



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 07:58 PM EDT

PDB ID : 3CCS  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A  
Authors : Blaha, G.; Gurel, G.  
Deposited on : unknown  
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

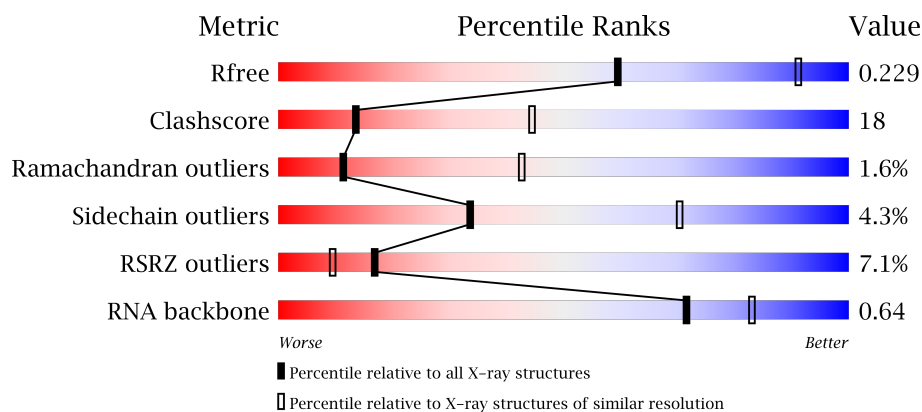
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)
RNA backbone	2435	1008 (3.30-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>3%</div> <div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>62%</div> <div>33%</div> <div>•</div> </div>
3	C	246	<div> <div>73%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>30%</div> <div>51%</div> <div>25%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8009	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8079	-	-	-	X
32	MG	0	8080	-	-	-	X
32	MG	0	8085	-	-	-	X
33	CL	0	8812	-	-	X	-
33	CL	0	8816	-	-	-	X
33	CL	B	8819	-	-	-	X
33	CL	Y	8820	-	-	X	-
34	SR	0	8903	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8926	-	-	-	X
34	SR	0	8943	-	-	-	X
34	SR	0	8975	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8992	-	-	-	X
34	SR	B	8987	-	-	-	X
34	SR	L	8969	-	-	-	X
34	SR	R	8912	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
36	K	0	8401	-	-	-	X
37	CD	3	8704	-	-	-	X
37	CD	U	8701	-	-	-	X
37	CD	Z	8703	-	-	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	2745			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	86	Total	Mg	0	0
			86	86		
32	9	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	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	92	Total Sr 92 92	0	0
34	1	2	Total Sr 2 2	0	0
34	H	1	Total Sr 1 1	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	2	Total Sr 2 2	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	L	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	S	1	Total 1	Sr 1	0	0
34	F	1	Total 1	Sr 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total 65	Na 65	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	119	Total 119	O 119	0	0
38	B	152	Total 152	O 152	0	0
38	C	185	Total 185	O 185	0	0
38	D	42	Total 42	O 42	0	0
38	E	43	Total 43	O 43	0	0
38	F	26	Total 26	O 26	0	0
38	G	19	Total 19	O 19	0	0
38	H	65	Total 65	O 65	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	58	Total 58	O 58	0	0
38	L	85	Total 85	O 85	0	0
38	M	127	Total 127	O 127	0	0
38	N	59	Total 59	O 59	0	0
38	O	39	Total 39	O 39	0	0

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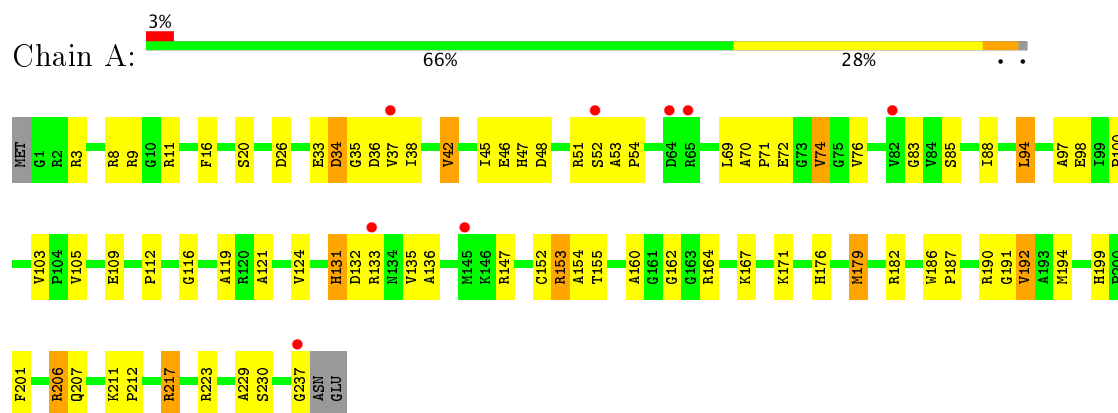
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	67	Total 67	O 67	0	0
38	Q	48	Total 48	O 48	0	0
38	R	77	Total 77	O 77	0	0
38	S	30	Total 30	O 30	0	0
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	31	Total 31	O 31	0	0
38	1	59	Total 59	O 59	0	0
38	2	43	Total 43	O 43	0	0
38	3	70	Total 70	O 70	0	0
38	0	5904	Total 5904	O 5904	0	0
38	9	149	Total 149	O 149	0	0

