:0:2388:C:H5'	19:Q:83:THR:O	2.16	0.45
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.51	0.45
1:0:1333:U:H2'	1:0:1334:C:H6	1.81	0.45
1:0:2720:C:O2	13:K:87:ARG:NH2	2.50	0.45
1:0:671:A:O2'	1:0:672:G:H2'	2.16	0.45
6:D:103:ASN:ND2	6:D:134:LEU:H	2.14	0.45
7:E:102:VAL:HG11	7:E:148:ILE:HD11	1.97	0.45
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.45
15:M:114:VAL:O	15:M:158:ARG:HD3	2.15	0.45
15:M:94:ARG:NH2	37:M:8581:HOH:O	2.35	0.45
16:N:159:TYR:CD2	16:N:163:PHE:HD2	2.35	0.45
26:X:70:ILE:O	26:X:70:ILE:HG23	2.16	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.17	0.45
21:S:6:LYS:HB2	21:S:27:ALA:O	2.15	0.45
24:V:55:ARG:NH2	37:V:4428:HOH:O	2.42	0.45
3:A:165:THR:HG22	37:A:8621:HOH:O	2.15	0.45
1:0:475:G:C5'	5:C:73:LEU:HD23	2.46	0.45
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.99	0.45
11:I:75:THR:OG1	11:I:112:LYS:HE2	2.16	0.45
15:M:107:ARG:NH1	37:M:8576:HOH:O	2.47	0.45
1:0:314:G:N2	1:0:316:A:H3'	2.32	0.45
1:0:338:C:H4'	5:C:174:ILE:HD12	1.98	0.45
2:9:56:A:C3'	2:9:57:A:H5''	2.46	0.45
5:C:164:ALA:O	5:C:167:ASP:HB2	2.16	0.45
6:D:169:THR:O	6:D:170:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:49:PRO:HG3	37:D:5828:HOH:O	2.15	0.45
6:D:92:GLU:HB2	37:D:3862:HOH:O	2.16	0.45
13:K:75:ARG:HH21	13:K:94:ALA:CB	2.30	0.45
14:L:130:ARG:HA	37:L:8557:HOH:O	2.17	0.45
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.99	0.45
1:0:1314:U:H2'	37:0:5374:HOH:O	2.16	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.16	0.45
1:0:1613:C:H2'	1:0:1614:G:O4'	2.16	0.45
1:0:2488:A:H2	37:0:6767:HOH:O	1.99	0.45
29:1:25:LYS:HD2	30:2:49:GLU:H	1.82	0.45
4:B:146:THR:O	4:B:159:PRO:HB3	2.16	0.45
4:B:280:VAL:HG13	4:B:333:GLU:O	2.17	0.45
7:E:132:THR:O	7:E:132:THR:HG23	2.16	0.45
7:E:80:TRP:O	7:E:134:SER:HA	2.17	0.45
26:X:18:ARG:NH1	37:X:4132:HOH:O	2.46	0.45
1:0:1681:G:H5''	1:0:1682:A:H5'	1.98	0.45
1:0:2515:C:H2'	1:0:2516:G:O4'	2.17	0.45
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.45
2:9:88:G:OP1	25:W:130:HIS:NE2	2.47	0.45
10:H:1:LYS:HA	10:H:2:PRO:HD3	1.84	0.45
10:H:38:LYS:HE2	10:H:42:ASP:HB3	1.98	0.45
11:I:112:LYS:C	11:I:114:PRO:HD2	2.36	0.45
12:J:6:PHE:O	12:J:8:ALA:N	2.50	0.45
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.81	0.45
16:N:5:ARG:HG3	19:Q:18:PRO:CB	2.47	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.32	0.45
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.32	0.45
1:0:1028:U:H1'	37:0:3152:HOH:O	2.17	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:585:C:H6	37:0:5595:HOH:O	1.99	0.45
6:D:55:LYS:HA	37:D:6752:HOH:O	2.16	0.45
11:I:103:ASP:HA	11:I:106:LYS:HD2	1.98	0.45
15:M:182:LYS:HD2	15:M:193:LYS:HB2	1.98	0.45
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.15	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.17	0.45
1:0:1006:A:N1	1:0:2311:A:H1'	2.32	0.45
1:0:283:U:H5''	1:0:284:C:P	2.57	0.45
1:0:2890:A:H1'	23:U:56:ARG:HH21	1.79	0.45
4:B:72:THR:HB	37:B:8610:HOH:O	2.16	0.45
5:C:236:THR:O	5:C:237:GLU:C	2.55	0.45
10:H:58:ARG:HG3	10:H:58:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.99	0.45
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.52	0.44
1:O:1342:C:O2'	1:O:1343:C:H5'	2.16	0.44
30:2:18:ASN:HA	30:2:18:ASN:HD22	1.59	0.44
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.82	0.44
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.32	0.44
4:B:74:ILE:HG13	37:B:8610:HOH:O	2.16	0.44
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.47	0.44
6:D:167:GLU:OE2	6:D:173:GLU:HG2	2.16	0.44
7:E:101:GLU:OE2	7:E:115:ARG:HD3	2.18	0.44
7:E:34:TRP:O	12:J:127:ILE:HD11	2.17	0.44
11:I:131:THR:HG23	37:I:7439:HOH:O	2.18	0.44
37:9:8464:HOH:O	16:N:147:ILE:HD12	2.17	0.44
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.52	0.44
1:O:141:C:P	37:O:3368:HOH:O	2.76	0.44
1:O:581:G:H5'	37:O:7175:HOH:O	2.16	0.44
4:B:279:THR:OG1	4:B:290:VAL:HB	2.17	0.44
4:B:41:PHE:CE1	4:B:79:MET:HG3	2.51	0.44
5:C:196:THR:HG23	37:C:8399:HOH:O	2.18	0.44
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.18	0.44
8:F:28:ALA:HB3	8:F:99:THR:O	2.16	0.44
9:G:64:ASN:N	9:G:64:ASN:ND2	2.64	0.44
10:H:36:LYS:HD3	37:H:8380:HOH:O	2.18	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.79	0.44
16:N:143:ARG:HH12	16:N:173:ASP:CG	2.21	0.44
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.38	0.44
23:U:13:ILE:HG12	23:U:32:CYS:CB	2.47	0.44
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.87	0.44
28:Z:23:ARG:NH1	37:Z:8404:HOH:O	2.45	0.44
1:O:2769:C:H2'	1:O:2770:G:H5'	2.00	0.44
1:O:790:A:H2'	1:O:791:A:O4'	2.18	0.44
5:C:170:ASP:O	5:C:171:GLU:HG3	2.17	0.44
6:D:57:THR:HG23	6:D:63:ILE:CB	2.47	0.44
6:D:86:THR:C	6:D:89:PRO:HD2	2.37	0.44
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.47	0.44
18:P:59:ARG:HD3	37:P:192:HOH:O	2.16	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.44
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.52	0.44
28:Z:13:ARG:NH1	28:Z:14:PHE:CE2	2.86	0.44
1:O:2001:G:O2'	1:O:2002:C:H5'	2.17	0.44
1:O:2005:G:OP2	1:O:2005:G:H3'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2326:U:H4'	1:0:2412:G:C4'	2.48	0.44
1:0:2667:G:H1'	1:0:2914:A:N3	2.32	0.44
1:0:2668:G:H2'	1:0:2669:U:C6	2.52	0.44
29:1:25:LYS:O	29:1:25:LYS:HG2	2.18	0.44
4:B:82:VAL:HG12	4:B:101:TRP:CE3	2.53	0.44
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.46	0.44
11:I:112:LYS:O	11:I:116:LEU:HG	2.18	0.44
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.47	0.44
25:W:139:GLY:O	25:W:141:HIS:CD2	2.69	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.53	0.44
1:0:2807:U:P	4:B:27:ASN:HD21	2.40	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.18	0.44
1:0:821:U:H5''	37:0:9556:HOH:O	2.15	0.44
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.33	0.44
2:9:39:U:H3'	2:9:40:C:H5''	1.99	0.44
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.47	0.44
5:C:39:GLN:O	5:C:43:LYS:HD3	2.17	0.44
11:I:87:THR:HG22	11:I:88:GLY:N	2.33	0.44
12:J:70:PHE:CD2	12:J:70:PHE:O	2.70	0.44
20:R:84:ALA:O	20:R:88:PHE:HD1	2.00	0.44
25:W:48:VAL:CG1	25:W:48:VAL:O	2.64	0.44
1:0:566:A:H2'	1:0:567:U:O4'	2.18	0.44
2:9:31:C:H1'	37:9:8392:HOH:O	2.17	0.44
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.18	0.44
4:B:315:VAL:HG23	4:B:316:ARG:HG2	1.99	0.44
4:B:7:ARG:NH1	4:B:11:LEU:CD2	2.81	0.44
10:H:26:SER:HA	10:H:59:HIS:CD2	2.53	0.44
11:I:75:THR:HG22	11:I:79:ILE:CD1	2.48	0.44
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.44
16:N:89:GLY:O	16:N:92:ALA:HB3	2.17	0.44
18:P:10:ALA:CA	18:P:13:VAL:HG12	2.45	0.44
1:0:1120:U:H5'	1:0:1121:G:OP2	2.17	0.44
1:0:1592:G:HO2'	1:0:1593:C:C4'	2.31	0.44
1:0:1634:G:H2'	1:0:1635:U:C6	2.53	0.44
1:0:1730:G:C5'	1:0:1731:C:H6	2.30	0.44
1:0:2401:A:H5'	37:0:9000:HOH:O	2.16	0.44
1:0:407:A:O5'	37:0:3965:HOH:O	2.21	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.16	0.44
7:E:84:MET:HE1	7:E:148:ILE:HD12	2.00	0.44
14:L:6:ARG:NH2	37:L:8548:HOH:O	2.46	0.44
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2559:C:H4'	37:0:6747:HOH:O	2.17	0.44
1:0:2730:G:O2'	1:0:2731:G:H5'	2.17	0.44
1:0:545:G:H2'	1:0:546:C:O4'	2.18	0.44
1:0:834:G:H4'	1:0:835:U:OP2	2.18	0.44
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.99	0.44
4:B:27:ASN:HB3	37:B:8633:HOH:O	2.17	0.44