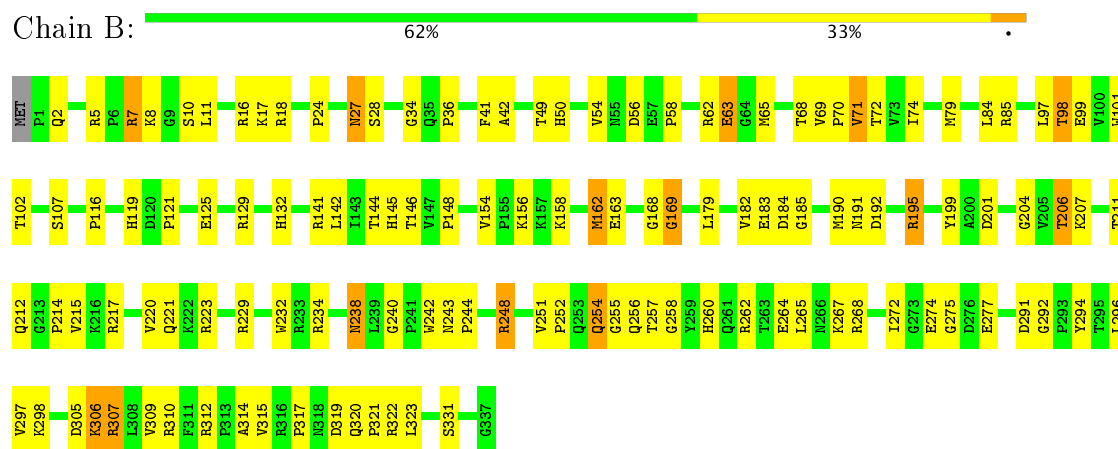
### 3 Residue-property plots

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

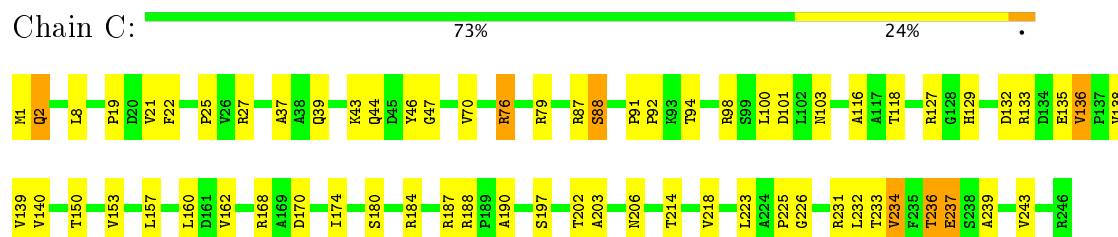
- Molecule 1: 50S ribosomal protein L2P



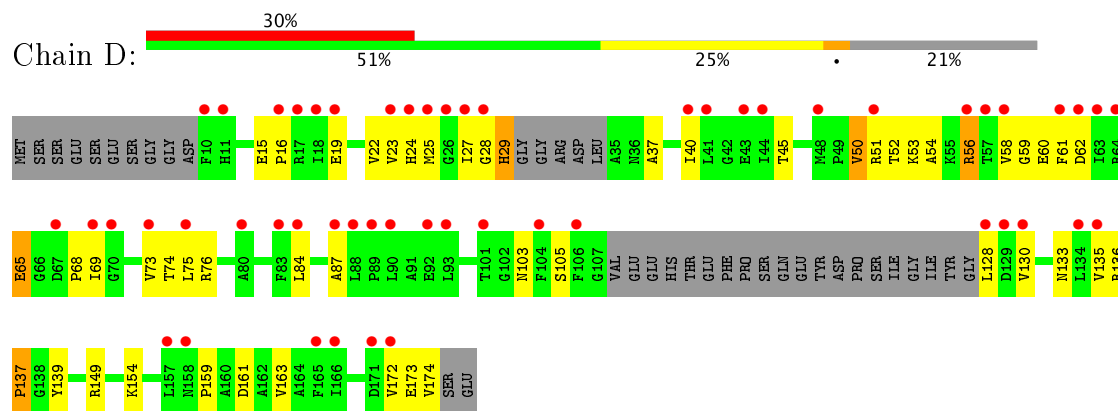
- Molecule 2: 50S ribosomal protein L3P



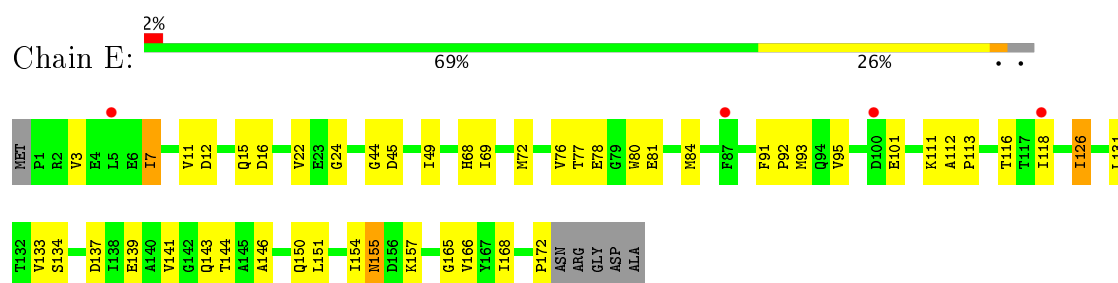
- Molecule 3: 50S ribosomal protein L4P



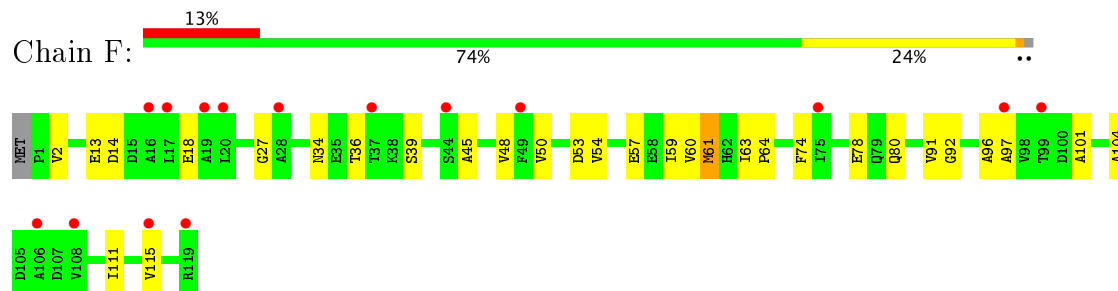
- Molecule 4: 50S ribosomal protein L5P



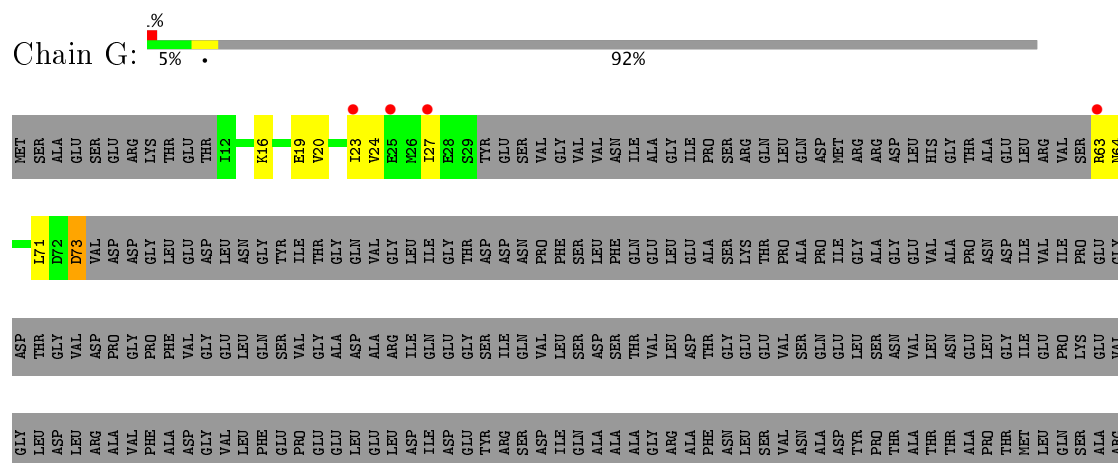
- Molecule 5: 50S ribosomal protein L6P



- Molecule 6: 50S ribosomal protein L7Ae



- Molecule 7: 50S ribosomal protein L10E

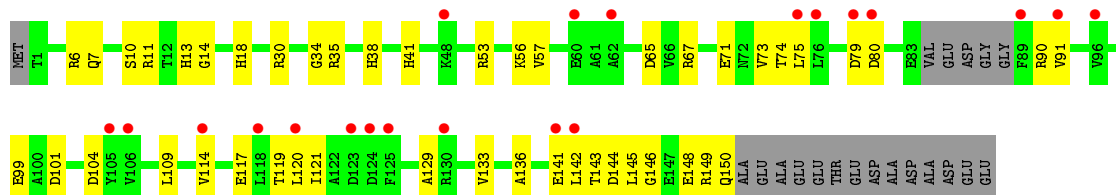




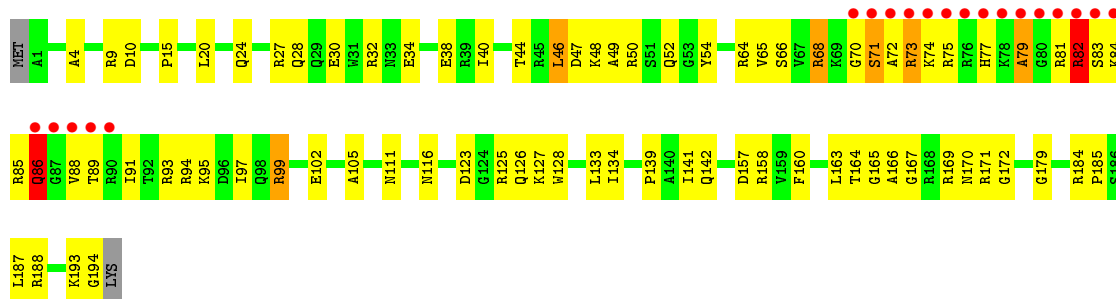




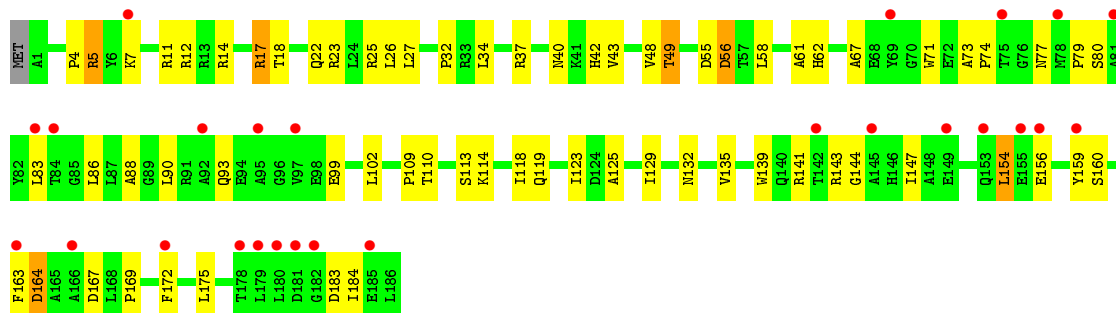
- Molecule 12: 50S ribosomal protein L15P



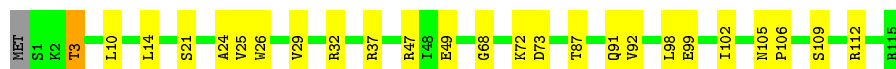
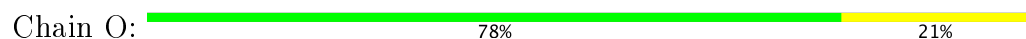
- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

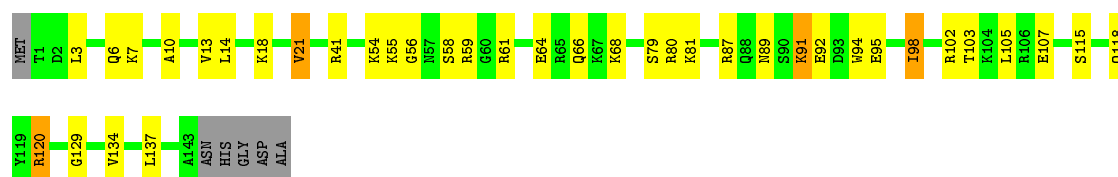


- Molecule 15: 50S ribosomal protein L18e

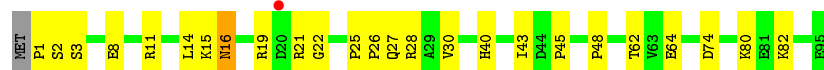
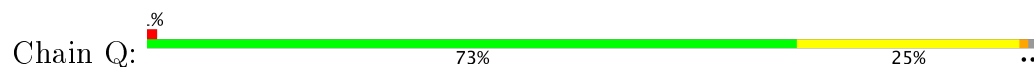


- Molecule 16: 50S ribosomal protein L19e

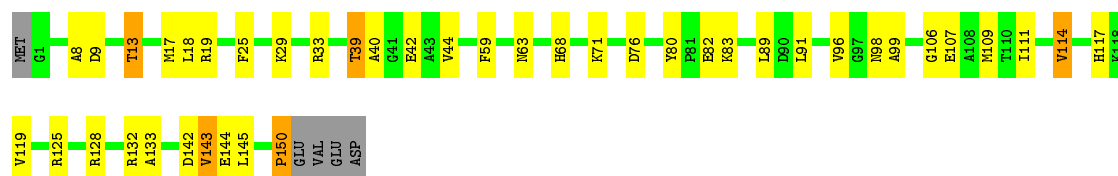




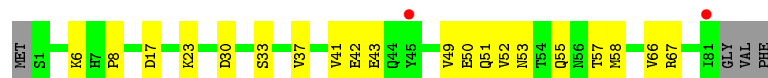
- Molecule 17: 50S ribosomal protein L21e



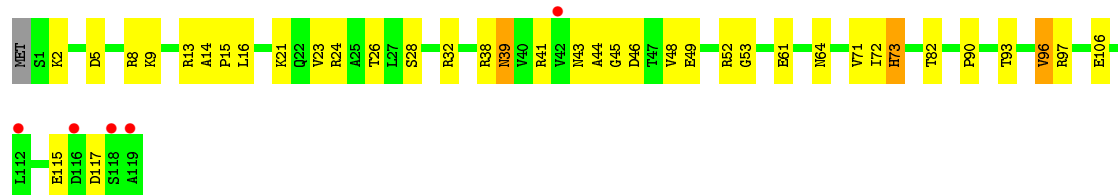
- Molecule 18: 50S ribosomal protein L22P



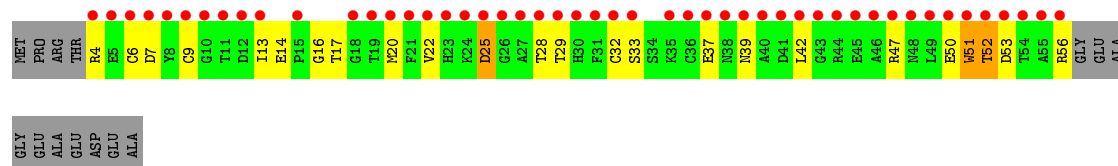
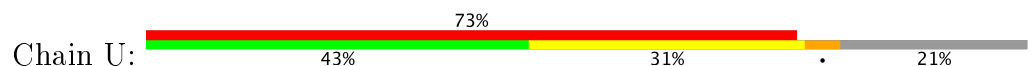
- Molecule 19: 50S ribosomal protein L23P



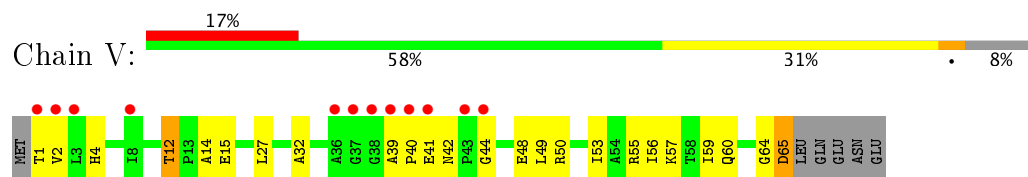
- Molecule 20: 50S ribosomal protein L24P



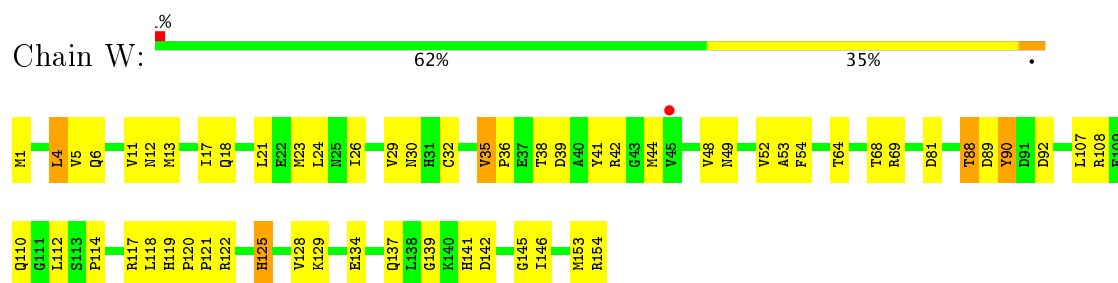
- Molecule 21: 50S ribosomal protein L24e



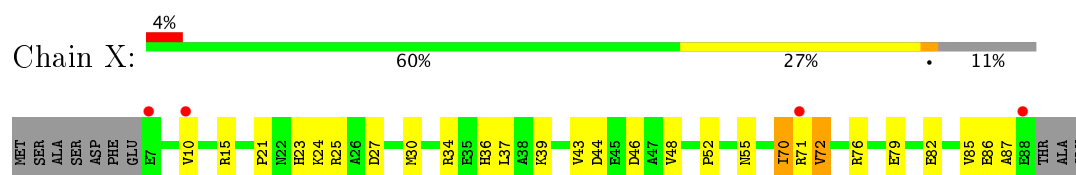
- Molecule 22: 50S ribosomal protein L29P



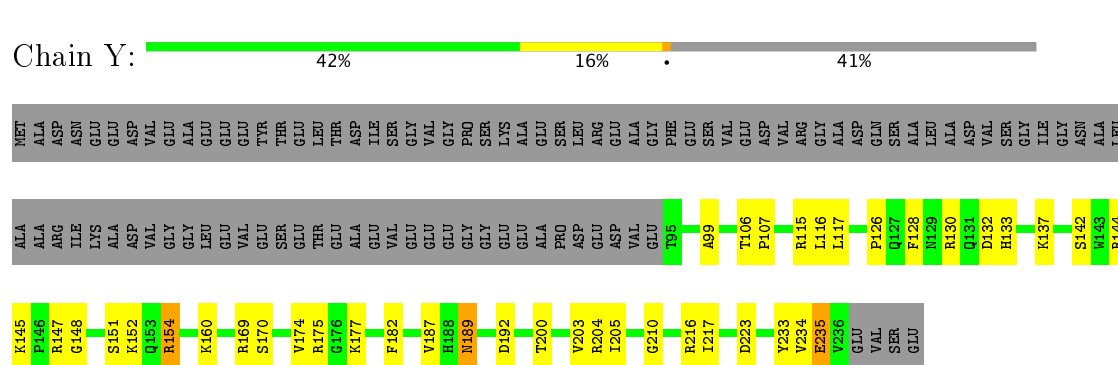
- Molecule 23: 50S ribosomal protein L30P



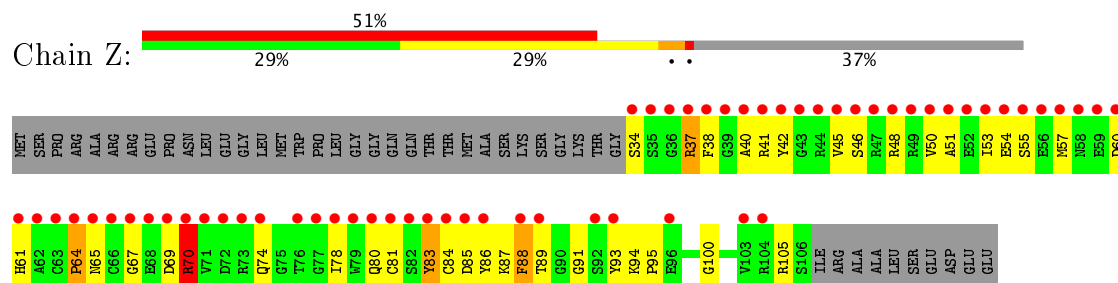
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae

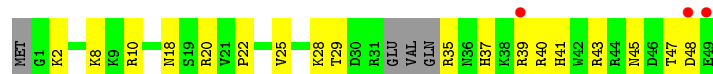


- Molecule 27: 50S ribosomal protein L37e

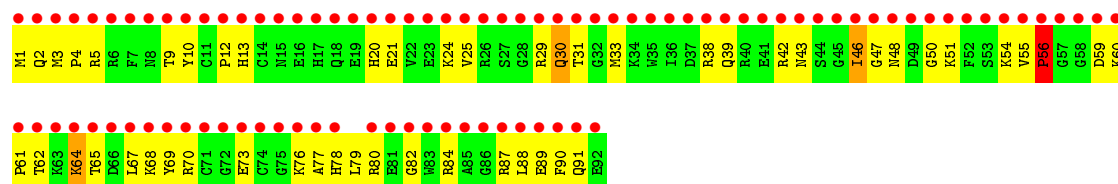
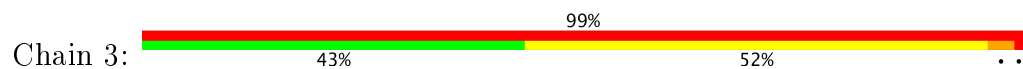




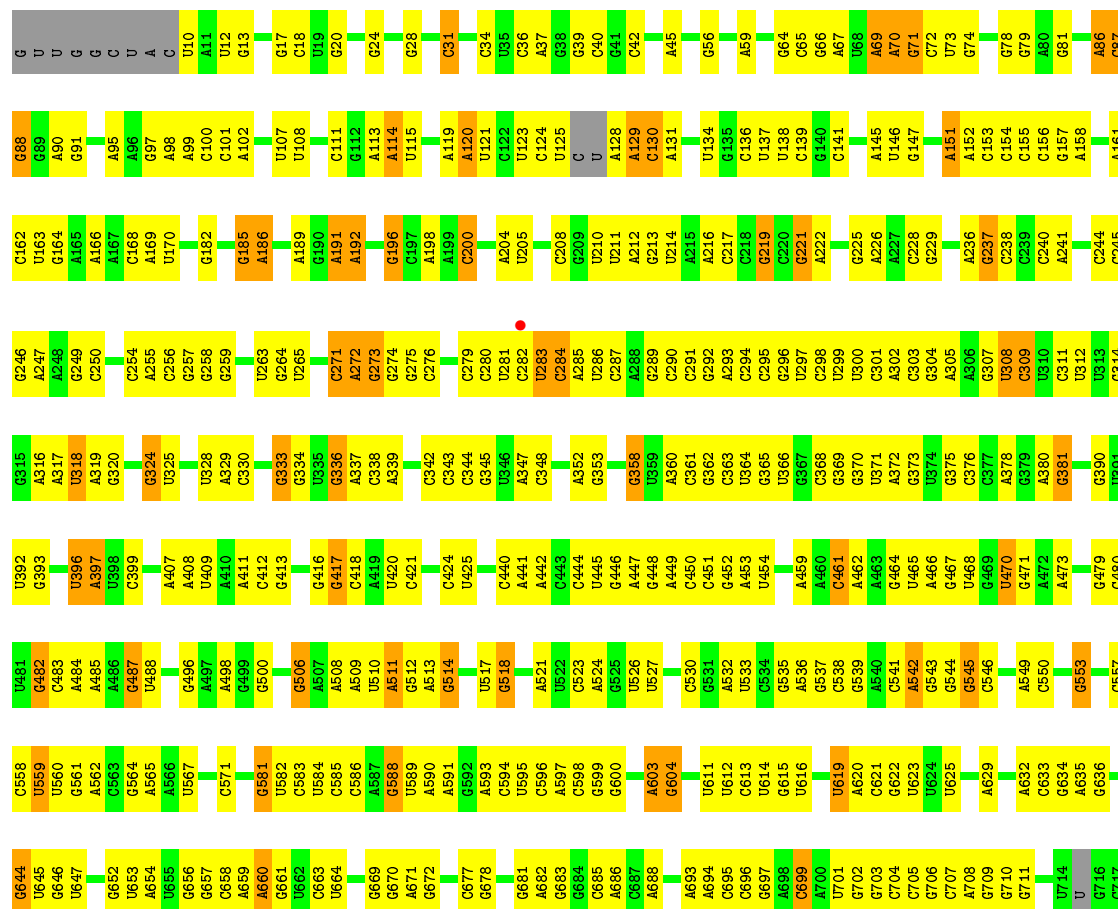
- Molecule 28: 50S ribosomal protein L39e



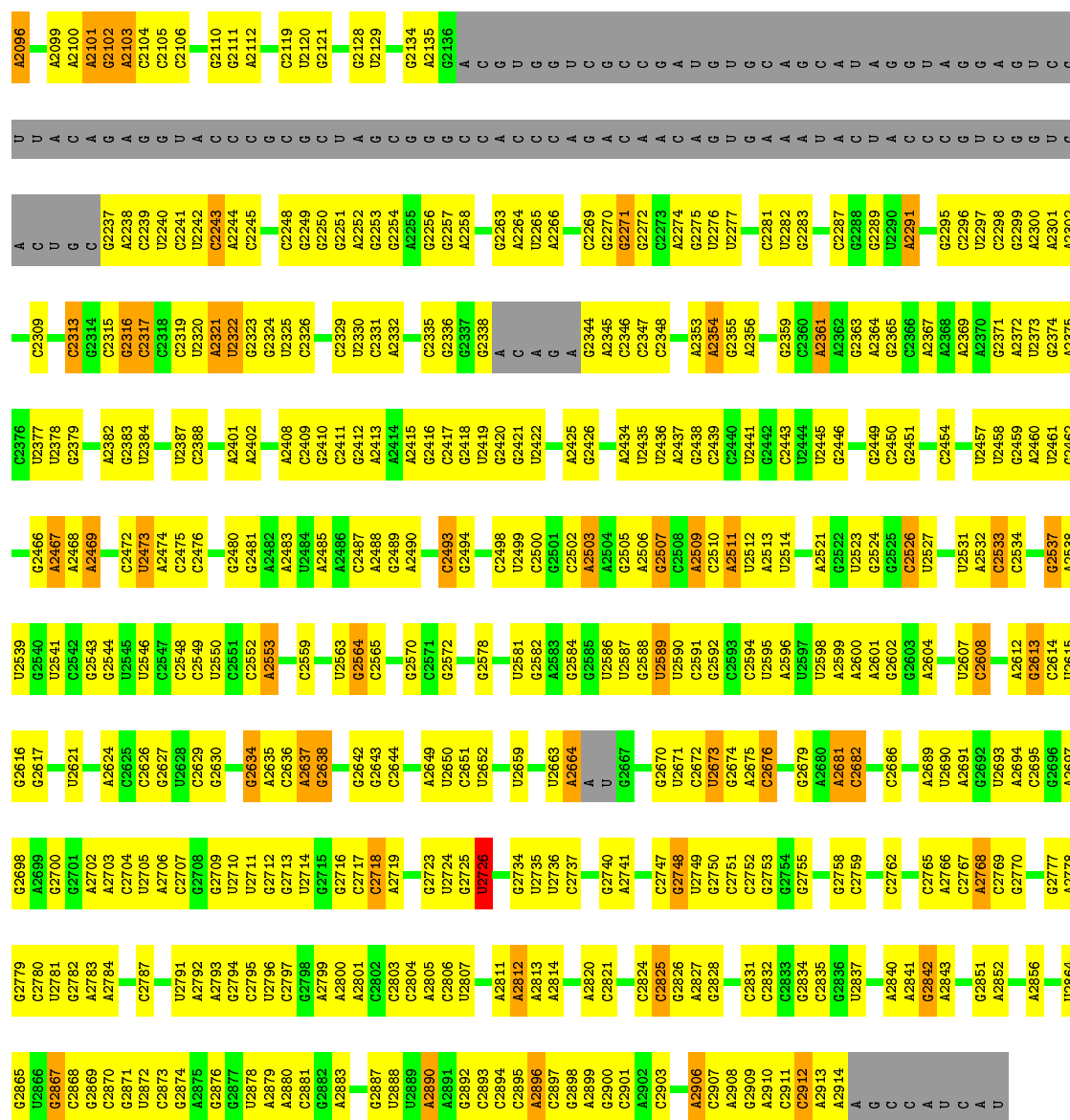
- Molecule 29: 50S ribosomal protein L44E



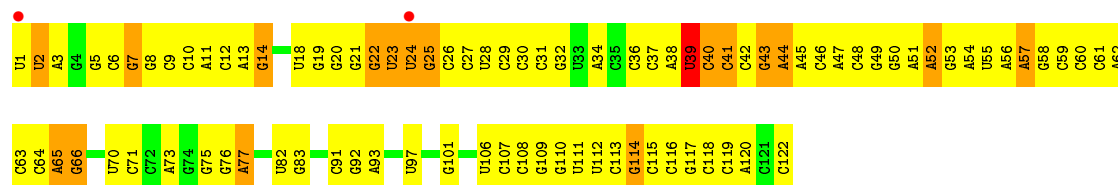
- Molecule 30: 23S RIBOSOMAL RNA







• Molecule 31: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.24Å 299.19Å 575.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 85.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 91.7 (85.59-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.179 , 0.238 0.177 , 0.229	Depositor DCC
$R_{free}$ test set	3430 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.8	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	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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, SR, 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	A	0.34	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.39	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.57	0/1498
5	E	0.34	0/1382	0.56	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.32	0/241	0.47	0/324
8	H	0.33	0/1302	0.62	0/1743
9	I	0.32	0/526	0.54	0/716
10	J	0.39	0/1136	0.61	0/1530
11	K	0.37	0/1004	0.66	0/1351
12	L	0.34	0/1130	0.61	0/1509
13	M	0.40	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.61	0/1999
15	O	0.37	0/874	0.62	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.64	0/1005
18	R	1.27	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.36	0/648	0.59	0/875
20	T	0.34	0/958	0.66	0/1289
21	U	0.45	0/417	0.60	0/562
22	V	0.34	0/502	0.53	0/675
23	W	0.38	0/1219	0.65	0/1655
24	X	0.36	0/664	0.61	0/895
25	Y	0.38	0/1146	0.62	0/1536
26	Z	0.43	0/584	0.63	0/781
27	1	0.47	0/438	0.64	0/578
28	2	0.36	0/401	0.61	0/529
29	3	0.46	0/771	0.60	0/1024
30	0	0.42	0/65956	0.68	7/102865 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.42	7/98700 (0.0%)	0.67	14/147584 (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
18	R	1	0
23	W	0	1
30	0	0	34
All	All	1	35