13:K:101:ASN:O	13:K:102:GLU:HB2	2.17	0.44
16:N:37:ARG:HD3	16:N:37:ARG:HA	1.72	0.44
16:N:32:PRO:HD2	16:N:99:GLU:O	2.18	0.44
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.74	0.44
25:W:5:VAL:HG22	25:W:32:CYS:HB2	2.00	0.44
1:0:1615:A:H4'	37:0:5386:HOH:O	2.17	0.44
1:0:2251:G:H4'	37:0:6900:HOH:O	2.16	0.44
2:9:28:U:H2'	2:9:29:C:C6	2.53	0.44
4:B:248:ARG:O	4:B:251:VAL:CG1	2.66	0.44
5:C:162:VAL:HG12	5:C:162:VAL:O	2.18	0.44
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.99	0.44
6:D:23:VAL:CG2	6:D:23:VAL:O	2.65	0.44
37:0:9133:HOH:O	8:F:38:LYS:HE2	2.18	0.44
9:G:64:ASN:O	9:G:68:GLU:HG3	2.17	0.44
16:N:154:LEU:O	16:N:155:GLU:CB	2.66	0.44
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.80	0.44
1:0:1211:G:O2'	1:0:1212:C:H5'	2.17	0.43
1:0:1406:A:H4'	1:0:1407:A:H5''	1.99	0.43
29:1:17:THR:HA	30:2:49:GLU:HA	1.99	0.43
6:D:10:PHE:N	37:D:7345:HOH:O	2.51	0.43
7:E:20:ILE:HD12	7:E:33:LEU:HD12	2.00	0.43
11:I:122:THR:O	11:I:125:ALA:HB3	2.18	0.43
13:K:49:LEU:HD21	13:K:74:VAL:O	2.18	0.43
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.21	0.43
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.99	0.43
1:0:1730:G:H5'	1:0:1731:C:H5	1.82	0.43
1:0:1787:C:H4'	1:0:2883:A:O4'	2.18	0.43
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.32	0.43
1:0:894:A:C2	5:C:87:ARG:NH2	2.86	0.43
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.47	0.43
8:F:113:ASP:O	8:F:117:GLU:HG3	2.18	0.43
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.00	0.43
16:N:154:LEU:CG	16:N:155:GLU:H	2.28	0.43
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.83	0.43
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5'	1.99	0.43
1:0:1329:A:C2	37:0:4183:HOH:O	2.56	0.43
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.43
1:0:2314:G:C2'	1:0:2315:C:H5'	2.48	0.43
29:1:2:GLY:O	29:1:6:PRO:HG2	2.18	0.43
3:A:100:PRO:O	3:A:103:VAL:HG23	2.17	0.43
4:B:254:GLN:HG2	4:B:255:GLY:N	2.32	0.43
4:B:60:SER:C	4:B:62:ARG:H	2.20	0.43
9:G:12:ILE:HG13	37:G:6833:HOH:O	2.16	0.43
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.38	0.43
16:N:67:ALA:C	16:N:69:TYR:H	2.21	0.43
22:T:37:GLN:OE1	22:T:118:SER:HA	2.17	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43
1:0:1171:A:H2'	1:0:1172:G:H5'	2.01	0.43
1:0:2443:C:H3'	37:0:9982:HOH:O	2.18	0.43
1:0:2672:C:H1'	37:B:8640:HOH:O	2.18	0.43
31:3:65:THR:HB	31:3:83:TRP:H	1.83	0.43
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.88	0.43
4:B:205:VAL:HA	4:B:260:HIS:O	2.18	0.43
6:D:84:LEU:C	6:D:86:THR:H	2.21	0.43
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.53	0.43
17:O:43:VAL:HG12	17:O:44:ASN:O	2.18	0.43
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.52	0.43
1:0:1172:G:H5''	37:0:6751:HOH:O	2.18	0.43
1:0:1656:A:H2'	1:0:1657:A:O4'	2.19	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.52	0.43
4:B:41:PHE:HB3	4:B:190:MET:CE	2.48	0.43
5:C:107:ARG:CZ	37:C:8457:HOH:O	2.64	0.43
6:D:18:ILE:HD13	6:D:84:LEU:HD12	2.00	0.43
8:F:21:GLU:O	8:F:24:ARG:HG3	2.17	0.43
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.48	0.43
16:N:149:GLU:O	16:N:152:GLU:HB2	2.19	0.43
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.43
17:O:54:GLU:O	17:O:55:ASP:HB2	2.19	0.43
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.86	0.43
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.19	0.43
1:0:1523:G:H2'	1:0:1524:U:C6	2.53	0.43
1:0:1857:A:N6	1:0:2247:C:H1'	2.34	0.43
1:0:2004:U:H1'	37:0:9700:HOH:O	2.19	0.43
1:0:1980:U:O2	1:0:2008:U:H4'	2.19	0.43
1:0:2825:C:H4'	1:0:2826:G:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
3:A:26:ASP:OD1	3:A:28:GLU:HG3	2.18	0.43
6:D:67:ASP:O	6:D:69:ILE:HG13	2.19	0.43
14:L:121:ILE:HG12	14:L:141:GLU:HB2	2.00	0.43
1:0:962:C:C1'	16:N:5:ARG:NH1	2.75	0.43
17:O:25:VAL:HG23	17:O:26:TRP:N	2.34	0.43
23:U:6:CYS:HA	23:U:13:ILE:HD11	2.00	0.43
25:W:88:THR:HG23	25:W:110:GLN:HB3	2.01	0.43
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.34	0.43
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.48	0.43
1:0:1163:G:N2	37:O:5548:HOH:O	2.52	0.43
1:0:1669:A:H2'	1:0:1670:G:H8	1.82	0.43
1:0:2653:A:H2'	1:0:2654:C:C6	2.54	0.43
4:B:243:ASN:HA	4:B:244:PRO:C	2.38	0.43
7:E:133:VAL:HG12	7:E:141:VAL:HG13	2.00	0.43
10:H:9:ILE:HG12	10:H:56:GLN:CG	2.49	0.43
10:H:66:ARG:HB3	37:H:8382:HOH:O	2.18	0.43
11:I:75:THR:CA	11:I:112:LYS:HE2	2.49	0.43
11:I:131:THR:HG22	11:I:131:THR:O	2.17	0.43
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.52	0.43
19:Q:11:ARG:NH1	37:Q:5620:HOH:O	2.51	0.43
1:0:1180:U:H2'	1:0:1181:A:O4'	2.19	0.43
1:0:2256:G:C2'	1:0:2257:G:H5'	2.48	0.43
1:0:284:C:C4'	1:0:285:A:O5'	2.64	0.43
1:0:590:A:H2'	1:0:591:A:H5'	2.01	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
4:B:125:GLU:OE2	4:B:129:ARG:NH1	2.51	0.43
4:B:62:ARG:CB	4:B:65:MET:HE3	2.49	0.43
37:O:9183:HOH:O	5:C:214:THR:HB	2.18	0.43
5:C:7:ASP:OD1	5:C:11:ASN:O	2.37	0.43
11:I:123:ASN:O	11:I:127:GLU:HG3	2.18	0.43
1:0:1242:A:C5'	12:J:82:THR:HG23	2.28	0.43
13:K:75:ARG:HG2	13:K:90:PHE:CD2	2.54	0.43
15:M:47:ASP:CG	15:M:48:LYS:N	2.72	0.43
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.83	0.43
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.43
1:0:151:A:H2'	1:0:152:A:O4'	2.19	0.43
1:0:1545:C:H2'	1:0:1546:G:O4'	2.19	0.43
1:0:1625:U:H5''	37:O:5522:HOH:O	2.19	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.43
1:0:377:C:H5	37:O:9815:HOH:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:834:G:H3'	1:0:835:U:H4'	2.00	0.43
31:3:15:ASN:ND2	37:3:8546:HOH:O	2.52	0.43
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.43
7:E:31:ARG:NH1	7:E:68:HIS:CD2	2.86	0.43
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.49	0.43
11:I:99:ASP:OD1	11:I:138:THR:HB	2.19	0.43
11:I:75:THR:HA	11:I:112:LYS:CE	2.49	0.43
12:J:103:VAL:CG1	37:J:5907:HOH:O	2.65	0.43
20:R:39:THR:CB	20:R:42:GLU:HG3	2.43	0.43
22:T:1:SER:N	37:T:5837:HOH:O	2.52	0.43
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.19	0.43
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.34	0.43
1:0:1058:A:H2'	1:0:1060:C:C5'	2.46	0.43
1:0:1636:G:O2'	1:0:1637:A:H5'	2.18	0.43
1:0:1878:G:H5''	37:0:9304:HOH:O	2.18	0.43
1:0:1947:G:H2'	1:0:1948:G:C8	2.54	0.43
1:0:2289:G:N2	1:0:2291:A:C2	2.78	0.43
1:0:2420:G:H4'	37:0:3598:HOH:O	2.19	0.43
1:0:588:G:O6	25:W:154:ARG:NH1	2.52	0.43
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.43
2:9:107:C:H2'	2:9:108:C:C6	2.53	0.43
5:C:133:ARG:HD2	37:C:8410:HOH:O	2.19	0.43
10:H:46:GLN:CB	10:H:167:PRO:HD2	2.25	0.43
15:M:125:ARG:NH1	37:M:8596:HOH:O	2.52	0.43
16:N:63:SER:O	16:N:66:LEU:HB2	2.18	0.43
24:V:60:GLN:O	24:V:65:ASP:N	2.51	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.18	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.42
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.42
1:0:559:U:H2'	1:0:560:C:O4'	2.19	0.42
3:A:35:GLY:O	3:A:36:ASP:CB	2.61	0.42
4:B:88:GLU:O	4:B:88:GLU:HG3	2.17	0.42
7:E:84:MET:HE1	7:E:133:VAL:HG21	2.00	0.42
10:H:151:ARG:HA	10:H:154:TYR:CE2	2.54	0.42
10:H:46:GLN:HB3	10:H:167:PRO:CD	2.27	0.42
13:K:27:ARG:HD2	37:K:4747:HOH:O	2.19	0.42
14:L:73:VAL:HG11	14:L:118:LEU:HD21	2.00	0.42
1:0:2365:G:H4'	19:Q:45:PRO:O	2.18	0.42
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.19	0.42