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.15	2.85	1.50
18	R	150	PRO	CA-C	-18.51	1.15	1.52
18	R	150	PRO	CG-CD	13.84	1.96	1.50
18	R	150	PRO	C-O	11.87	1.47	1.23
18	R	150	PRO	N-CA	11.57	1.67	1.47
18	R	150	PRO	N-CD	10.73	1.62	1.47
18	R	150	PRO	CA-CB	7.84	1.69	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.43	55.92	112.00
18	R	150	PRO	N-CA-C	-19.45	61.53	112.10
18	R	150	PRO	CA-N-CD	12.27	128.88	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.27	100.34	120.20
18	R	150	PRO	CA-CB-CG	-6.08	92.45	104.00
30	0	871	G	C5'-C4'-O4'	-5.70	102.26	109.10
30	0	1504	A	C1'-O4'-C4'	-5.64	105.39	109.90
30	0	1942	A	C5'-C4'-C3'	5.59	124.94	116.00
30	0	1971	G	N9-C1'-C2'	5.38	121.00	114.00
30	0	1819	G	C5'-C4'-C3'	5.29	124.46	116.00
30	0	2726	U	N1-C1'-C2'	5.20	120.75	114.00
30	0	2313	C	O4'-C4'-C3'	-5.12	98.88	104.00
31	9	39	U	N1-C1'-C2'	5.09	120.62	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1236	A	Sidechain
30	0	1260	G	Sidechain
30	0	1430	G	Sidechain
30	0	1524	U	Sidechain
30	0	1599	U	Sidechain
30	0	1736	A	Sidechain
30	0	1741	U	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1878	G	Sidechain
30	0	196	G	Sidechain
30	0	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2316	G	Sidechain
30	0	2473	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2552	C	Sidechain
30	0	2599	A	Sidechain
30	0	2630	G	Sidechain
30	0	2673	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	324	G	Sidechain
30	0	333	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	506	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	85	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	63	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	39	0
6	F	890	0	843	19	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	14	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	34	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	95	0
14	N	1445	0	1401	73	0
15	O	865	0	873	22	0
16	P	1136	0	1123	34	0
17	Q	735	0	729	28	0
18	R	1149	0	1122	41	0
19	S	641	0	605	15	0
20	T	950	0	924	36	0
21	U	410	0	368	26	0
22	V	499	0	511	21	0
23	W	1196	0	1137	58	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	39	0
26	Z	573	0	535	50	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	732	57	0
30	0	59019	0	29809	1661	0
31	9	2599	0	1325	127	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	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	10	0	0	3	0
33	3	1	0	0	1	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	2	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	L	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5904	0	0	251	0
38	1	59	0	0	3	0
38	2	43	0	0	2	0
38	3	70	0	0	3	0
38	9	149	0	0	10	0
38	A	119	0	0	7	0
38	B	152	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	185	0	0	18	0
38	D	42	0	0	4	0
38	E	43	0	0	1	0
38	F	26	0	0	1	0
38	G	19	0	0	1	0
38	H	65	0	0	4	0
38	I	8	0	0	1	0
38	J	53	0	0	1	0
38	K	58	0	0	3	0
38	L	85	0	0	9	0
38	M	127	0	0	13	0
38	N	59	0	0	2	0
38	O	39	0	0	2	0
38	P	67	0	0	3	0
38	Q	48	0	0	1	0
38	R	77	0	0	2	0
38	S	30	0	0	2	0
38	T	36	0	0	3	0
38	U	28	0	0	4	0
38	V	13	0	0	2	0
38	W	67	0	0	3	0
38	X	21	0	0	2	0
38	Y	100	0	0	5	0
38	Z	31	0	0	7	0
All	All	99121	0	59922	2675	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 18.