1:0:653:C:H2'	1:0:654:A:C8	2.53	0.42
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.42
4:B:71:VAL:CG1	4:B:296:LEU:HB3	2.46	0.42
6:D:76:ARG:O	6:D:77:ASP:HB2	2.19	0.42
11:I:78:LEU:HD12	11:I:112:LYS:NZ	2.34	0.42
12:J:121:LEU:HD11	12:J:126:ASN:ND2	2.34	0.42
1:0:1109:U:O4	12:J:21:ARG:HA	2.19	0.42
14:L:128:GLY:O	14:L:132:LYS:HG3	2.19	0.42
25:W:38:THR:HB	37:W:5390:HOH:O	2.18	0.42
25:W:90:TYR:N	25:W:90:TYR:CD1	2.86	0.42
1:0:1123:A:C2	1:0:1129:C:H4'	2.54	0.42
1:0:1641:A:C2'	1:0:1642:A:H5'	2.49	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.83	0.42
1:0:2266:A:H2'	1:0:2267:G:C8	2.55	0.42
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.42
3:A:17:ARG:HD2	37:A:8542:HOH:O	2.20	0.42
3:A:33:GLU:CD	3:A:33:GLU:H	2.22	0.42
13:K:99:ASP:OD1	13:K:101:ASN:N	2.51	0.42
15:M:78:LYS:HD3	37:M:8637:HOH:O	2.19	0.42
15:M:95:LYS:HG2	15:M:99:ARG:HB3	2.01	0.42
16:N:67:ALA:C	16:N:69:TYR:N	2.73	0.42
17:O:77:ALA:HA	17:O:96:VAL:O	2.19	0.42
1:0:1423:C:O2'	1:0:1424:A:H5'	2.20	0.42
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.42
1:0:306:A:P	22:T:38:ARG:HH21	2.42	0.42
1:0:513:A:H3'	37:0:3359:HOH:O	2.19	0.42
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.42
1:0:870:G:C3'	1:0:871:G:H5''	2.49	0.42
3:A:51:ARG:NH2	3:A:69:LEU:HD13	2.34	0.42
5:C:33:LYS:HE2	37:C:8359:HOH:O	2.19	0.42
6:D:77:ASP:HB3	6:D:78:GLU:H	1.57	0.42
9:G:27:ILE:HD12	9:G:70:ALA:HB1	2.02	0.42
11:I:102:VAL:HG12	11:I:106:LYS:HE3	2.02	0.42
15:M:167:GLY:O	15:M:171:ARG:HG3	2.19	0.42
1:0:793:A:H5''	18:P:83:LYS:HG2	2.02	0.42
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.52	0.42
1:0:1168:C:H5'	37:I:5128:HOH:O	2.20	0.42
1:0:1555:G:H4'	1:0:1630:A:H2	1.85	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42
1:0:2649:A:H5'	1:0:2649:A:H8	1.84	0.42
1:0:2691:A:OP1	1:0:2691:A:H8	2.01	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:C:H1'	37:0:4176:HOH:O	2.19	0.42
1:0:736:A:H2'	1:0:737:A:O4'	2.19	0.42
1:0:814:G:H4'	37:0:9639:HOH:O	2.19	0.42
1:0:90:A:H2'	1:0:91:G:O4'	2.19	0.42
4:B:268:ARG:NE	37:B:8612:HOH:O	2.51	0.42
4:B:279:THR:CG2	4:B:280:VAL:N	2.82	0.42
1:0:2561:C:OP1	7:E:153:ARG:NH2	2.53	0.42
7:E:84:MET:HB2	7:E:131:LEU:HB2	2.01	0.42
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.75	0.42
12:J:130:VAL:CG1	12:J:131:THR:N	2.81	0.42
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.43	0.42
24:V:39:ALA:C	24:V:41:GLU:N	2.73	0.42
25:W:76:ASP:O	25:W:77:ALA:C	2.57	0.42
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.42
1:0:2356:A:H2'	1:0:2357:G:O4'	2.19	0.42
1:0:2359:G:H3'	37:0:5190:HOH:O	2.19	0.42
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.42
1:0:289:G:O2'	1:0:290:C:H5'	2.20	0.42
1:0:40:C:H4'	37:0:6492:HOH:O	2.20	0.42
6:D:64:ARG:NE	6:D:67:ASP:HB3	2.34	0.42
1:0:262:A:OP2	8:F:91:VAL:HG11	2.19	0.42
1:0:1162:G:O2'	11:I:117:LEU:HG	2.19	0.42
12:J:22:VAL:O	12:J:26:VAL:HG23	2.18	0.42
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.83	0.42
16:N:47:LEU:HD12	16:N:92:ALA:CB	2.49	0.42
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.83	0.42
25:W:14:HIS:HB2	25:W:17:ILE:HD12	2.02	0.42
1:0:249:G:O2'	1:0:250:C:H5'	2.20	0.42
1:0:2777:G:O2'	1:0:2778:A:H5'	2.20	0.42
3:A:169:PHE:O	3:A:171:LYS:N	2.48	0.42
4:B:254:GLN:NE2	37:B:8594:HOH:O	2.49	0.42
11:I:113:HIS:NE2	11:I:121:LEU:HD22	2.35	0.42
11:I:81:ASP:O	11:I:84:GLY:N	2.53	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.19	0.42
25:W:146:ILE:HG22	25:W:147:ASP:N	2.34	0.42
25:W:64:THR:O	25:W:68:THR:HG22	2.19	0.42
1:0:1609:C:H2'	1:0:1610:G:C8	2.55	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.42
31:3:91:GLN:O	31:3:92:GLU:HB2	2.19	0.42
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.42
4:B:168:GLY:N	4:B:174:ARG:HD3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:305:ASP:O	4:B:306:LYS:CB	2.66	0.42
5:C:139:VAL:CG1	37:C:8447:HOH:O	2.61	0.42
5:C:165:ASP:O	5:C:168:ARG:HB3	2.20	0.42
1:O:968:G:C1'	10:H:32:LYS:HZ1	2.25	0.42
10:H:96:ARG:NH2	37:H:8336:HOH:O	2.51	0.42
11:I:102:VAL:O	11:I:106:LYS:HG3	2.20	0.42
12:J:63:ILE:HG22	12:J:64:GLY:N	2.33	0.42
14:L:104:ASP:O	14:L:105:TYR:HB3	2.20	0.42
16:N:73:ALA:N	37:N:8565:HOH:O	2.52	0.42
22:T:40:VAL:HG22	22:T:41:ARG:N	2.35	0.42
22:T:48:VAL:HG22	22:T:97:ARG:O	2.20	0.42
1:O:1159:G:H1	1:O:1208:C:H42	1.67	0.42
1:O:1268:C:O2'	1:O:1269:G:H5'	2.19	0.42
1:O:1883:U:O2'	1:O:1884:G:H5'	2.19	0.42
1:O:92:G:H4'	24:V:44:GLY:HA3	2.02	0.42
3:A:105:VAL:CG1	3:A:106:CYS:N	2.82	0.42
4:B:55:ASN:HB3	4:B:64:GLY:H	1.85	0.42
6:D:166:ILE:O	6:D:169:THR:N	2.53	0.42
8:F:58:GLU:HA	8:F:61:MET:HE2	2.02	0.42
16:N:100:ALA:O	16:N:129:ILE:HG23	2.20	0.42
16:N:159:TYR:HD2	16:N:163:PHE:HD2	1.67	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.82	0.42
1:O:1139:U:H2'	1:O:1140:C:C6	2.55	0.42
1:O:2361:A:H2'	1:O:2362:A:C8	2.55	0.42
1:O:2741:A:H2'	1:O:2742:G:O4'	2.20	0.42
1:O:827:A:H2'	1:O:828:G:O4'	2.20	0.42
1:O:88:G:N7	30:2:28:LYS:HD2	2.34	0.42
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.91	0.42
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.55	0.42
20:R:132:ARG:NH2	37:R:8582:HOH:O	2.52	0.42
26:X:51:ASP:O	26:X:53:SER:N	2.53	0.42
1:O:1943:C:O4'	3:A:212:PRO:HA	2.20	0.41
1:O:2115:U:H2'	1:O:2116:U:C6	2.55	0.41
1:O:2237:G:H1'	37:O:4354:HOH:O	2.19	0.41
1:O:2842:G:C2'	1:O:2843:A:H5'	2.49	0.41
4:B:221:GLN:HE22	13:K:42:ASN:ND2	2.11	0.41
5:C:153:VAL:O	5:C:157:LEU:HG	2.20	0.41
7:E:156:ASP:OD2	7:E:157:LYS:HG3	2.18	0.41
7:E:47:VAL:HG11	7:E:69:ILE:HD13	2.01	0.41
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.35	0.41
11:I:85:PHE:N	11:I:85:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:19:MET:HE2	12:J:79:PHE:HA	2.02	0.41
14:L:148:GLU:HB2	37:L:8592:HOH:O	2.19	0.41
17:O:41:ALA:HA	37:O:5104:HOH:O	2.18	0.41
1:O:1014:A:H5''	2:9:101:G:O2'	2.20	0.41
1:O:777:U:O2'	29:1:11:LYS:HG2	2.20	0.41
3:A:48:ASP:HB3	37:A:8609:HOH:O	2.21	0.41
3:A:97:ALA:HB2	3:A:150:PRO:HB2	2.01	0.41
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.86	0.41
5:C:234:VAL:HG22	5:C:234:VAL:O	2.20	0.41
12:J:131:THR:HB	12:J:134:GLU:HG3	2.01	0.41
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.41
15:M:164:THR:CG2	15:M:165:GLY:N	2.84	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.85	0.41
1:O:1098:A:H2'	1:O:1099:G:O4'	2.20	0.41
1:O:1235:G:C1'	12:J:63:ILE:HG23	2.50	0.41
1:O:1973:A:H5'	1:O:1973:A:C8	2.46	0.41
1:O:321:A:H1'	37:O:6525:HOH:O	2.21	0.41
31:3:74:CYS:N	37:3:8559:HOH:O	2.52	0.41
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.36	0.41
6:D:59:GLY:O	6:D:61:PHE:N	2.46	0.41
10:H:162:ARG:NH1	37:H:8383:HOH:O	2.52	0.41
13:K:55:VAL:HG12	13:K:56:SER:H	1.83	0.41
23:U:9:CYS:O	23:U:52:THR:HG23	2.21	0.41
1:O:1477:C:C5'	1:O:1868:G:H5''	2.51	0.41
1:O:245:C:H2'	1:O:246:G:H5'	2.01	0.41
31:3:84:ARG:HD3	37:3:8549:HOH:O	2.21	0.41
3:A:36:ASP:CB	3:A:83:GLY:HA3	2.51	0.41
7:E:152:THR:HG21	7:E:165:GLY:HA2	2.01	0.41
14:L:144:ASP:HA	14:L:147:GLU:HG3	2.02	0.41
15:M:133:LEU:O	15:M:134:ILE:HD13	2.20	0.41
16:N:175:LEU:HD12	16:N:175:LEU:HA	1.87	0.41
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.56	0.41
22:T:78:THR:HB	22:T:87:VAL:O	2.21	0.41
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.32	0.41
1:O:130:C:H5'	37:O:4710:HOH:O	2.20	0.41
1:O:157:G:H4'	15:M:95:LYS:HE3	2.02	0.41
1:O:1966:U:H2'	1:O:1967:U:C6	2.54	0.41
1:O:2019:A:H5'	37:O:4042:HOH:O	2.20	0.41
37:O:3915:HOH:O	3:A:11:ARG:CZ	2.69	0.41
4:B:277:GLU:N	4:B:278:PRO:HD2	2.35	0.41
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:20:ILE:O	7:E:30:THR:HA	2.20	0.41
8:F:119:ARG:OXT	8:F:119:ARG:HD3	2.21	0.41
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.02	0.41
25:W:129:LYS:HG2	37:W:1990:HOH:O	2.21	0.41
27:Y:174:VAL:HG12	27:Y:174:VAL:O	2.20	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.68	0.41
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.55	0.41
1:O:1878:G:H5''	37:O:4663:HOH:O	2.19	0.41
1:O:1923:G:H4'	31:3:31:THR:O	2.20	0.41
1:O:2415:A:N3	16:N:26:LEU:HD13	2.36	0.41
1:O:2909:G:H2'	1:O:2910:A:H8	1.86	0.41
6:D:20:LYS:HD3	6:D:76:ARG:NH2	2.35	0.41
6:D:53:LYS:HA	6:D:67:ASP:O	2.20	0.41
8:F:1:PRO:HB2	37:F:5897:HOH:O	2.21	0.41
10:H:20:ILE:CG2	10:H:120:ILE:CD1	2.99	0.41
1:O:2413:A:N7	16:N:109:PRO:HB3	2.35	0.41
16:N:43:VAL:HG13	16:N:118:ILE:HD11	2.03	0.41
20:R:125:ARG:HG2	37:R:8542:HOH:O	2.21	0.41
23:U:52:THR:HG21	23:U:54:THR:HB	2.02	0.41
24:V:55:ARG:NE	37:V:4428:HOH:O	2.38	0.41
26:X:12:ILE:HG23	26:X:36:HIS:CG	2.55	0.41
28:Z:60:CYS:O	28:Z:61:ASP:CB	2.69	0.41
1:O:2011:A:H4'	1:O:2012:U:O5'	2.20	0.41
1:O:396:U:H5'	31:3:42:ARG:NH1	2.35	0.41
1:O:613:C:H2'	1:O:614:U:H6	1.85	0.41
1:O:934:C:H2'	1:O:935:G:C8	2.56	0.41
12:J:39:VAL:HG13	12:J:106:GLY:O	2.20	0.41
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.20	0.41
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.84	0.41
24:V:1:THR:HG23	24:V:2:VAL:N	2.25	0.41
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.47	0.41
1:O:1385:G:O3'	26:X:49:ARG:NH1	2.53	0.41
37:O:3694:HOH:O	27:Y:186:ARG:HD2	2.21	0.41
28:Z:27:ALA:O	28:Z:31:SER:HB2	2.21	0.41
1:O:1116:U:H3	1:O:1246:A:N6	2.01	0.41
1:O:2251:G:H2'	1:O:2252:A:H8	1.86	0.41
1:O:2255:A:H2'	1:O:2256:G:O4'	2.21	0.41
1:O:2712:G:H5'	37:K:4183:HOH:O	2.19	0.41
1:O:370:G:O2'	1:O:371:U:H5'	2.21	0.41
1:O:412:C:H2'	1:O:413:G:O4'	2.21	0.41
1:O:820:G:O2'	1:O:856:G:H4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:949:U:H4'	19:Q:95:GLU:HA	2.02	0.41
4:B:41:PHE:CG	4:B:190:MET:HE3	2.56	0.41
4:B:82:VAL:CG1	4:B:82:VAL:O	2.67	0.41
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.56	0.41
10:H:83:TYR:CD1	10:H:83:TYR:C	2.94	0.41
11:I:128:VAL:C	11:I:130:GLY:N	2.74	0.41
22:T:45:GLY:C	37:T:3851:HOH:O	2.59	0.41
25:W:29:VAL:O	25:W:30:ASN:HB2	2.20	0.41
1:0:625:U:H5''	1:0:1044:C:N4	2.35	0.41
1:0:1515:A:H2'	1:0:1516:C:C6	2.55	0.41
1:0:2421:G:H3'	1:0:2422:U:C5'	2.51	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.56	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.21	0.41
2:9:14:G:O2'	16:N:1:ALA:HB2	2.21	0.41
3:A:88:ILE:CD1	3:A:100:PRO:HD3	2.43	0.41
4:B:127:GLN:HG3	37:B:8648:HOH:O	2.20	0.41
10:H:88:ARG:NH1	10:H:135:THR:OG1	2.54	0.41
11:I:87:THR:HG22	11:I:88:GLY:H	1.85	0.41
14:L:10:SER:O	14:L:11:ARG:HB3	2.21	0.41
14:L:143:THR:HG21	37:L:8537:HOH:O	2.20	0.41
14:L:72:ASN:O	14:L:76:LEU:HG	2.21	0.41
18:P:13:VAL:HG13	18:P:14:LEU:N	2.36	0.41
1:0:56:G:H5''	24:V:50:ARG:NH1	2.36	0.41
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.56	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.21	0.41
1:0:2782:G:O6	1:0:2790:C:H5''	2.21	0.41
1:0:2858:U:H2'	1:0:2859:C:C6	2.55	0.41
1:0:324:G:O2'	1:0:325:U:H5'	2.21	0.41
1:0:40:C:H6	1:0:40:C:O5'	2.04	0.41
1:0:611:U:H2'	1:0:612:U:C6	2.56	0.41
29:1:25:LYS:HD2	30:2:49:GLU:N	2.35	0.41
2:9:8:G:O6	16:N:11:ARG:NH1	2.53	0.41
3:A:103:VAL:HA	3:A:104:PRO:HD3	1.89	0.41
4:B:129:ARG:NH2	4:B:176:ASP:OD1	2.51	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.21	0.41
8:F:32:GLY:N	37:F:3111:HOH:O	2.52	0.41
12:J:75:PRO:HD3	12:J:136:SER:OG	2.20	0.41
14:L:146:GLY:C	14:L:148:GLU:H	2.25	0.41
21:S:32:ALA:HA	21:S:36:GLU:OE1	2.20	0.41
22:T:48:VAL:HG13	22:T:49:GLU:N	2.35	0.41
37:K:7438:HOH:O	23:U:20:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.36	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.89	0.41
26:X:15:ARG:CB	26:X:15:ARG:HH11	2.32	0.41
26:X:78:GLU:CG	26:X:79:GLU:N	2.82	0.41
28:Z:30:GLU:HG2	28:Z:33:MET:HE3	2.03	0.41
1:0:1175:G:H1'	1:0:1193:A:H2'	2.02	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.21	0.41
1:0:2679:G:H2'	1:0:2681:A:OP2	2.21	0.41
1:0:794:U:H3	1:0:819:A:H61	1.68	0.41
2:9:1:U:H5''	2:9:3:A:OP1	2.21	0.41
2:9:2:U:OP2	2:9:3:A:H5'	2.20	0.41
4:B:53:LEU:HD12	4:B:327:VAL:HA	2.02	0.41
5:C:115:LEU:HA	5:C:115:LEU:HD12	1.89	0.41
7:E:35:TYR:HA	12:J:127:ILE:HD12	2.03	0.41
10:H:112:GLY:N	37:H:8390:HOH:O	2.54	0.41
10:H:9:ILE:HD12	10:H:54:THR:CG2	2.47	0.41
13:K:101:ASN:O	13:K:102:GLU:CB	2.69	0.41
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.93	0.41
1:0:1367:A:H2'	1:0:1368:U:O4'	2.21	0.40
1:0:1592:G:O2'	1:0:1593:C:O5'	2.38	0.40
1:0:2419:U:H5''	1:0:2420:G:C5'	2.50	0.40
1:0:2478:U:O2'	1:0:2479:A:H5'	2.21	0.40
1:0:2589:U:H2'	1:0:2590:U:C6	2.56	0.40
1:0:2820:A:H2'	1:0:2821:C:O4'	2.21	0.40
1:0:517:U:H1'	37:0:7067:HOH:O	2.21	0.40
3:A:36:ASP:HB2	3:A:84:VAL:N	2.36	0.40
1:0:2821:C:H4'	4:B:116:PRO:CB	2.51	0.40
4:B:81:ALA:O	4:B:186:GLY:HA3	2.21	0.40
4:B:275:GLY:C	37:B:8657:HOH:O	2.60	0.40
6:D:19:GLU:HG3	37:D:6165:HOH:O	2.20	0.40
6:D:20:LYS:HA	6:D:75:LEU:O	2.22	0.40
6:D:38:GLU:OE2	6:D:51:ARG:CZ	2.70	0.40
10:H:24:PRO:HD3	10:H:120:ILE:HG22	2.04	0.40
13:K:72:VAL:HG11	13:K:121:PHE:CD1	2.56	0.40
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.02	0.40
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.40
16:N:164:ASP:OD1	16:N:164:ASP:C	2.59	0.40
16:N:184:ILE:O	16:N:184:ILE:HG23	2.22	0.40
17:O:23:GLY:C	37:O:3062:HOH:O	2.59	0.40
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.35	0.40
23:U:17:THR:CG2	23:U:18:GLY:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.86	0.40
25:W:151:GLU:O	25:W:154:ARG:HB3	2.21	0.40
1:0:290:C:O2'	1:0:291:C:H5'	2.21	0.40
1:0:475:G:H5'	5:C:73:LEU:HD23	2.03	0.40
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.53	0.40
1:0:926:A:O2'	14:L:41:HIS:CD2	2.74	0.40
37:O:7200:HOH:O	5:C:94:THR:HG21	2.19	0.40
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.51	0.40
6:D:67:ASP:HA	6:D:68:PRO:HD3	1.94	0.40
7:E:79:GLY:HA3	37:E:7046:HOH:O	2.20	0.40
10:H:138:CYS:SG	10:H:146:VAL:HG11	2.61	0.40
15:M:59:GLY:HA3	15:M:141:ILE:HD12	2.03	0.40
16:N:66:LEU:HA	16:N:66:LEU:HD12	1.95	0.40
19:Q:16:ASN:HA	19:Q:16:ASN:HD22	1.76	0.40
21:S:76:GLU:HB3	37:S:8343:HOH:O	2.20	0.40
25:W:1:MET:HB2	25:W:103:GLU:HG2	2.02	0.40
1:0:1165:G:H1'	1:0:1174:A:H1'	2.03	0.40
1:0:1438:G:HO2'	1:0:1684:A:H2	1.69	0.40
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.35	0.40
2:9:24:U:H3'	2:9:25:G:C5'	2.52	0.40
5:C:16:VAL:CG1	5:C:17:ASP:N	2.83	0.40
6:D:23:VAL:HG23	6:D:41:LEU:HD22	2.03	0.40
6:D:18:ILE:HD13	6:D:84:LEU:CD1	2.52	0.40
12:J:39:VAL:HG11	12:J:107:ASN:HB2	2.04	0.40
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.36	0.40
14:L:1:THR:N	37:L:8539:HOH:O	2.55	0.40
20:R:7:GLU:HG3	37:R:8580:HOH:O	2.21	0.40
1:0:317:A:OP1	22:T:52:ARG:O	2.40	0.40
1:0:1413:A:H2'	1:0:1414:A:O4'	2.22	0.40
1:0:1753:C:O2	4:B:229:ARG:NH2	2.49	0.40
1:0:2050:G:H5''	20:R:80:TYR:O	2.21	0.40
1:0:2281:C:C2'	1:0:2282:U:H5'	2.51	0.40
1:0:2851:G:C2'	1:0:2852:A:H5'	2.52	0.40