All (2675) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.41
30:0:871:G:C8	30:0:871:G:H5'	1.77	1.19
10:J:82:THR:HG23	30:0:1242:A:H5'	1.23	1.16
30:0:1165:G:H1'	30:0:1174:A:H1'	1.17	1.14
31:9:56:A:H2'	31:9:57:A:H5''	1.19	1.13
30:0:1559:A:H1'	38:0:5849:HOH:O	1.45	1.13
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.13
31:9:29:C:H2'	31:9:30:C:H5'	1.32	1.10
15:O:3:THR:HG22	30:0:656:G:H5'	1.19	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ARG:HD3	30:0:156:C:H5''	1.28	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.80	1.09
30:0:871:G:H8	30:0:871:G:H5'	0.99	1.08
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.17	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.69	1.07
31:9:76:G:H3'	31:9:77:A:H5''	1.33	1.05
30:0:545:G:H8	30:0:545:G:H5'	1.22	1.05
14:N:37:ARG:NH1	31:9:6:C:H5''	1.71	1.03
30:0:1603:A:H5'	30:0:1605:G:O4'	1.60	1.02
30:0:1641:A:H2'	30:0:1642:A:H5'	1.44	0.99
21:U:56:ARG:HD2	30:0:2890:A:C8	1.98	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.63	0.98
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.43	0.98
11:K:10:GLN:H	11:K:10:GLN:HE21	0.99	0.97
30:0:1979:G:H2'	38:0:9283:HOH:O	1.65	0.97
30:0:381:G:H5''	38:0:4317:HOH:O	1.64	0.96
30:0:871:G:H8	30:0:871:G:C5'	1.78	0.96
30:0:1165:G:H21	30:0:1173:A:H5''	1.30	0.96
13:M:70:GLY:HA3	13:M:73:ARG:NH2	1.80	0.96
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.47	0.96
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.05	0.95
31:9:56:A:C2'	31:9:57:A:H5''	1.95	0.95
30:0:1474:C:H6	30:0:1474:C:H5'	1.30	0.95
31:9:14:G:H5'	31:9:14:G:H8	1.32	0.94
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.50	0.94
30:0:236:A:H4'	30:0:237:G:H5'	1.49	0.94
2:B:264:GLU:HG2	2:B:267:LYS:HE3	1.50	0.94
30:0:1165:G:H21	30:0:1173:A:C5'	1.81	0.93
16:P:115:SER:H	16:P:118:GLN:HE21	1.11	0.93
30:0:2505:G:H2'	30:0:2506:A:H5'	1.50	0.93
30:0:2717:C:C2'	30:0:2718:C:H5''	1.99	0.93
30:0:2502:C:H2'	30:0:2503:A:H5'	1.52	0.92
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.35	0.92
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.52	0.91
3:C:27:ARG:HG2	3:C:27:ARG:HH11	1.36	0.91
30:0:2321:A:H2	30:0:2378:U:H3	1.14	0.91
15:O:3:THR:CG2	30:0:656:G:H5'	2.00	0.91
30:0:2710:U:H1'	38:0:7613:HOH:O	1.71	0.90
30:0:282:C:O2'	30:0:283:U:H5'	1.71	0.90
30:0:1118:A:H62	30:0:1244:U:H3	1.14	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:236:THR:HG22	3:C:239:ALA:H	1.35	0.90
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.90
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.53	0.90
30:0:2812:A:H2	30:0:2814:A:H62	1.19	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.54	0.90
30:0:545:G:C8	30:0:545:G:H5'	2.06	0.89
30:0:2321:A:H8	30:0:2322:U:HO2'	1.13	0.89
30:0:2502:C:C2'	30:0:2503:A:H5'	2.03	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.88
33:Y:8820:CL:CL	38:0:4953:HOH:O	2.27	0.88
30:0:1119:G:H22	30:0:1246:A:H2	1.16	0.88
30:0:2700:G:H3'	38:0:3569:HOH:O	1.73	0.88
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.88
31:9:92:G:H2'	31:9:93:A:C8	2.07	0.88
13:M:79:ALA:HB3	13:M:81:ARG:HH12	1.38	0.88
30:0:1118:A:H3'	30:0:1118:A:C8	2.08	0.88
30:0:1206:U:H6	30:0:1206:U:H5'	1.39	0.88
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.35	0.88
30:0:506:G:H22	30:0:509:A:C5'	1.85	0.87
30:0:1474:C:C6	30:0:1474:C:H5'	2.10	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.73	0.87
30:0:542:A:H5'	30:0:542:A:H8	1.39	0.87
30:0:1118:A:H3'	30:0:1118:A:H8	1.39	0.87
30:0:2321:A:H4'	30:0:2322:U:OP1	1.73	0.87
30:0:363:C:H1'	38:0:5273:HOH:O	1.75	0.86
30:0:1278:A:H4'	30:0:1279:U:C4	2.10	0.86
30:0:2505:G:C2'	30:0:2506:A:H5'	2.04	0.86
1:A:70:ALA:HB1	26:Z:89:THR:HG21	1.57	0.86
30:0:1701:A:H4'	30:0:1702:U:H5''	1.55	0.86
13:M:70:GLY:HA2	30:0:2263:G:H4'	1.59	0.85
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.58	0.85
30:0:506:G:H22	30:0:509:A:H5''	1.42	0.85
30:0:1205:U:H2'	30:0:1206:U:H5'	1.58	0.85
30:0:1641:A:C2'	30:0:1642:A:H5'	2.06	0.85
26:Z:70:ARG:NH1	26:Z:83:TYR:HB2	1.91	0.85
30:0:2717:C:H2'	30:0:2718:C:H5''	1.59	0.85
30:0:1666:C:H2'	30:0:1667:A:H5'	1.58	0.84
30:0:2717:C:O2'	30:0:2718:C:H5''	1.76	0.84
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.60	0.84
30:0:2637:A:H4'	38:0:4923:HOH:O	1.78	0.83
30:0:2043:U:H3'	38:0:6696:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.58	0.83
23:W:125:HIS:NE2	30:0:1097:A:H5''	1.93	0.83
30:0:2010:A:H2'	38:0:5942:HOH:O	1.77	0.83
1:A:167:LYS:HE2	26:Z:50:VAL:HG13	1.61	0.83
30:0:380:A:H2'	38:0:7216:HOH:O	1.77	0.83
29:3:64:LYS:HA	29:3:84:ARG:HA	1.57	0.83
13:M:68:ARG:NH2	13:M:73:ARG:HD3	1.94	0.83
11:K:10:GLN:H	11:K:10:GLN:NE2	1.77	0.83
11:K:39:GLY:HA2	38:0:5215:HOH:O	1.76	0.83
30:0:2454:C:H5''	38:0:7719:HOH:O	1.79	0.82
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.61	0.82
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:1667:A:H8	30:0:1667:A:H5'	1.44	0.82
13:M:27:ARG:HH22	13:M:44:THR:HG23	1.44	0.82
30:0:541:C:C2'	30:0:542:A:H5''	2.09	0.82
30:0:541:C:H2'	30:0:542:A:C5'	2.08	0.82
30:0:1300:G:H1'	38:0:4678:HOH:O	1.80	0.81
29:3:31:THR:O	30:0:1923:G:H4'	1.79	0.81
30:0:1184:C:H1'	38:0:7461:HOH:O	1.80	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.81
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.62	0.81
30:0:2769:C:O2'	30:0:2770:G:H5'	1.81	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.80	0.81
30:0:559:U:H5'	30:0:559:U:H6	1.45	0.81
31:9:29:C:C2'	31:9:30:C:H5'	2.08	0.81
3:C:139:VAL:HG13	38:C:8658:HOH:O	1.79	0.81
30:0:1174:A:C6	30:0:1201:C:H4'	2.14	0.81
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.25	0.81
18:R:39:THR:HG22	18:R:42:GLU:H	1.46	0.81
30:0:1205:U:H2'	30:0:1206:U:C5'	2.10	0.81
30:0:1119:G:N2	30:0:1246:A:C2	2.47	0.81
30:0:681:G:H5'	30:0:681:G:N3	1.96	0.81
30:0:1641:A:H2'	30:0:1642:A:C5'	2.09	0.81
30:0:1801:A:H3'	38:0:7607:HOH:O	1.81	0.80
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.47	0.80
30:0:2748:G:H2'	38:0:7534:HOH:O	1.81	0.80
30:0:1593:C:H1'	38:0:6089:HOH:O	1.80	0.80
28:2:41:HIS:H	28:2:45:ASN:HD22	1.27	0.80
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.96	0.80
15:O:3:THR:HG22	30:0:656:G:C5'	2.09	0.80
25:Y:115:ARG:NH2	30:0:1266:U:H4'	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2783:A:H3'	38:0:5225:HOH:O	1.81	0.80
31:9:39:U:H1'	31:9:44:A:H61	1.45	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.80
31:9:14:G:H5'	31:9:14:G:C8	2.16	0.80
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.63	0.80
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.62	0.80
30:0:586:C:H5''	38:0:7275:HOH:O	1.81	0.80
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.63	0.79
13:M:27:ARG:NH2	13:M:44:THR:HG23	1.96	0.79
6:F:91:VAL:HG12	6:F:92:GLY:H	1.46	0.79
38:N:8842:HOH:O	31:9:49:G:H5''	1.83	0.79
10:J:82:THR:CG2	30:0:1242:A:H5'	2.09	0.79
30:0:2419:U:H5''	30:0:2420:G:H5'	1.65	0.79
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.79
30:0:1183:C:H2'	38:0:6224:HOH:O	1.82	0.79
30:0:255:A:H2'	30:0:256:C:H6	1.48	0.79
3:C:1:MET:HG2	3:C:2:GLN:H	1.47	0.78
30:0:2635:A:O2'	30:0:2636:C:H5'	1.82	0.78
30:0:308:U:H5'	30:0:309:C:OP1	1.82	0.78
30:0:659:A:H5''	38:0:7089:HOH:O	1.83	0.78
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.48	0.78
30:0:123:U:H5'	38:0:6637:HOH:O	1.82	0.78
30:0:1372:A:H3'	38:0:7180:HOH:O	1.81	0.78
30:0:2485:A:H3'	38:0:5838:HOH:O	1.82	0.78
4:D:154:LYS:HD2	4:D:154:LYS:H	1.48	0.78
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.31	0.78
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.66	0.78
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.80	0.78
30:0:960:G:H4'	38:0:7423:HOH:O	1.83	0.78
30:0:1595:G:O2'	30:0:1596:U:H5'	1.84	0.78
30:0:2291:A:C8	30:0:2309:C:H5'	2.19	0.78
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.82	0.78
30:0:2469:A:H1'	38:0:3229:HOH:O	1.83	0.77
30:0:541:C:H2'	30:0:542:A:H5''	1.65	0.77
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.77
30:0:1189:A:H3'	38:0:7669:HOH:O	1.83	0.77
30:0:2420:G:O2'	30:0:2421:G:H5'	1.85	0.77
30:0:1116:U:H3	30:0:1246:A:H62	1.33	0.77
30:0:558:C:C2'	30:0:559:U:H5''	2.14	0.77
30:0:564:G:H1'	38:0:6295:HOH:O	1.84	0.77
30:0:2769:C:C2'	30:0:2770:G:H5'	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:O2'	30:0:559:U:H5''	1.85	0.77
30:0:1632:A:H2'	30:0:1633:C:H5'	1.67	0.76
30:0:1973:A:H5'	30:0:1973:A:H8	1.48	0.76
30:0:2703:A:H2'	30:0:2704:C:H6	1.50	0.76
30:0:283:U:H5	30:0:284:C:C4	2.02	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
31:9:1:U:H4'	31:9:3:A:OP1	1.84	0.76
30:0:2468:A:H3'	38:0:5449:HOH:O	1.84	0.76
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.33	0.76
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.68	0.76
30:0:2506:A:O2'	30:0:2507:G:H8	1.68	0.76
38:C:8633:HOH:O	30:0:338:C:H5''	1.86	0.76
30:0:969:G:H1	30:0:999:C:H42	1.34	0.76
13:M:71:SER:HB3	30:0:2264:A:OP1	1.85	0.75
30:0:899:C:H5'	38:0:3190:HOH:O	1.85	0.75
4:D:105:SER:OG	30:0:2338:G:H1'	1.85	0.75
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.66	0.75
30:0:2505:G:H2'	30:0:2506:A:C5'	2.17	0.75
30:0:282:C:H1'	30:0:368:C:N4	2.01	0.75
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.52	0.75
30:0:1170:U:H2'	30:0:1172:G:OP2	1.87	0.75
30:0:2908:A:H2'	30:0:2909:G:O4'	1.87	0.74
26:Z:70:ARG:HB2	26:Z:70:ARG:HH11	1.51	0.74
30:0:1741:U:O2'	30:0:2723:G:H4'	1.87	0.74
30:0:544:G:H2'	30:0:545:G:H5''	1.68	0.74
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.52	0.74
3:C:218:VAL:HG12	38:C:8637:HOH:O	1.87	0.74
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.52	0.74
30:0:1834:C:H2'	30:0:1840:A:N6	2.02	0.74
33:0:8813:CL:CL	38:0:4678:HOH:O	2.43	0.74
30:0:2781:U:C2'	30:0:2782:G:H5'	2.18	0.74
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.69	0.74
30:0:2793:A:H1'	38:0:6312:HOH:O	1.88	0.74
14:N:11:ARG:HD3	31:9:114:G:O6	1.88	0.74
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.92	0.73
3:C:140:VAL:HB	38:C:8660:HOH:O	1.86	0.73
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.70	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.36	0.73