29:1:28:HIS:HD2	29:1:31:LYS:H	1.69	0.40
5:C:91:PRO:O	5:C:93:LYS:HG3	2.21	0.40
10:H:40:ALA:HB1	10:H:137:TYR:CE2	2.57	0.40
11:I:134:SER:CB	37:I:7330:HOH:O	2.70	0.40
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.04	0.40
22:T:26:THR:HA	22:T:39:ASN:HB3	2.03	0.40
25:W:5:VAL:O	25:W:52:VAL:CG2	2.70	0.40
1:0:1298:U:H2'	1:0:1299:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.40
1:0:1972:U:C2'	1:0:1973:A:H5''	2.51	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.22	0.40
1:0:2462:G:N7	31:3:60:LYS:NZ	2.67	0.40
1:0:475:G:OP1	5:C:73:LEU:CD2	2.70	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.57	0.40
2:9:59:C:H6	2:9:59:C:O5'	2.05	0.40
3:A:72:GLU:HG3	28:Z:66:GLY:HA2	2.04	0.40
7:E:11:VAL:HG11	7:E:22:VAL:HG13	2.02	0.40
15:M:59:GLY:C	15:M:141:ILE:HD11	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	217 (92%)	15 (6%)	3 (1%)	12	17
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	7	8
5	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
6	D	134/177 (76%)	104 (78%)	23 (17%)	7 (5%)	2	1
7	E	170/178 (96%)	159 (94%)	10 (6%)	1 (1%)	25	36
8	F	117/120 (98%)	105 (90%)	10 (8%)	2 (2%)	9	11
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/171 (91%)	145 (93%)	9 (6%)	2 (1%)	12	17
11	I	68/162 (42%)	53 (78%)	12 (18%)	3 (4%)	2	2
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	7	8
13	K	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	10	14
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	22	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
16	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	5	5
17	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	32
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	3
25	W	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	22	32
26	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	5	6
27	Y	140/241 (58%)	140 (100%)	0	0	100	100
28	Z	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	15
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	42 (100%)	0	0	100	100
31	3	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	6	7
All	All	3705/4420 (84%)	3442 (93%)	218 (6%)	45 (1%)	13	19

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	137	PRO
6	D	173	GLU
10	H	166	SER
10	H	168	ALA
14	L	80	ASP
16	N	154	LEU
28	Z	81	ARG
3	A	34	ASP
3	A	37	VAL
3	A	132	ASP
4	B	34	GLY
4	B	169	GLY
4	B	184	ASP

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Mol	Chain	Res	Type
6	D	171	ASP
12	J	5	GLU
16	N	167	ASP
24	V	43	PRO
31	3	56	PRO
31	3	57	GLY
6	D	61	PHE
8	F	101	ALA
11	I	80	LYS
12	J	7	ASP
12	J	143	LYS
13	K	126	SER
16	N	139	TRP
16	N	164	ASP
25	W	77	ALA
26	X	77	PHE
4	B	107	SER
8	F	64	PRO
13	K	119	GLN
16	N	65	ASP
4	B	185	GLY
6	D	27	ILE
6	D	170	TYR
24	V	40	PRO
4	B	2	GLN
7	E	44	GLY
6	D	16	PRO
11	I	74	PRO
11	I	92	PRO
20	R	81	PRO
26	X	52	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	166 (93%)	13 (7%)	14	22
4	B	282/283 (100%)	263 (93%)	19 (7%)	16	26
5	C	193/193 (100%)	179 (93%)	14 (7%)	14	22
6	D	117/148 (79%)	108 (92%)	9 (8%)	13	20
7	E	152/156 (97%)	148 (97%)	4 (3%)	46	66
8	F	93/94 (99%)	93 (100%)	0	100	100
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	125 (95%)	7 (5%)	22	37
11	I	58/130 (45%)	54 (93%)	4 (7%)	15	25
12	J	118/121 (98%)	110 (93%)	8 (7%)	16	25
13	K	106/106 (100%)	103 (97%)	3 (3%)	43	63
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	55
15	M	158/158 (100%)	151 (96%)	7 (4%)	28	45
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	42
17	O	93/94 (99%)	88 (95%)	5 (5%)	22	36
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	65
19	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	66
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	100 (95%)	5 (5%)	25	41
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	74
25	W	130/130 (100%)	122 (94%)	8 (6%)	18	29
26	X	66/74 (89%)	63 (96%)	3 (4%)	27	44
27	Y	120/196 (61%)	110 (92%)	10 (8%)	11	17
28	Z	60/60 (100%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	51
All	All	3093/3603 (86%)	2948 (95%)	145 (5%)	26	42

All (145) 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	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	206	ARG
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	97	LEU
4	B	98	THR
4	B	103	ASP
4	B	162	MET
4	B	190	MET
4	B	234	ARG
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	264	GLU
4	B	277	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
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP

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Mol	Chain	Res	Type
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS
6	D	61	PHE
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	12	ASP
7	E	102	VAL
7	E	164	ASP
10	H	1	LYS
10	H	84	LYS
10	H	88	ARG
10	H	132	GLN
10	H	146	VAL
10	H	154	TYR
10	H	170	ASN
11	I	86	GLU
11	I	93	GLN
11	I	138	THR
11	I	140	GLU
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	120	SER
12	J	125	SER
12	J	127	ILE
13	K	7	ASP
13	K	10	GLN
13	K	98	VAL
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP

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Mol	Chain	Res	Type
14	L	117	GLU
15	M	46	LEU
15	M	68	ARG
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	158	ARG
15	M	164	THR
16	N	26	LEU
16	N	127	LEU
16	N	128	ASP
16	N	135	VAL
16	N	152	GLU
16	N	163	PHE
16	N	180	LEU
17	O	3	THR
17	O	25	VAL
17	O	28	ASP
17	O	98	LEU
17	O	111	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	73	HIS
22	T	96	VAL
24	V	43	PRO
25	W	4	LEU
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	142	ASP

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Mol	Chain	Res	Type
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	72	VAL
27	Y	141	THR
27	Y	154	ARG
27	Y	163	THR
27	Y	172	THR
27	Y	186	ARG
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	231	PRO
30	2	18	ASN
31	3	14	CYS
31	3	42	ARG
31	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) 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
4	B	256	GLN
4	B	260	HIS
4	B	318	ASN
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
5	C	163	HIS
6	D	103	ASN
6	D	133	ASN
7	E	15	GLN

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Mol	Chain	Res	Type
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	56	GLN
10	H	59	HIS
10	H	70	ASN
10	H	132	GLN
10	H	170	ASN
11	I	123	ASN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	21	HIS
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
21	S	53	ASN
22	T	39	ASN

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Mol	Chain	Res	Type
22	T	73	HIS
23	U	39	ASN
24	V	60	GLN
25	W	27	HIS
25	W	59	GLN
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	236 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	2 (1%)
All	All	2867/3044 (94%)	253 (8%)	36 (1%)

All (253) 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

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Mol	Chain	Res	Type
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	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
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
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
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	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

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Mol	Chain	Res	Type
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	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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	11	A
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
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	103	A
2	9	114	G
2	9	122	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U

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Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
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
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	65	A
2	9	103	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	0	2621	1	17,21,22	1.50	3 (17%)	20,30,33	5.44	4 (20%)
1	OMG	0	2588	1	18,26,27	1.12	2 (11%)	20,38,41	2.62	5 (25%)
1	UR3	0	2619	1	14,22,23	0.86	0	15,32,35	0.66	0
1	OMU	0	2587	1	14,22,23	1.03	1 (7%)	14,31,34	1.16	1 (7%)
1	1MA	0	628	1	15,25,26	0.71	0	15,37,40	1.38	1 (6%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.56	1.48	1.52
1	0	2588	OMG	C6-N1	3.52	1.39	1.33
1	0	2621	PSU	C4-N3	2.84	1.38	1.33
1	0	2587	OMU	C4-N3	2.74	1.37	1.33
1	0	2621	PSU	C2-N1	2.54	1.43	1.38
1	0	2588	OMG	C8-N7	-2.03	1.31	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.10	114.84	128.43
1	0	2621	PSU	C4-N3-C2	14.53	127.41	115.14
1	0	2588	OMG	C5-C6-N1	-8.73	111.50	123.43
1	0	2621	PSU	C5-C4-N3	-8.35	114.60	125.36
1	0	2588	OMG	C6-N1-C2	5.88	125.27	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	628	1MA	C2-N3-C4	-4.75	110.64	116.58
1	0	2587	OMU	C5-C4-N3	-3.89	114.75	123.31
1	0	2588	OMG	C2-N3-C4	-3.04	111.88	115.36
1	0	2621	PSU	C6-N1-C2	2.63	119.70	115.36
1	0	2588	OMG	N3-C2-N1	-2.38	124.05	127.22
1	0	2588	OMG	C6-C5-C4	-2.01	118.88	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.38	56 (2%) 65 63	18, 37, 80, 136	0
2	9	122/122 (100%)	-0.39	5 (4%) 37 36	32, 54, 75, 144	0
3	A	237/240 (98%)	0.38	20 (8%) 11 10	20, 39, 73, 93	0
4	B	337/338 (99%)	0.38	15 (4%) 33 31	21, 46, 72, 83	0
5	C	246/246 (100%)	0.32	11 (4%) 33 31	15, 36, 58, 70	0
6	D	140/177 (79%)	2.55	82 (58%) 0 0	44, 89, 112, 117	0
7	E	172/178 (96%)	0.60	13 (7%) 13 12	38, 59, 78, 83	0
8	F	119/120 (99%)	0.92	24 (20%) 1 0	38, 58, 83, 90	0
9	G	29/348 (8%)	2.54	20 (68%) 0 0	65, 81, 89, 93	0
10	H	160/171 (93%)	0.57	20 (12%) 3 3	32, 47, 77, 88	0
11	I	70/162 (43%)	5.30	67 (95%) 0 0	88, 102, 119, 122	0
12	J	142/145 (97%)	0.25	4 (2%) 53 51	30, 43, 63, 85	0
13	K	132/132 (100%)	0.15	6 (4%) 33 31	28, 43, 62, 71	0
14	L	145/165 (87%)	0.73	17 (11%) 4 4	20, 55, 93, 106	0
15	M	194/194 (100%)	-0.11	1 (0%) 91 89	19, 32, 46, 54	0
16	N	186/187 (99%)	0.62	17 (9%) 9 8	32, 51, 94, 109	0
17	O	115/116 (99%)	0.00	2 (1%) 70 68	28, 44, 61, 69	0
18	P	143/149 (95%)	0.12	0 100 100	31, 45, 57, 64	0
19	Q	95/96 (98%)	0.09	1 (1%) 80 79	27, 35, 52, 59	0
20	R	150/155 (96%)	-0.03	0 100 100	23, 36, 54, 63	0
21	S	81/85 (95%)	0.50	10 (12%) 4 3	32, 47, 68, 72	0
22	T	119/120 (99%)	0.42	5 (4%) 36 35	29, 46, 67, 82	0
23	U	53/66 (80%)	0.36	2 (3%) 40 39	34, 47, 64, 73	0
24	V	65/71 (91%)	1.63	12 (18%) 1 1	40, 59, 99, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.35	6 (3%) 39 38	28, 42, 58, 67	0
26	X	82/92 (89%)	0.43	4 (4%) 29 28	36, 49, 74, 91	0
27	Y	142/241 (58%)	0.01	5 (3%) 44 43	22, 36, 60, 75	0
28	Z	73/73 (100%)	0.39	4 (5%) 25 24	37, 49, 68, 85	0
29	1	56/57 (98%)	0.20	0 100 100	18, 25, 33, 37	0
30	2	46/50 (92%)	0.52	6 (13%) 3 3	29, 50, 75, 86	0
31	3	92/92 (100%)	0.19	3 (3%) 46 45	24, 45, 59, 73	0
All	All	6646/7464 (89%)	0.15	438 (6%) 18 17	15, 42, 85, 144	0

All (438) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	96	PHE	14.9
24	V	1	THR	11.9
11	I	71	GLY	11.5
11	I	133	THR	10.5
11	I	109	ALA	10.1
11	I	85	PHE	9.9
24	V	39	ALA	9.6
6	D	63	ILE	9.5
11	I	79	ILE	8.8
11	I	93	GLN	8.7
11	I	83	ALA	8.1
11	I	113	HIS	7.8
11	I	105	VAL	7.7
11	I	102	VAL	7.5
24	V	40	PRO	7.5
11	I	95	ASP	7.4
11	I	114	PRO	7.4
11	I	75	THR	7.3
26	X	88	GLU	7.2
11	I	94	GLU	7.2
3	A	37	VAL	7.2
6	D	10	PHE	7.1
11	I	84	GLY	7.1
16	N	166	ALA	7.0
21	S	81	ILE	6.7
11	I	82	GLU	6.6
11	I	108	ILE	6.5
11	I	121	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
11	I	137	VAL	6.4
6	D	57	THR	6.3
6	D	93	LEU	6.2
11	I	111	GLN	6.1
2	9	1	U	5.9
11	I	91	GLU	5.8
6	D	69	ILE	5.8
11	I	97	VAL	5.8
11	I	76	ALA	5.7
6	D	18	ILE	5.7
11	I	88	GLY	5.6
6	D	170	TYR	5.6
6	D	61	PHE	5.6
11	I	103	ASP	5.6
24	V	38	GLY	5.6
6	D	166	ILE	5.6
6	D	66	GLY	5.5
11	I	92	PRO	5.5
6	D	95	THR	5.5
3	A	237	GLY	5.4
26	X	80	GLU	5.3
11	I	116	LEU	5.2
6	D	85	GLN	5.1
11	I	107	GLN	5.1
6	D	172	VAL	5.1
24	V	43	PRO	5.0
11	I	104	GLN	5.0
11	I	117	LEU	5.0
9	G	23	ILE	5.0
11	I	132	CYS	4.8
6	D	44	ILE	4.8
8	F	119	ARG	4.8
1	0	1198	U	4.8
11	I	72	VAL	4.8
4	B	1	PRO	4.8
6	D	92	GLU	4.7
11	I	136	GLY	4.7
6	D	165	PHE	4.7
1	0	284	C	4.7
11	I	129	VAL	4.7
6	D	88	LEU	4.6
1	0	282	C	4.6

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Mol	Chain	Res	Type	RSRZ
1	0	1202	A	4.6
9	G	70	ALA	4.6
11	I	73	PRO	4.6
3	A	35	GLY	4.6
7	E	87	PHE	4.6
6	D	75	LEU	4.5
1	0	1200	A	4.5
11	I	89	SER	4.5
11	I	119	TYR	4.4
6	D	64	ARG	4.4
3	A	36	ASP	4.4
11	I	80	LYS	4.4
6	D	58	VAL	4.4
1	0	1174	A	4.3
11	I	118	SER	4.3
11	I	126	LYS	4.3
11	I	125	ALA	4.3
2	9	23	U	4.3
1	0	1172	G	4.3
11	I	87	THR	4.3
1	0	1171	A	4.2
6	D	81	GLU	4.2
11	I	74	PRO	4.2
11	I	81	ASP	4.2
11	I	86	GLU	4.2
11	I	139	ILE	4.2
6	D	104	PHE	4.2
10	H	73	LEU	4.2
27	Y	235	GLU	4.2
6	D	106	PHE	4.1
6	D	62	ASP	4.0
1	0	960	G	4.0
1	0	1199	A	4.0
14	L	80	ASP	4.0
11	I	135	LEU	4.0
1	0	1177	A	3.9
9	G	71	LEU	3.9
11	I	77	GLU	3.9
2	9	24	U	3.9
9	G	26	MET	3.9
11	I	115	ASP	3.9
6	D	102	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
11	I	128	VAL	3.9
1	0	1525	G	3.8
14	L	81	VAL	3.8
11	I	106	LYS	3.8
5	C	135	GLU	3.8
6	D	68	PRO	3.8
9	G	12	ILE	3.8
30	2	49	GLU	3.8
16	N	183	ASP	3.8
6	D	134	LEU	3.7
23	U	47	ARG	3.7
6	D	40	ILE	3.7
11	I	98	ALA	3.7
16	N	152	GLU	3.6
6	D	27	ILE	3.6
11	I	78	LEU	3.6
6	D	101	THR	3.6
28	Z	80	ARG	3.6
1	0	1201	C	3.6
6	D	171	ASP	3.6
1	0	1173	A	3.6
6	D	84	LEU	3.6
11	I	123	ASN	3.6
6	D	17	ARG	3.5
24	V	41	GLU	3.5
6	D	11	HIS	3.5
6	D	67	ASP	3.5
11	I	110	GLU	3.5
6	D	73	VAL	3.5
9	G	24	VAL	3.5
16	N	163	PHE	3.5
6	D	98	PHE	3.5
1	0	1170	U	3.5
3	A	31	LYS	3.5
1	0	1951	G	3.4
6	D	50	VAL	3.4
1	0	1169	U	3.4
30	2	31	ARG	3.4
10	H	37	GLN	3.4
24	V	2	VAL	3.4
6	D	157	LEU	3.4
6	D	80	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
11	I	138	THR	3.4
1	0	970	U	3.4
12	J	5	GLU	3.4
1	0	2237	G	3.4
6	D	65	GLU	3.3
8	F	107	ASP	3.3
9	G	73	ASP	3.3
11	I	122	THR	3.3
21	S	2	TRP	3.3
6	D	51	ARG	3.3
16	N	68	GLU	3.3
13	K	132	VAL	3.3
3	A	85	SER	3.3
16	N	162	ASP	3.3
17	O	23	GLY	3.3
6	D	99	ASP	3.3
5	C	132	ASP	3.3
6	D	74	THR	3.2
10	H	162	ARG	3.2
11	I	99	ASP	3.2
6	D	78	GLU	3.2
4	B	57	GLU	3.2
21	S	1	SER	3.2
6	D	26	GLY	3.2
7	E	45	ASP	3.2
11	I	120	ASP	3.2
6	D	132	VAL	3.2
11	I	90	GLY	3.2
6	D	94	ALA	3.2
8	F	115	VAL	3.2
15	M	194	ALA	3.2
6	D	173	GLU	3.2
6	D	103	ASN	3.2
1	0	1179	C	3.1
14	L	148	GLU	3.1
1	0	10	U	3.1
7	E	170	ARG	3.1
9	G	25	GLU	3.1
11	I	112	LYS	3.1
3	A	64	ASP	3.1
13	K	119	GLN	3.1
7	E	169	THR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	F	105	ASP	3.1
11	I	100	LEU	3.1