30:0:1525:G:H5'	30:0:1526:A:OP2	1.89	0.73
30:0:2578:G:H5'	30:0:2578:G:H8	1.52	0.73
31:9:92:G:H2'	31:9:93:A:H8	1.50	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.52	0.73
21:U:56:ARG:HH11	21:U:56:ARG:HG3	1.54	0.73
30:0:2748:G:H1'	38:0:7889:HOH:O	1.88	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.70	0.73
30:0:1279:U:O2	30:0:1279:U:H2'	1.89	0.72
30:0:2768:A:O2'	30:0:2769:C:H5'	1.89	0.72
30:0:619:U:H3'	38:0:3270:HOH:O	1.88	0.72
30:0:2524:G:H21	30:0:2526:C:N4	1.85	0.72
30:0:2871:G:H2'	30:0:2872:U:H6	1.54	0.72
14:N:37:ARG:HH12	31:9:6:C:H5''	1.55	0.72
30:0:271:C:H41	30:0:378:A:H2	1.33	0.72
30:0:558:C:H2'	30:0:559:U:C5'	2.20	0.72
30:0:1921:A:O2'	30:0:1922:A:H5'	1.89	0.72
30:0:2766:A:H5'	38:0:9565:HOH:O	1.88	0.72
2:B:179:LEU:O	2:B:183:GLU:HG2	1.89	0.72
30:0:1166:A:P	30:0:1174:A:H4'	2.29	0.72
31:9:29:C:H2'	31:9:30:C:C5'	2.17	0.72
30:0:2533:C:H5'	30:0:2533:C:H6	1.53	0.72
30:0:877:G:H5'	30:0:878:G:OP1	1.89	0.72
30:0:2712:G:H5'	38:0:5215:HOH:O	1.90	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.20	0.72
30:0:836:G:H5''	38:0:9285:HOH:O	1.89	0.72
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.70	0.72
13:M:79:ALA:H	13:M:81:ARG:HH22	1.37	0.72
29:3:2:GLN:O	30:0:2320:U:H2'	1.90	0.71
31:9:54:A:O2'	31:9:55:U:H5'	1.89	0.71
2:B:145:HIS:HD2	2:B:146:THR:O	1.73	0.71
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.24	0.71
14:N:159:TYR:HE1	31:9:50:G:H5''	1.55	0.71
30:0:281:U:H2'	30:0:282:C:O4'	1.90	0.71
30:0:702:G:O2'	30:0:703:G:H5'	1.90	0.71
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.72	0.71
30:0:2534:C:H1'	38:0:3477:HOH:O	1.91	0.71
30:0:821:U:H3'	38:0:3759:HOH:O	1.90	0.71
30:0:2426:G:H1'	38:0:6075:HOH:O	1.90	0.71
30:0:1165:G:N2	30:0:1173:A:C5'	2.53	0.71
30:0:221:G:H5''	38:0:5725:HOH:O	1.90	0.71
38:I:6825:HOH:O	30:0:1166:A:H2	1.73	0.71
30:0:1835:U:C5	30:0:1840:A:N7	2.57	0.71
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.55	0.71
30:0:1132:A:N6	30:0:1229:C:H2'	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1589:G:N2	30:0:1605:G:H1'	2.05	0.71
30:0:1979:G:H3'	38:0:3282:HOH:O	1.88	0.71
14:N:5:ARG:HB2	14:N:5:ARG:HH11	1.56	0.71
30:0:2487:C:H5	38:0:4880:HOH:O	1.73	0.70
30:0:2514:U:OP1	30:0:2572:G:H1'	1.90	0.70
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.56	0.70
30:0:2505:G:O2'	30:0:2506:A:H5'	1.90	0.70
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.55	0.70
30:0:1666:C:H2'	30:0:1667:A:C5'	2.21	0.70
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.20	0.70
26:Z:70:ARG:HH12	26:Z:83:TYR:HB2	1.55	0.70
17:Q:11:ARG:NH2	30:0:2297:U:H4'	2.07	0.70
30:0:1189:A:H1'	30:0:1209:C:C1'	2.21	0.70
30:0:1209:C:H2'	30:0:1210:G:H8	1.57	0.70
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.06	0.70
30:0:2237:G:H1'	30:0:2238:A:C8	2.27	0.70
13:M:188:ARG:HD3	30:0:155:C:OP2	1.92	0.70
26:Z:80:GLN:HG3	26:Z:81:CYS:H	1.56	0.70
30:0:31:C:H2'	38:0:7677:HOH:O	1.90	0.70
38:Q:6286:HOH:O	30:0:1019:C:H5'	1.91	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.27	0.69
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.07	0.69
30:0:138:U:H5''	30:0:139:C:OP2	1.93	0.69
30:0:1451:C:H5'	30:0:1505:U:C5	2.27	0.69
30:0:1562:C:O2	30:0:1562:C:H2'	1.91	0.69
30:0:42:C:H3'	38:0:4166:HOH:O	1.92	0.69
2:B:36:PRO:HG3	2:B:169:GLY:H	1.57	0.69
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.57	0.69
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.74	0.69
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.55	0.69
14:N:49:THR:HB	14:N:58:LEU:HD11	1.74	0.69
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.69
30:0:2102:G:H4'	38:0:5631:HOH:O	1.92	0.69
30:0:2102:G:N2	30:0:2103:A:N1	2.40	0.69
30:0:2871:G:H2'	30:0:2872:U:C6	2.28	0.69
30:0:287:C:H42	30:0:365:G:H1	1.41	0.69
30:0:407:A:H2'	30:0:408:A:C8	2.28	0.69
30:0:961:A:H4'	38:0:6759:HOH:O	1.91	0.69
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.72	0.69
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.06	0.69
14:N:141:ARG:HH21	31:9:48:C:H4'	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.75	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.69
31:9:39:U:H3'	31:9:40:C:H5''	1.75	0.69
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.75	0.69
30:0:2511:A:H2'	30:0:2512:U:O4'	1.93	0.69
30:0:2781:U:H2'	30:0:2782:G:H5'	1.73	0.69
2:B:18:ARG:HE	2:B:256:GLN:HE21	1.41	0.69
30:0:1589:G:H22	30:0:1605:G:H1'	1.55	0.69
30:0:969:G:H1	30:0:999:C:N4	1.91	0.69
13:M:68:ARG:HD3	13:M:68:ARG:O	1.93	0.69
30:0:317:A:H5'	38:0:3761:HOH:O	1.91	0.68
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.59	0.68
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.92	0.68
22:V:50:ARG:HH12	30:0:56:G:H5''	1.58	0.68
30:0:1474:C:C5'	30:0:1474:C:H6	2.06	0.68
30:0:2781:U:O2'	30:0:2782:G:H5'	1.93	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.22	0.68
14:N:40:ASN:ND2	31:9:28:U:H5''	2.08	0.68
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.87	0.68
30:0:962:C:H2'	30:0:963:C:H5'	1.74	0.68
29:3:59:ASP:HA	30:0:2460:A:H5''	1.74	0.68
2:B:254:GLN:HG3	38:0:9697:HOH:O	1.92	0.68
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.75	0.68
30:0:255:A:H2'	30:0:256:C:C6	2.29	0.68
30:0:390:G:H5'	38:0:7539:HOH:O	1.94	0.68
28:2:35:ARG:HB2	38:2:2691:HOH:O	1.92	0.68
10:J:131:THR:HB	10:J:134:GLU:HG3	1.75	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.28	0.68
30:0:1634:G:H2'	30:0:1635:U:H6	1.57	0.68
30:0:1702:U:H1'	38:0:5758:HOH:O	1.93	0.68
30:0:283:U:H5	30:0:284:C:N3	1.91	0.68
12:L:6:ARG:HD3	30:0:1299:G:O6	1.94	0.68
13:M:171:ARG:CD	30:0:156:C:H5''	2.15	0.68
30:0:2374:G:H2'	30:0:2375:A:C8	2.29	0.68
30:0:440:C:H2'	30:0:441:A:C8	2.29	0.68
13:M:83:SER:HA	38:M:8877:HOH:O	1.94	0.68
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.91	0.68
26:Z:70:ARG:HB3	38:Z:8728:HOH:O	1.93	0.68
30:0:1666:C:C2'	30:0:1667:A:H5''	2.23	0.67
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.93	0.67
2:B:264:GLU:CG	2:B:267:LYS:HE3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1158:G:C2'	30:0:1159:G:H5'	2.24	0.67
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.75	0.67
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.08	0.67
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.31	0.67
30:0:1634:G:H2'	30:0:1635:U:C6	2.29	0.67
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.76	0.67
31:9:24:U:H3'	31:9:25:G:H5'	1.75	0.67
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.74	0.67
30:0:283:U:C5	30:0:284:C:C4	2.83	0.67
20:T:2:LYS:HG2	30:0:447:A:OP1	1.95	0.67
30:0:1632:A:C2'	30:0:1633:C:H5'	2.24	0.67
30:0:1762:C:O2'	30:0:1763:C:H5'	1.95	0.67
30:0:735:C:C5	30:0:736:A:C4	2.82	0.67
31:9:91:C:H1'	38:9:9143:HOH:O	1.95	0.67
30:0:1268:C:H2'	30:0:1269:G:H8	1.59	0.67
30:0:541:C:H2'	30:0:542:A:H5'	1.75	0.67
30:0:221:G:H2'	30:0:222:A:C8	2.30	0.67
30:0:603:A:H5''	30:0:604:G:OP1	1.94	0.67
1:A:72:GLU:HG2	26:Z:100:GLY:HA3	1.76	0.67
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.95	0.67
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.67
9:I:96:SER:H	9:I:99:GLN:NE2	1.93	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.77	0.66
30:0:2073:G:OP2	30:0:2490:A:H5'	1.95	0.66
30:0:506:G:H22	30:0:509:A:H5'	1.60	0.66
30:0:613:C:H2'	30:0:614:U:H6	1.61	0.66
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.78	0.66
23:W:44:MET:CE	30:0:944:G:H21	2.09	0.66
30:0:2488:A:C2	38:0:7265:HOH:O	2.48	0.66
30:0:451:C:O2'	30:0:452:G:H5'	1.95	0.66
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.77	0.66
30:0:1158:G:O2'	30:0:1159:G:H5'	1.96	0.66
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.76	0.66
30:0:849:C:H1'	38:0:6602:HOH:O	1.95	0.66
31:9:55:U:H4'	31:9:56:A:C8	2.31	0.66
22:V:50:ARG:NH1	30:0:56:G:H5''	2.10	0.66
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.96	0.66
30:0:2461:U:O2	30:0:2466:G:H1'	1.96	0.66
30:0:2321:A:C2	30:0:2378:U:N3	2.57	0.66
30:0:735:C:H2'	30:0:736:A:O4'	1.96	0.66
30:0:558:C:H2'	30:0:559:U:H5'	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.61	0.66
9:I:87:PRO:HD2	30:0:1180:U:H1'	1.77	0.66
9:I:110:ASP:O	30:0:1163:G:H5'	1.96	0.65
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.10	0.65
3:C:233:THR:HG22	3:C:234:VAL:H	1.61	0.65
4:D:103:ASN:HD22	4:D:133:ASN:HA	1.60	0.65
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.11	0.65
21:U:56:ARG:NE	30:0:2890:A:H1'	2.11	0.65
30:0:567:U:H5''	38:0:5280:HOH:O	1.97	0.65
30:0:635:A:H2'	30:0:636:G:H5''	1.77	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
30:0:1940:C:H1'	38:0:9376:HOH:O	1.96	0.65
30:0:1950:G:H2'	30:0:1951:G:C8	2.32	0.65
30:0:1925:G:O2'	30:0:1926:G:H5'	1.96	0.65
30:0:625:U:H5''	30:0:1044:C:N4	2.11	0.65
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.27	0.65
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.97	0.65
30:0:2869:G:H2'	30:0:2870:C:C6	2.31	0.65
30:0:1165:G:H1'	30:0:1174:A:C1'	2.11	0.65
14:N:144:GLY:O	14:N:147:ILE:HG22	1.97	0.65
22:V:39:ALA:N	22:V:40:PRO:HD2	2.12	0.65
30:0:1972:U:H2'	30:0:1973:A:C5'	2.27	0.65
30:0:2458:U:H3'	38:0:3239:HOH:O	1.96	0.64
17:Q:19:ARG:HH21	31:9:11:A:P	2.19	0.64
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.78	0.64
30:0:1165:G:H21	30:0:1173:A:H5'	1.63	0.64
30:0:128:A:O2'	30:0:129:A:H5'	1.97	0.64
30:0:2672:C:O2'	30:0:2673:U:H5'	1.97	0.64
30:0:2896:A:H5''	38:0:6082:HOH:O	1.96	0.64
30:0:583:C:H2'	30:0:584:U:H6	1.62	0.64
30:0:125:U:H2'	38:0:3755:HOH:O	1.97	0.64
30:0:369:G:O2'	30:0:370:G:H5'	1.98	0.64
30:0:660:A:H4'	30:0:661:G:O5'	1.98	0.64
30:0:69:A:H5'	30:0:69:A:C8	2.32	0.64
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.79	0.64
30:0:200:C:H2'	38:0:3428:HOH:O	1.96	0.64
30:0:2488:A:H2	38:0:7265:HOH:O	1.81	0.64
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.79	0.64
30:0:1167:G:H2'	30:0:1168:C:O4'	1.98	0.64
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.79	0.64
13:M:70:GLY:CA	30:0:2263:G:H4'	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:36:C:H5'	38:9:9047:HOH:O	1.98	0.64