14	L	147	GLU	3.1
1	0	1180	U	3.1
8	F	110	ASP	3.1
22	T	119	ALA	3.1
9	G	27	ILE	3.0
6	D	158	ASN	3.0
4	B	183	GLU	3.0
16	N	181	ASP	3.0
25	W	93	ILE	3.0
1	0	1196	C	3.0
6	D	45	THR	3.0
6	D	23	VAL	3.0
27	Y	108	ASP	3.0
25	W	38	THR	3.0
1	0	1625	U	2.9
3	A	236	GLY	2.9
7	E	86	VAL	2.9
16	N	139	TRP	2.9
16	N	160	SER	2.9
6	D	56	ARG	2.9
6	D	167	GLU	2.9
8	F	16	ALA	2.9
31	3	92	GLU	2.9
3	A	97	ALA	2.9
14	L	150	GLN	2.9
10	H	167	PRO	2.9
8	F	118	LEU	2.9
11	I	124	ALA	2.9
22	T	1	SER	2.9
2	9	2	U	2.9
8	F	12	LEU	2.9
28	Z	24	ARG	2.9
16	N	179	LEU	2.9
16	N	164	ASP	2.8
26	X	85	VAL	2.8
1	0	1175	G	2.8
5	C	14	GLY	2.8
6	D	22	VAL	2.8
8	F	117	GLU	2.8
3	A	133	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
4	B	184	ASP	2.8
6	D	89	PRO	2.8
1	0	1165	G	2.8
9	G	69	ARG	2.8
9	G	66	LEU	2.8
6	D	130	VAL	2.8
4	B	117	GLU	2.8
6	D	55	LYS	2.8
9	G	21	ASP	2.8
9	G	28	GLU	2.7
1	0	1181	A	2.7
6	D	41	LEU	2.7
9	G	72	ASP	2.7
14	L	102	ASP	2.7
7	E	88	TYR	2.7
4	B	104	GLU	2.7
6	D	25	MET	2.7
11	I	101	SER	2.7
30	2	39	ARG	2.7
8	F	22	VAL	2.7
9	G	18	GLU	2.7
14	L	130	ARG	2.7
6	D	77	ASP	2.7
7	E	10	ASP	2.7
7	E	100	ASP	2.7
1	0	1178	G	2.7
9	G	68	GLU	2.7
24	V	37	GLY	2.7
3	A	34	ASP	2.7
4	B	180	ASP	2.7
12	J	4	ALA	2.6
16	N	184	ILE	2.6
10	H	35	ARG	2.6
6	D	96	SER	2.6
21	S	77	VAL	2.6
5	C	143	ASP	2.6
1	0	1195	G	2.6
30	2	35	ARG	2.6
1	0	1163	G	2.6
1	0	1203	G	2.6
4	B	120	ASP	2.6
14	L	75	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
26	X	71	ARG	2.6
4	B	133	GLU	2.6
8	F	10	ALA	2.6
1	0	283	U	2.6
1	0	1950	G	2.6
27	Y	236	VAL	2.6
9	G	15	TRP	2.6
3	A	32	VAL	2.5
6	D	47	GLN	2.5
5	C	134	ASP	2.5
1	0	2238	A	2.5
10	H	83	TYR	2.5
1	0	1168	C	2.5
6	D	86	THR	2.5
6	D	43	GLU	2.5
8	F	103	GLU	2.5
10	H	32	LYS	2.5
1	0	2508	C	2.5
2	9	122	C	2.5
10	H	47	ILE	2.5
6	D	169	THR	2.5
8	F	28	ALA	2.5
10	H	171	ALA	2.5
1	0	1192	A	2.5
8	F	99	THR	2.5
6	D	53	LYS	2.5
4	B	123	ALA	2.5
14	L	104	ASP	2.5
4	B	115	VAL	2.5
6	D	135	VAL	2.5
9	G	20	VAL	2.5
8	F	108	VAL	2.4
22	T	82	THR	2.4
21	S	76	GLU	2.4
22	T	80	GLU	2.4
16	N	177	GLU	2.4
27	Y	95	THR	2.4
10	H	80	GLU	2.4
14	L	105	TYR	2.4
21	S	45	TYR	2.4
31	3	56	PRO	2.4
6	D	87	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	0	735	C	2.4
14	L	91	VAL	2.4
6	D	29	HIS	2.4
6	D	156	ARG	2.4
14	L	145	LEU	2.4
3	A	134	ASN	2.4
8	F	15	ASP	2.4
8	F	106	ALA	2.4
8	F	17	LEU	2.4
1	0	2004	U	2.3
11	I	130	GLY	2.3
10	H	45	VAL	2.3
1	0	1279	U	2.3
3	A	38	ILE	2.3
6	D	48	MET	2.3
9	G	14	GLU	2.3
10	H	141	GLU	2.3
5	C	61	PHE	2.3
17	O	1	SER	2.3
7	E	127	ASP	2.3
8	F	100	ASP	2.3
25	W	86	GLU	2.3
1	0	1208	C	2.3
14	L	149	ARG	2.3
10	H	39	ASP	2.3
14	L	89	PHE	2.3
6	D	164	ALA	2.3
1	0	1166	A	2.3
5	C	162	VAL	2.3
21	S	80	ARG	2.3
24	V	42	ASN	2.3
24	V	45	ARG	2.3
31	3	26	ARG	2.3
3	A	60	PHE	2.3
16	N	186	LEU	2.3
10	H	33	MET	2.3
13	K	101	ASN	2.3
13	K	125	ALA	2.3
25	W	92	ASP	2.3
28	Z	81	ARG	2.2
27	Y	98	GLN	2.2
4	B	118	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
10	H	166	SER	2.2
8	F	18	GLU	2.2
9	G	17	GLN	2.2
10	H	82	ASP	2.2
13	K	108	GLU	2.2
6	D	54	ALA	2.2
8	F	49	PHE	2.2
25	W	95	GLY	2.2
3	A	65	ARG	2.2
3	A	89	ALA	2.2
30	2	44	ARG	2.2
1	0	1948	G	2.2
21	S	46	ASP	2.2
25	W	91	ASP	2.2
10	H	36	LYS	2.2
14	L	97	VAL	2.2
19	Q	95	GLU	2.2
7	E	121	ASP	2.2
1	0	1965	C	2.2
1	0	2769	C	2.2
6	D	162	ALA	2.2
14	L	83	GLU	2.2
5	C	13	ASP	2.2
6	D	83	PHE	2.2
8	F	11	ASP	2.2
6	D	90	LEU	2.2
3	A	66	ARG	2.2
28	Z	20	ARG	2.2
10	H	137	TYR	2.1
16	N	167	ASP	2.1
5	C	141	SER	2.1
4	B	92	TYR	2.1
8	F	7	ASP	2.1
12	J	7	ASP	2.1
30	2	20	ARG	2.1
1	0	1966	U	2.1
1	0	1967	U	2.1
1	0	1167	G	2.1
1	0	736	A	2.1
5	C	198	ASP	2.1
3	A	63	GLY	2.1
6	D	70	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	138	U	2.1
10	H	74	ILE	2.1
6	D	38	GLU	2.1
7	E	11	VAL	2.1
11	I	127	GLU	2.1
12	J	39	VAL	2.1
1	0	999	C	2.1
1	0	1949	G	2.1
4	B	181	ILE	2.1
6	D	59	GLY	2.1
16	N	185	GLU	2.1
16	N	134	ASP	2.0
1	0	281	U	2.0
1	0	1162	G	2.0
1	0	2254	G	2.0
3	A	94	LEU	2.0
7	E	42	VAL	2.0
13	K	129	THR	2.0
21	S	43	GLU	2.0
21	S	79	SER	2.0
24	V	27	LEU	2.0
8	F	25	ASP	2.0
7	E	129	GLU	2.0
10	H	79	GLU	2.0
22	T	104	GLU	2.0
4	B	134	ALA	2.0
1	0	280	C	2.0
5	C	73	LEU	2.0
24	V	49	LEU	2.0
14	L	144	ASP	2.0
23	U	12	ASP	2.0
6	D	159	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMG	0	2588	24/25	0.98	0.13	22,25,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	UR3	0	2619	21/22	0.98	0.14	23,27,31,37	0
1	OMU	0	2587	21/22	0.98	0.13	24,26,28,30	0
1	1MA	0	628	23/24	0.98	0.17	21,24,25,27	0
1	PSU	0	2621	20/21	0.99	0.15	20,25,28,28	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8087	1/1	0.52	0.31	71,71,71,71	0
32	MG	0	8050	1/1	0.64	0.15	62,62,62,62	0
32	MG	0	8072	1/1	0.71	0.10	51,51,51,51	0
32	MG	0	8103	1/1	0.73	0.27	57,57,57,57	0
32	MG	9	8095	1/1	0.77	0.14	67,67,67,67	0
34	NA	0	8371	1/1	0.78	0.37	52,52,52,52	0
34	NA	0	8384	1/1	0.79	0.16	54,54,54,54	0
32	MG	0	8102	1/1	0.80	0.10	54,54,54,54	0
34	NA	0	8370	1/1	0.82	0.43	60,60,60,60	0
32	MG	0	8070	1/1	0.83	0.14	41,41,41,41	0
32	MG	0	8047	1/1	0.83	0.10	55,55,55,55	0
34	NA	0	8329	1/1	0.83	0.13	50,50,50,50	0
34	NA	C	8304	1/1	0.84	0.20	32,32,32,32	0
32	MG	0	8094	1/1	0.84	0.07	62,62,62,62	0
32	MG	0	8049	1/1	0.85	0.12	55,55,55,55	0
34	NA	9	8351	1/1	0.86	0.15	43,43,43,43	0
34	NA	R	8386	1/1	0.87	0.41	75,75,75,75	0
32	MG	0	8112	1/1	0.87	0.13	38,38,38,38	0
34	NA	0	8311	1/1	0.87	0.14	48,48,48,48	0
34	NA	H	8322	1/1	0.87	0.26	53,53,53,53	0
32	MG	0	8034	1/1	0.87	0.09	32,32,32,32	0
34	NA	0	8308	1/1	0.88	0.20	43,43,43,43	0
32	MG	0	8101	1/1	0.88	0.29	48,48,48,48	0
34	NA	0	8307	1/1	0.88	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	9	8383	1/1	0.88	0.22	44,44,44,44	0
34	NA	0	8363	1/1	0.89	0.31	52,52,52,52	0
32	MG	0	8052	1/1	0.89	0.07	47,47,47,47	0
32	MG	0	8066	1/1	0.90	0.49	76,76,76,76	0
32	MG	0	8090	1/1	0.90	0.34	55,55,55,55	0
32	MG	0	8089	1/1	0.90	0.08	52,52,52,52	0
34	NA	0	8376	1/1	0.90	0.40	40,40,40,40	0
34	NA	0	8341	1/1	0.91	0.13	38,38,38,38	0
34	NA	0	8372	1/1	0.91	0.45	55,55,55,55	0
34	NA	0	8327	1/1	0.91	0.26	38,38,38,38	0
32	MG	0	8077	1/1	0.91	0.13	24,24,24,24	0
32	MG	0	8076	1/1	0.91	0.05	43,43,43,43	0
32	MG	0	8067	1/1	0.91	0.14	35,35,35,35	0
34	NA	0	8373	1/1	0.91	0.13	44,44,44,44	0
32	MG	0	8014	1/1	0.92	0.09	25,25,25,25	0
32	MG	0	8116	1/1	0.92	0.16	38,38,38,38	0
34	NA	0	8358	1/1	0.92	0.38	67,67,67,67	0
32	MG	0	8043	1/1	0.92	0.06	34,34,34,34	0
32	MG	0	8045	1/1	0.92	0.07	51,51,51,51	0
34	NA	0	8324	1/1	0.92	0.15	51,51,51,51	0
32	MG	0	8062	1/1	0.92	0.07	42,42,42,42	0
34	NA	0	8314	1/1	0.92	0.30	39,39,39,39	0
32	MG	0	8085	1/1	0.92	0.08	35,35,35,35	0
34	NA	0	8385	1/1	0.92	0.38	48,48,48,48	0
34	NA	0	8340	1/1	0.92	0.25	46,46,46,46	0
34	NA	0	8350	1/1	0.92	0.36	36,36,36,36	0
34	NA	0	8382	1/1	0.93	0.10	66,66,66,66	0
35	CL	J	8521	1/1	0.93	0.17	48,48,48,48	0
34	NA	0	8325	1/1	0.93	0.24	49,49,49,49	0
32	MG	0	8022	1/1	0.93	0.12	31,31,31,31	0
34	NA	0	8310	1/1	0.93	0.12	28,28,28,28	0
32	MG	0	8082	1/1	0.93	0.19	59,59,59,59	0
32	MG	0	8080	1/1	0.93	0.07	42,42,42,42	0
34	NA	0	8357	1/1	0.93	0.09	40,40,40,40	0
32	MG	0	8068	1/1	0.93	0.04	45,45,45,45	0
34	NA	0	8369	1/1	0.93	0.21	41,41,41,41	0
32	MG	0	8071	1/1	0.93	0.04	61,61,61,61	0
32	MG	B	8055	1/1	0.93	0.07	43,43,43,43	0
32	MG	0	8012	1/1	0.94	0.14	34,34,34,34	0
34	NA	S	8312	1/1	0.94	0.08	28,28,28,28	0
32	MG	0	8016	1/1	0.94	0.09	32,32,32,32	0
32	MG	K	8069	1/1	0.94	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8377	1/1	0.94	0.23	51,51,51,51	0
34	NA	0	8361	1/1	0.94	0.22	38,38,38,38	0
32	MG	0	8051	1/1	0.94	0.11	56,56,56,56	0
34	NA	0	8321	1/1	0.94	0.24	40,40,40,40	0
32	MG	0	8046	1/1	0.94	0.06	38,38,38,38	0
34	NA	0	8362	1/1	0.94	0.35	51,51,51,51	0
34	NA	0	8356	1/1	0.94	0.20	37,37,37,37	0
32	MG	0	8093	1/1	0.94	0.12	37,37,37,37	0
34	NA	0	8365	1/1	0.94	0.19	30,30,30,30	0
34	NA	A	8345	1/1	0.94	0.09	47,47,47,47	0
34	NA	0	8313	1/1	0.94	0.11	48,48,48,48	0
34	NA	0	8302	1/1	0.94	0.20	45,45,45,45	0
32	MG	0	8099	1/1	0.94	0.23	43,43,43,43	0
32	MG	0	8013	1/1	0.95	0.15	22,22,22,22	0
32	MG	0	8079	1/1	0.95	0.16	20,20,20,20	0
34	NA	0	8349	1/1	0.95	0.17	36,36,36,36	0
34	NA	0	8318	1/1	0.95	0.29	51,51,51,51	0
34	NA	0	8334	1/1	0.95	0.09	35,35,35,35	0
34	NA	0	8364	1/1	0.95	0.26	38,38,38,38	0
34	NA	0	8333	1/1	0.95	0.09	25,25,25,25	0
34	NA	0	8315	1/1	0.95	0.18	32,32,32,32	0
34	NA	0	8366	1/1	0.95	0.24	57,57,57,57	0
32	MG	0	8104	1/1	0.95	0.14	47,47,47,47	0
34	NA	0	8368	1/1	0.95	0.15	50,50,50,50	0
32	MG	0	8006	1/1	0.95	0.07	27,27,27,27	0
33	K	0	8201	1/1	0.95	0.15	64,64,64,64	0
32	MG	0	8039	1/1	0.95	0.07	34,34,34,34	0
32	MG	0	8028	1/1	0.95	0.06	26,26,26,26	0
34	NA	0	8326	1/1	0.95	0.19	38,38,38,38	0
32	MG	0	8064	1/1	0.95	0.14	26,26,26,26	0
35	CL	0	8515	1/1	0.95	0.10	50,50,50,50	0
34	NA	0	8355	1/1	0.96	0.35	48,48,48,48	0
34	NA	L	8380	1/1	0.96	0.34	42,42,42,42	0
32	MG	0	8097	1/1	0.96	0.08	32,32,32,32	0
34	NA	0	8330	1/1	0.96	0.08	38,38,38,38	0
34	NA	0	8317	1/1	0.96	0.11	27,27,27,27	0
34	NA	R	8337	1/1	0.96	0.08	34,34,34,34	0
34	NA	0	8379	1/1	0.96	0.45	49,49,49,49	0
32	MG	0	8091	1/1	0.96	0.09	42,42,42,42	0
34	NA	0	8336	1/1	0.96	0.07	37,37,37,37	0
35	CL	J	8502	1/1	0.96	0.12	53,53,53,53	0
34	NA	0	8316	1/1	0.96	0.21	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8037	1/1	0.96	0.06	34,34,34,34	0
32	MG	0	8105	1/1	0.96	0.13	43,43,43,43	0
34	NA	Q	8348	1/1	0.96	0.07	32,32,32,32	0
32	MG	0	8098	1/1	0.96	0.06	27,27,27,27	0
32	MG	3	8078	1/1	0.96	0.09	40,40,40,40	0
32	MG	0	8023	1/1	0.96	0.13	31,31,31,31	0
34	NA	0	8303	1/1	0.97	0.18	34,34,34,34	0
34	NA	0	8319	1/1	0.97	0.11	29,29,29,29	0
35	CL	R	8506	1/1	0.97	0.12	40,40,40,40	0
34	NA	0	8378	1/1	0.97	0.18	42,42,42,42	0
32	MG	0	8061	1/1	0.97	0.15	34,34,34,34	0
32	MG	0	8044	1/1	0.97	0.09	33,33,33,33	0
32	MG	0	8020	1/1	0.97	0.09	25,25,25,25	0
34	NA	0	8359	1/1	0.97	0.26	40,40,40,40	0
34	NA	0	8381	1/1	0.97	0.14	42,42,42,42	0
34	NA	0	8342	1/1	0.97	0.26	33,33,33,33	0
34	NA	0	8352	1/1	0.97	0.13	40,40,40,40	0
34	NA	M	8347	1/1	0.97	0.17	20,20,20,20	0
35	CL	0	8522	1/1	0.97	0.17	46,46,46,46	0
32	MG	0	8113	1/1	0.97	0.10	36,36,36,36	0
32	MG	0	8106	1/1	0.97	0.03	31,31,31,31	0
35	CL	3	8504	1/1	0.97	0.07	45,45,45,45	0
32	MG	0	8033	1/1	0.97	0.10	20,20,20,20	0
32	MG	0	8040	1/1	0.97	0.12	38,38,38,38	0
32	MG	0	8096	1/1	0.97	0.12	38,38,38,38	0
34	NA	T	8343	1/1	0.97	0.06	31,31,31,31	0
32	MG	0	8018	1/1	0.97	0.06	29,29,29,29	0
34	NA	0	8331	1/1	0.97	0.28	40,40,40,40	0
34	NA	0	8360	1/1	0.97	0.17	43,43,43,43	0
32	MG	0	8107	1/1	0.97	0.07	65,65,65,65	0
32	MG	0	8031	1/1	0.97	0.12	24,24,24,24	0
34	NA	0	8335	1/1	0.97	0.19	32,32,32,32	0
32	MG	0	8081	1/1	0.97	0.10	39,39,39,39	0
34	NA	0	8301	1/1	0.97	0.12	35,35,35,35	0
32	MG	0	8002	1/1	0.97	0.08	28,28,28,28	0
32	MG	0	8063	1/1	0.97	0.14	62,62,62,62	0
32	MG	0	8042	1/1	0.97	0.09	29,29,29,29	0
32	MG	0	8059	1/1	0.97	0.08	26,26,26,26	0
35	CL	L	8510	1/1	0.97	0.10	38,38,38,38	0
34	NA	0	8367	1/1	0.97	0.28	45,45,45,45	0
32	MG	0	8027	1/1	0.97	0.07	36,36,36,36	0
32	MG	0	8011	1/1	0.97	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8332	1/1	0.97	0.12	33,33,33,33	0
32	MG	Y	8108	1/1	0.97	0.09	27,27,27,27	0
34	NA	0	8374	1/1	0.97	0.20	44,44,44,44	0
32	MG	0	8001	1/1	0.97	0.11	25,25,25,25	0
32	MG	0	8032	1/1	0.97	0.06	24,24,24,24	0
32	MG	0	8074	1/1	0.97	0.06	35,35,35,35	0
35	CL	Y	8520	1/1	0.97	0.14	39,39,39,39	0
32	MG	0	8084	1/1	0.98	0.07	39,39,39,39	0
32	MG	0	8092	1/1	0.98	0.11	68,68,68,68	0
35	CL	0	8505	1/1	0.98	0.11	42,42,42,42	0
32	MG	0	8053	1/1	0.98	0.10	29,29,29,29	0
36	CD	O	8405	1/1	0.98	0.08	73,73,73,73	0
32	MG	0	8038	1/1	0.98	0.13	23,23,23,23	0
32	MG	0	8041	1/1	0.98	0.10	34,34,34,34	0
35	CL	0	8503	1/1	0.98	0.17	42,42,42,42	0
32	MG	0	8088	1/1	0.98	0.08	21,21,21,21	0
32	MG	0	8036	1/1	0.98	0.09	36,36,36,36	0
35	CL	J	8501	1/1	0.98	0.09	46,46,46,46	0
32	MG	0	8003	1/1	0.98	0.10	22,22,22,22	0
34	NA	0	8344	1/1	0.98	0.11	25,25,25,25	0
35	CL	O	8508	1/1	0.98	0.08	53,53,53,53	0
34	NA	0	8306	1/1	0.98	0.13	31,31,31,31	0
32	MG	0	8029	1/1	0.98	0.09	36,36,36,36	0
34	NA	0	8339	1/1	0.98	0.20	21,21,21,21	0
35	CL	0	8511	1/1	0.98	0.11	38,38,38,38	0
32	MG	0	8083	1/1	0.98	0.08	30,30,30,30	0
32	MG	T	8073	1/1	0.98	0.05	39,39,39,39	0
32	MG	0	8010	1/1	0.98	0.16	25,25,25,25	0
35	CL	M	8518	1/1	0.98	0.20	35,35,35,35	0
32	MG	0	8048	1/1	0.98	0.07	40,40,40,40	0
35	CL	0	8517	1/1	0.98	0.10	50,50,50,50	0
32	MG	0	8058	1/1	0.98	0.06	28,28,28,28	0
32	MG	0	8114	1/1	0.98	0.07	37,37,37,37	0
34	NA	0	8354	1/1	0.98	0.17	26,26,26,26	0
32	MG	0	8115	1/1	0.98	0.09	44,44,44,44	0
32	MG	0	8054	1/1	0.98	0.15	18,18,18,18	0
32	MG	0	8019	1/1	0.98	0.05	25,25,25,25	0
34	NA	0	8305	1/1	0.98	0.23	33,33,33,33	0
35	CL	N	8507	1/1	0.98	0.09	46,46,46,46	0
34	NA	H	8309	1/1	0.98	0.09	28,28,28,28	0
32	MG	0	8035	1/1	0.98	0.07	37,37,37,37	0
32	MG	0	8100	1/1	0.98	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8015	1/1	0.98	0.18	27,27,27,27	0
32	MG	0	8007	1/1	0.98	0.15	22,22,22,22	0
32	MG	0	8008	1/1	0.98	0.10	24,24,24,24	0
32	MG	0	8009	1/1	0.98	0.14	25,25,25,25	0
32	MG	0	8021	1/1	0.98	0.09	24,24,24,24	0
34	NA	J	8346	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8075	1/1	0.98	0.06	30,30,30,30	0
32	MG	0	8026	1/1	0.98	0.16	27,27,27,27	0
32	MG	0	8057	1/1	0.98	0.12	36,36,36,36	0
35	CL	0	8514	1/1	0.98	0.20	38,38,38,38	0
35	CL	0	8513	1/1	0.99	0.11	45,45,45,45	0
35	CL	B	8519	1/1	0.99	0.14	34,34,34,34	0
34	NA	0	8323	1/1	0.99	0.15	32,32,32,32	0
36	CD	Z	8403	1/1	0.99	0.14	48,48,48,48	0
32	MG	0	8109	1/1	0.99	0.13	26,26,26,26	0
32	MG	0	8024	1/1	0.99	0.15	23,23,23,23	0
35	CL	A	8509	1/1	0.99	0.11	49,49,49,49	0
32	MG	0	8025	1/1	0.99	0.09	37,37,37,37	0
36	CD	1	8402	1/1	0.99	0.07	44,44,44,44	0
32	MG	0	8086	1/1	0.99	0.09	33,33,33,33	0
33	K	0	8202	1/1	0.99	0.07	38,38,38,38	0
34	NA	0	8320	1/1	0.99	0.30	38,38,38,38	0
32	MG	0	8005	1/1	0.99	0.12	24,24,24,24	0
32	MG	A	8065	1/1	0.99	0.07	24,24,24,24	0
32	MG	0	8111	1/1	0.99	0.09	25,25,25,25	0
35	CL	0	8512	1/1	0.99	0.12	35,35,35,35	0
34	NA	0	8353	1/1	0.99	0.14	20,20,20,20	0
32	MG	0	8110	1/1	0.99	0.11	32,32,32,32	0
36	CD	U	8401	1/1	0.99	0.11	52,52,52,52	0
34	NA	0	8328	1/1	0.99	0.12	30,30,30,30	0
32	MG	0	8060	1/1	0.99	0.22	32,32,32,32	0
36	CD	3	8404	1/1	0.99	0.09	49,49,49,49	0
32	MG	0	8056	1/1	0.99	0.04	31,31,31,31	0
35	CL	0	8516	1/1	0.99	0.14	42,42,42,42	0
32	MG	0	8004	1/1	0.99	0.14	22,22,22,22	0
34	NA	0	8338	1/1	0.99	0.06	38,38,38,38	0
34	NA	0	8375	1/1	0.99	0.22	43,43,43,43	0
32	MG	0	8017	1/1	1.00	0.14	13,13,13,13	0
32	MG	0	8030	1/1	1.00	0.07	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.