30:0:285:A:H2'	30:0:286:U:O4'	1.97	0.64
30:0:1119:G:N2	30:0:1246:A:H2	1.89	0.64
30:0:2781:U:H2'	30:0:2782:G:C5'	2.27	0.64
30:0:1181:A:H2'	30:0:1182:C:H5'	1.78	0.64
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.64
31:9:5:G:O2'	31:9:6:C:H5'	1.97	0.64
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.12	0.64
30:0:1213:C:O2'	30:0:1214:G:H5'	1.98	0.64
18:R:132:ARG:HH21	30:0:2055:A:H4'	1.61	0.64
30:0:2436:U:H2'	30:0:2437:A:C8	2.33	0.64
30:0:2878:U:H5''	38:0:4165:HOH:O	1.98	0.64
30:0:2887:G:H2'	30:0:2888:U:C6	2.32	0.64
30:0:2377:U:O2'	30:0:2378:U:H5'	1.98	0.63
30:0:2613:G:O2'	30:0:2614:C:H5'	1.99	0.63
31:9:24:U:H3'	31:9:25:G:C5'	2.28	0.63
12:L:143:THR:HG22	12:L:144:ASP:H	1.62	0.63
30:0:2281:C:C2'	30:0:2282:U:H5'	2.28	0.63
30:0:2831:C:C2'	30:0:2832:C:H5'	2.28	0.63
30:0:585:C:H5''	38:0:4864:HOH:O	1.98	0.63
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.81	0.63
14:N:141:ARG:NH2	31:9:48:C:H4'	2.13	0.63
21:U:4:ARG:O	21:U:13:ILE:HG22	1.98	0.63
30:0:1170:U:H1'	30:0:1172:G:N7	2.13	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.97	0.63
30:0:2869:G:H5'	38:0:5487:HOH:O	1.97	0.63
13:M:99:ARG:HE	13:M:170:ASN:ND2	1.96	0.63
30:0:1204:C:H1'	38:0:4741:HOH:O	1.98	0.63
30:0:1268:C:H2'	30:0:1269:G:C8	2.34	0.63
30:0:1904:A:C2	30:0:1905:U:H1'	2.34	0.63
30:0:2336:G:H2'	38:0:6280:HOH:O	1.98	0.63
30:0:2868:C:H1'	38:0:7114:HOH:O	1.97	0.63
13:M:81:ARG:HB3	13:M:85:ARG:HB2	1.80	0.63
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.79	0.63
30:0:820:G:H5'	30:0:821:U:H5'	1.80	0.63
29:3:55:VAL:HB	29:3:56:PRO:HD2	1.81	0.63
3:C:174:ILE:CD1	30:0:338:C:H4'	2.29	0.63
30:0:1528:A:H2'	30:0:1529:G:O4'	1.98	0.63
30:0:2321:A:H8	30:0:2322:U:O2'	1.80	0.63
30:0:2831:C:H2'	30:0:2832:C:H5'	1.79	0.63
30:0:424:C:H2'	30:0:425:U:H6	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1950:G:H2'	30:0:1951:G:H8	1.64	0.63
30:0:2401:A:H2'	30:0:2402:A:C8	2.34	0.63
30:0:280:C:H2'	30:0:281:U:O4'	1.99	0.63
31:9:36:C:C5	31:9:37:C:C5	2.87	0.63
31:9:2:U:OP2	31:9:3:A:H5'	1.99	0.63
4:D:25:MET:SD	4:D:40:ILE:HD11	2.39	0.63
30:0:558:C:C2'	30:0:559:U:C5'	2.77	0.62
18:R:9:ASP:O	18:R:13:THR:HB	1.99	0.62
30:0:2594:C:O2'	30:0:2595:U:H5'	1.99	0.62
30:0:2827:A:H2'	30:0:2828:G:O4'	1.99	0.62
30:0:2894:C:O2'	30:0:2895:C:H5'	1.99	0.62
30:0:834:G:H4'	30:0:835:U:OP2	1.99	0.62
2:B:238:ASN:HD22	2:B:240:GLY:H	1.45	0.62
2:B:272:ILE:HG22	38:B:9132:HOH:O	2.00	0.62
12:L:79:ASP:HB3	38:L:9022:HOH:O	1.98	0.62
13:M:179:GLY:O	30:0:399:C:H5'	1.98	0.62
18:R:39:THR:HG23	18:R:107:GLU:O	1.99	0.62
30:0:1829:A:H2'	30:0:1830:C:H5'	1.81	0.62
30:0:2505:G:C2'	30:0:2506:A:C5'	2.76	0.62
30:0:308:U:C4	30:0:342:C:H1'	2.34	0.62
11:K:66:ARG:HH22	30:0:1994:A:P	2.21	0.62
30:0:1797:A:H4'	30:0:1798:C:C5	2.33	0.62
30:0:249:G:O2'	30:0:250:C:H5'	1.99	0.62
30:0:256:C:H2'	30:0:257:G:O4'	2.00	0.62
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.82	0.62
30:0:506:G:N2	30:0:509:A:H5''	2.14	0.62
25:Y:204:ARG:HH22	30:0:553:G:P	2.22	0.62
30:0:1087:G:H4'	30:0:1088:A:OP1	2.00	0.62
30:0:1230:A:OP1	30:0:1230:A:H8	1.83	0.62
30:0:2705:U:H2'	30:0:2706:A:C8	2.35	0.62
17:Q:11:ARG:HH21	30:0:2297:U:H4'	1.62	0.62
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.81	0.62
30:0:418:C:H5	38:0:5765:HOH:O	1.82	0.62
30:0:1625:U:H5''	38:0:6005:HOH:O	2.00	0.62
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.35	0.62
30:0:2248:C:H3'	38:0:5435:HOH:O	1.98	0.62
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.48	0.62
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.11	0.62
30:0:1165:G:N2	30:0:1173:A:H5''	2.09	0.62
30:0:303:C:O2'	30:0:304:G:H5'	2.00	0.62
15:O:37:ARG:HD2	30:0:656:G:OP2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1477:C:H5'	30:0:1868:G:H5'	1.81	0.62
30:0:289:G:O2'	30:0:290:C:H5'	1.98	0.62
8:H:168:VAL:HG13	38:H:9006:HOH:O	2.00	0.62
13:M:79:ALA:H	13:M:81:ARG:NH2	1.96	0.62
31:9:110:G:C6	31:9:111:U:C5	2.88	0.61
23:W:44:MET:HE2	30:0:944:G:H21	1.63	0.61
30:0:545:G:H8	30:0:545:G:C5'	2.08	0.61
30:0:807:A:O2'	30:0:808:A:H5'	1.99	0.61
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.82	0.61
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.34	0.61
3:C:27:ARG:NH1	3:C:27:ARG:HG2	2.12	0.61
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.31	0.61
12:L:90:ARG:HA	12:L:119:THR:HB	1.82	0.61
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.82	0.61
20:T:9:LYS:HD2	38:0:3744:HOH:O	2.00	0.61
28:2:41:HIS:HE1	30:0:1439:C:H5''	1.65	0.61
30:0:1596:U:H2'	30:0:1598:A:OP2	2.00	0.61
30:0:2102:G:N2	30:0:2104:C:C2	2.69	0.61
30:0:39:G:N2	30:0:444:C:C2	2.68	0.61
31:9:107:C:O2'	31:9:108:C:H5'	2.00	0.61
30:0:1245:C:O5'	30:0:1245:C:H6	1.84	0.61
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.35	0.61
30:0:1015:C:H2'	30:0:1016:U:H6	1.64	0.61
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.00	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.84	0.61
26:Z:40:ALA:HA	30:0:1773:G:C8	2.35	0.61
30:0:2502:C:H2'	30:0:2503:A:C5'	2.29	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.12	0.61
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.61
30:0:24:G:N2	30:0:518:G:H1'	2.16	0.61
30:0:559:U:H5'	30:0:559:U:C6	2.32	0.61
29:3:60:LYS:CG	29:3:61:PRO:HD2	2.29	0.61
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.83	0.61
30:0:272:A:H5'	30:0:273:G:OP2	2.01	0.61
30:0:2766:A:O2'	30:0:2767:C:H5'	2.00	0.61
30:0:424:C:H2'	30:0:425:U:C6	2.35	0.61
30:0:735:C:H5	30:0:736:A:C4	2.18	0.61
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.16	0.61
26:Z:78:ILE:HD12	38:Z:8714:HOH:O	2.01	0.61
30:0:1015:C:H2'	30:0:1016:U:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:657:G:H2'	30:0:658:C:H6	1.64	0.61
30:0:946:C:H2'	30:0:947:U:H6	1.65	0.61
29:3:4:PRO:HA	29:3:91:GLN:HB2	1.82	0.61
30:0:1741:U:H5'	30:0:1742:A:OP1	2.01	0.60
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.49	0.60
30:0:1165:G:N2	30:0:1173:A:H5'	2.15	0.60
30:0:1972:U:H2'	30:0:1973:A:H5'	1.83	0.60
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.60
15:O:32:ARG:HD3	15:O:32:ARG:O	2.01	0.60
30:0:1181:A:C2'	30:0:1182:C:H5'	2.30	0.60
28:2:10:ARG:NH2	30:0:121:U:OP2	2.34	0.60
30:0:1603:A:C5'	30:0:1605:G:H5'	2.29	0.60
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.01	0.60
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.83	0.60
30:0:1183:C:N4	30:0:1184:C:H41	1.98	0.60
30:0:1603:A:C5'	30:0:1605:G:O4'	2.45	0.60
30:0:1622:G:H2'	30:0:1623:C:H5'	1.83	0.60
30:0:192:A:H5'	38:0:7634:HOH:O	1.99	0.60
30:0:2102:G:C8	30:0:2538:A:O4'	2.54	0.60
30:0:2281:C:H2'	30:0:2282:U:H5'	1.83	0.60
30:0:272:A:H3'	38:0:7522:HOH:O	2.00	0.60
31:9:20:G:O2'	31:9:21:G:H5'	2.02	0.60
31:9:76:G:C3'	31:9:77:A:H5''	2.21	0.60
8:H:29:SER:HA	8:H:62:HIS:HD2	1.66	0.60
30:0:851:C:O2	30:0:2022:A:H2	1.85	0.60
30:0:396:U:H3'	38:0:3920:HOH:O	2.00	0.60
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.84	0.60
10:J:107:ASN:HD22	10:J:109:TYR:H	1.48	0.60
13:M:84:LYS:HA	29:3:46:ILE:O	2.01	0.60
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.84	0.60
30:0:182:G:H5'	38:0:5152:HOH:O	2.01	0.60
30:0:2659:U:H5''	38:0:4122:HOH:O	2.02	0.60
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.60
30:0:333:G:O2'	30:0:334:G:H5'	2.01	0.60
30:0:946:C:H2'	30:0:947:U:C6	2.35	0.60
29:3:3:MET:SD	29:3:88:LEU:HD11	2.41	0.60
13:M:77:HIS:HB2	13:M:81:ARG:HH21	1.66	0.60
30:0:228:C:H2'	30:0:229:G:H5'	1.82	0.60
5:E:24:GLY:HA3	5:E:76:VAL:HB	1.82	0.60
16:P:115:SER:N	16:P:118:GLN:HE21	1.92	0.60
30:0:671:A:O2'	30:0:672:G:H2'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:90:A:H2'	30:0:91:G:O4'	2.01	0.60
30:0:2793:A:H2'	38:0:4488:HOH:O	2.02	0.60
30:0:293:A:O2'	30:0:294:C:H5'	2.02	0.60
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.84	0.60
19:S:33:SER:O	19:S:37:VAL:HG23	2.02	0.60
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.30	0.60
30:0:1183:C:H42	30:0:1184:C:H41	1.50	0.60
30:0:2769:C:H2'	30:0:2770:G:C5'	2.31	0.60
3:C:184:ARG:NH2	30:0:450:C:OP1	2.29	0.60
30:0:453:A:H5''	38:0:3254:HOH:O	2.02	0.60
26:Z:37:ARG:HB2	30:0:819:A:C4'	2.32	0.60
26:Z:53:ILE:O	26:Z:57:MET:HB2	2.02	0.60
27:1:9:GLY:HA2	30:0:1687:C:O2	2.02	0.59
1:A:35:GLY:O	1:A:36:ASP:HB3	2.02	0.59
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.83	0.59
21:U:39:ASN:HB3	38:U:3805:HOH:O	2.02	0.59
30:0:2812:A:H1'	38:0:5773:HOH:O	2.01	0.59
31:9:63:C:O2'	31:9:64:C:H5'	2.02	0.59
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.31	0.59
2:B:258:GLY:H	2:B:260:HIS:CE1	2.20	0.59
30:0:1058:A:H2'	30:0:1060:C:H5''	1.83	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.82	0.59
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.59
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.01	0.59
27:1:1:THR:HB	38:0:7134:HOH:O	2.02	0.59
14:N:159:TYR:CE1	31:9:50:G:H5''	2.37	0.59
30:0:2321:A:H2	30:0:2378:U:N3	1.92	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.02	0.59
30:0:747:G:H5'	38:0:4947:HOH:O	2.02	0.59
31:9:39:U:H1'	31:9:44:A:N6	2.15	0.59
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.32	0.59
30:0:247:A:H2'	38:0:3921:HOH:O	2.02	0.59
30:0:2498:C:O2'	30:0:2499:U:H5'	2.03	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
30:0:2689:A:H2'	30:0:2690:U:H5'	1.85	0.59
17:Q:11:ARG:NH2	30:0:2363:G:H4'	2.18	0.59
30:0:468:U:H3'	38:0:7561:HOH:O	2.03	0.59
29:3:51:LYS:HB3	30:0:219:G:O2'	2.03	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
13:M:9:ARG:HD2	30:0:380:A:OP2	2.02	0.59
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:CYS:SG	21:U:32:CYS:HB3	2.43	0.59
26:Z:64:PRO:HB2	26:Z:86:TYR:CE2	2.38	0.59
30:0:1201:C:H5''	38:0:6132:HOH:O	2.02	0.59
30:0:1904:A:H2'	30:0:1905:U:O4'	2.02	0.59
30:0:1116:U:HO2'	30:0:1118:A:H2	0.72	0.59
30:0:1377:C:H6	30:0:1377:C:H5'	1.67	0.59
30:0:214:U:H5'	38:0:6123:HOH:O	2.01	0.59
17:Q:26:PRO:O	17:Q:30:VAL:HG22	2.02	0.59
30:0:1187:U:H2'	38:0:6882:HOH:O	2.02	0.59
30:0:1634:G:H3'	38:0:3889:HOH:O	2.02	0.59
30:0:2250:G:H2'	30:0:2251:G:O4'	2.03	0.59
30:0:319:A:H4'	30:0:338:C:C4	2.38	0.59
4:D:62:ASP:HA	38:D:4233:HOH:O	2.03	0.59
15:O:25:VAL:HG12	30:0:709:G:O2'	2.03	0.59
30:0:827:A:H1'	38:0:6196:HOH:O	2.02	0.59
30:0:1118:A:C8	30:0:1118:A:C3'	2.74	0.58
30:0:1175:G:H1'	30:0:1193:A:C2'	2.31	0.58
29:3:3:MET:O	29:3:90:PHE:HA	2.03	0.58
18:R:40:ALA:O	18:R:44:VAL:HG23	2.03	0.58
20:T:48:VAL:HG11	20:T:96:VAL:HG13	1.85	0.58
2:B:68:THR:HG21	21:U:16:GLY:HA3	1.85	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:2353:A:H4'	30:0:2354:A:O5'	2.02	0.58
30:0:542:A:H5'	30:0:542:A:C8	2.29	0.58
2:B:195:ARG:HE	2:B:323:LEU:HD13	1.68	0.58
30:0:1393:A:H2'	30:0:1394:C:C6	2.38	0.58
30:0:1929:G:H1'	38:0:5153:HOH:O	2.03	0.58
30:0:482:G:H4'	30:0:508:A:N1	2.18	0.58
30:0:669:G:O2'	30:0:670:G:H5'	2.03	0.58
30:0:918:G:H5''	38:0:9099:HOH:O	2.01	0.58
31:9:54:A:C2'	31:9:55:U:H5'	2.33	0.58
2:B:256:GLN:HG2	38:B:9129:HOH:O	2.03	0.58
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.84	0.58
30:0:1127:C:C5	30:0:1128:U:C4	2.91	0.58
30:0:1161:A:O5'	30:0:1161:A:H8	1.85	0.58
30:0:657:G:H2'	30:0:658:C:C6	2.38	0.58
1:A:199:HIS:CD2	1:A:201:PHE:H	2.21	0.58
30:0:812:A:H2'	30:0:813:C:C6	2.38	0.58
30:0:962:C:H2'	30:0:963:C:C5'	2.33	0.58
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.19	0.58
3:C:2:GLN:HB3	38:C:8594:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:133:VAL:HA	38:L:9035:HOH:O	2.04	0.58
12:L:30:ARG:HD2	30:0:164:G:H5''	1.85	0.58
13:M:68:ARG:HH21	13:M:73:ARG:HD3	1.65	0.58
30:0:2256:G:O2'	30:0:2257:G:H5'	2.04	0.58
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.58
30:0:2900:G:H2'	30:0:2901:C:O4'	2.03	0.58
30:0:416:G:H3'	38:0:9910:HOH:O	2.02	0.58
30:0:696:C:O2'	30:0:697:G:H5'	2.03	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.69	0.58
30:0:814:G:H4'	38:0:3124:HOH:O	2.03	0.58
30:0:858:U:H5	38:0:5421:HOH:O	1.86	0.58
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.39	0.58
7:G:64:ASN:N	7:G:64:ASN:HD22	1.99	0.58
12:L:80:ASP:HB2	12:L:90:ARG:O	2.03	0.58
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.68	0.58
30:0:2276:U:H1'	38:0:9608:HOH:O	2.04	0.58
30:0:244:C:H6	30:0:244:C:O5'	1.87	0.58
30:0:541:C:O2'	30:0:542:A:H5''	2.03	0.58
28:2:41:HIS:CD2	28:2:43:ARG:H	2.22	0.58
2:B:125:GLU:O	2:B:129:ARG:HG3	2.03	0.58
3:C:236:THR:HA	38:C:8660:HOH:O	2.04	0.58
25:Y:133:HIS:HD2	38:Y:8886:HOH:O	1.85	0.58
30:0:1221:G:H8	38:0:5971:HOH:O	1.87	0.58
30:0:1819:G:H2'	30:0:1820:G:C5'	2.34	0.58
30:0:2064:U:H5'	30:0:2652:U:H4'	1.86	0.58
31:9:1:U:C4'	31:9:3:A:OP1	2.52	0.58
1:A:109:GLU:HG2	1:A:116:GLY:H	1.69	0.58
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.58
13:M:81:ARG:HG3	30:0:161:A:OP1	2.04	0.58
29:3:60:LYS:HB2	30:0:2460:A:OP1	2.04	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
30:0:1205:U:C2'	30:0:1206:U:C5'	2.81	0.58
30:0:2867:G:H2'	30:0:2868:C:C6	2.39	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.35	0.58
13:M:28:GLN:O	13:M:32:ARG:HG3	2.02	0.58
22:V:1:THR:HG23	22:V:2:VAL:H	1.69	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
30:0:1829:A:C2'	30:0:1830:C:H5'	2.34	0.57
5:E:143:GLN:NE2	30:0:2779:G:H21	2.01	0.57
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.57
3:C:25:PRO:HG2	38:C:8522:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.04	0.57
26:Z:80:GLN:HG3	26:Z:81:CYS:N	2.20	0.57
30:0:1626:A:H2'	30:0:1627:G:C5'	2.35	0.57
30:0:1664:A:H8	30:0:1664:A:OP1	1.87	0.57
30:0:2499:U:H2'	30:0:2500:C:H6	1.69	0.57
30:0:553:G:H5'	38:0:3481:HOH:O	2.04	0.57
30:0:695:C:O2'	30:0:696:C:H5'	2.04	0.57
31:9:108:C:H2'	31:9:109:G:C8	2.38	0.57
30:0:1197:G:H1'	30:0:1203:G:N2	2.19	0.57
12:L:14:GLY:O	30:0:1295:G:H5''	2.04	0.57
30:0:1494:A:C4	30:0:1495:C:C5	2.93	0.57
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.86	0.57
30:0:1395:C:H2'	30:0:1396:C:C6	2.39	0.57
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.19	0.57
16:P:81:LYS:O	30:0:1761:U:H5'	2.04	0.57
30:0:2269:C:C2'	30:0:2270:G:H5'	2.34	0.57
30:0:544:G:C3'	30:0:545:G:H5''	2.35	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.81	0.57
29:3:69:TYR:HD1	29:3:78:HIS:O	1.87	0.57
31:9:49:G:O2'	31:9:50:G:H5'	2.05	0.57
20:T:26:THR:HA	20:T:39:ASN:HB3	1.86	0.57
30:0:2563:U:H2'	30:0:2565:C:O5'	2.04	0.57
30:0:2840:A:H3'	38:0:7638:HOH:O	2.04	0.57
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.57
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.34	0.57
30:0:1919:A:H4'	38:0:4844:HOH:O	2.04	0.57
30:0:2300:A:H4'	30:0:2301:A:O5'	2.05	0.57
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.52	0.57
30:0:1165:G:O3'	30:0:1174:A:H4'	2.04	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.85	0.57
30:0:957:A:H8	30:0:957:A:O5'	1.88	0.57
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.85	0.57
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.57
25:Y:130:ARG:HD2	38:Y:8857:HOH:O	2.04	0.57
30:0:2531:U:O2'	30:0:2532:A:H5'	2.05	0.57
31:9:114:G:H2'	31:9:115:C:C6	2.39	0.57
3:C:101:ASP:HB2	30:0:750:A:O3'	2.05	0.57
8:H:146:ALA:O	8:H:149:VAL:HG12	2.04	0.57
14:N:4:PRO:HD2	38:0:6759:HOH:O	2.04	0.57
30:0:1200:A:H3'	38:0:5738:HOH:O	2.05	0.57
30:0:1482:A:H1'	38:0:9425:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2032:U:H2'	30:0:2033:G:C5'	2.35	0.57
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.57
5:E:69:ILE:HA	5:E:72:MET:HE3	1.86	0.57
15:O:73:ASP:HA	15:O:92:VAL:O	2.05	0.57
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.04	0.57
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.05	0.57
30:0:1697:G:H4'	38:0:9342:HOH:O	2.05	0.57
30:0:2437:A:H2'	30:0:2438:G:C8	2.40	0.57
30:0:2768:A:H2'	30:0:2769:C:O4'	2.05	0.57
30:0:2831:C:H2'	30:0:2832:C:C5'	2.35	0.57
29:3:25:VAL:HG12	38:0:9267:HOH:O	2.04	0.57
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.85	0.57
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.57
30:0:1202:A:H2'	30:0:1203:G:C5'	2.34	0.56
30:0:1748:U:C5	30:0:1749:U:C5	2.92	0.56
30:0:2324:G:H1'	38:0:6095:HOH:O	2.04	0.56
30:0:589:U:H2'	30:0:590:A:H8	1.69	0.56
2:B:307:ARG:HB3	38:B:9126:HOH:O	2.04	0.56
30:0:1511:U:O2'	30:0:1512:G:H5'	2.05	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.04	0.56
30:0:2758:G:H2'	30:0:2759:C:C6	2.40	0.56
30:0:2824:C:O3'	30:0:2825:C:H6	1.88	0.56
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.04	0.56
2:B:297:VAL:HB	38:B:9075:HOH:O	2.03	0.56
3:C:214:THR:HG23	38:C:8649:HOH:O	2.04	0.56
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.56
22:V:39:ALA:H	22:V:40:PRO:HD2	1.69	0.56
26:Z:45:VAL:HA	26:Z:48:ARG:HB3	1.87	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.14	0.56
30:0:1426:C:H2'	38:0:9592:HOH:O	2.04	0.56
30:0:962:C:C2'	30:0:963:C:H5'	2.35	0.56
31:9:38:A:H2'	31:9:39:U:C6	2.41	0.56
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.87	0.56
2:B:244:PRO:HB3	30:0:1234:U:N3	2.20	0.56
3:C:138:VAL:HG11	3:C:160:LEU:HD13	1.87	0.56
30:0:594:C:O2'	30:0:595:U:H5'	2.05	0.56
30:0:708:A:H2'	30:0:709:G:O4'	2.05	0.56
31:9:18:U:H2'	31:9:19:G:C8	2.40	0.56
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.87	0.56
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.40	0.56
8:H:31:ILE:HD11	8:H:65:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.88	0.56
21:U:56:ARG:HD2	30:0:2890:A:N9	2.20	0.56
24:X:71:ARG:HD3	38:X:2171:HOH:O	2.04	0.56
30:0:1202:A:C2'	30:0:1203:G:H5'	2.35	0.56
30:0:1236:A:C2'	30:0:1237:U:H5'	2.36	0.56
30:0:28:G:H1'	38:0:4676:HOH:O	2.04	0.56
30:0:31:C:H4'	38:0:7417:HOH:O	2.04	0.56
30:0:1523:G:H2'	30:0:1524:U:C6	2.41	0.56
30:0:2248:C:H2'	30:0:2249:G:H8	1.70	0.56
30:0:2703:A:H2'	30:0:2704:C:C6	2.37	0.56
30:0:941:G:C5	30:0:942:U:C4	2.94	0.56
29:3:67:LEU:HD21	29:3:88:LEU:HD21	1.86	0.56
5:E:93:MET:HE1	5:E:165:GLY:N	2.21	0.56
30:0:1559:A:OP2	30:0:1559:A:H8	1.87	0.56
38:B:9106:HOH:O	30:0:2672:C:H1'	2.05	0.56
14:N:58:LEU:N	14:N:58:LEU:HD12	2.20	0.56
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.06	0.56
22:V:55:ARG:O	22:V:59:ILE:HG12	2.06	0.56
26:Z:37:ARG:HD3	26:Z:37:ARG:H	1.71	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.35	0.56
30:0:1504:A:H5'	38:0:4410:HOH:O	2.06	0.56
30:0:711:G:C2	30:0:718:C:C2	2.93	0.56
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.56
13:M:24:GLN:HE21	13:M:27:ARG:NH1	2.03	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.56
30:0:1537:C:H1'	38:0:6573:HOH:O	2.05	0.56
30:0:1574:C:H2'	30:0:1575:C:H6	1.70	0.56
30:0:2559:C:H4'	38:0:7245:HOH:O	2.06	0.56
19:S:37:VAL:O	19:S:41:VAL:HG23	2.04	0.56
21:U:56:ARG:NH1	21:U:56:ARG:HG3	2.18	0.56
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.05	0.56
30:0:1202:A:H2'	30:0:1203:G:O4'	2.06	0.56
28:2:41:HIS:CE1	30:0:1439:C:H5''	2.41	0.56
30:0:1574:C:H2'	30:0:1575:C:C6	2.41	0.56
30:0:1622:G:C2'	30:0:1623:C:H5'	2.36	0.56
30:0:1850:U:O4'	30:0:1941:A:C2	2.59	0.56
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.40	0.56
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
30:0:2897:C:O2'	30:0:2898:G:H5'	2.06	0.56
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.04	0.56
30:0:1060:C:H6	30:0:1060:C:H5'	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1159:G:H21	30:0:1189:A:H8	1.53	0.56
30:0:1778:A:H2'	30:0:1779:A:H5'	1.87	0.56
30:0:2004:U:H2'	30:0:2004:U:O2	2.05	0.56
30:0:2291:A:N9	30:0:2309:C:H5'	2.21	0.56
30:0:290:C:O2'	30:0:291:C:H5'	2.05	0.56
30:0:2316:G:H4'	38:0:6075:HOH:O	2.06	0.55
30:0:2906:A:H5'	30:0:2907:C:O4'	2.07	0.55
29:3:12:PRO:HD3	38:3:9032:HOH:O	2.05	0.55
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.46	0.55
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.01	0.55
26:Z:34:SER:HA	30:0:797:A:H4'	1.88	0.55
30:0:1594:C:O2'	30:0:1607:A:H4'	2.07	0.55
30:0:299:U:C2	30:0:300:U:C6	2.95	0.55
30:0:304:G:H1'	30:0:347:A:N6	2.21	0.55
30:0:485:A:N3	30:0:487:G:H5''	2.20	0.55
30:0:595:U:O2'	30:0:596:C:H5'	2.05	0.55
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.75	0.55
13:M:77:HIS:HB2	13:M:81:ARG:HE	1.72	0.55
14:N:49:THR:HG22	14:N:56:ASP:HB3	1.88	0.55
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.06	0.55
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.55
30:0:1972:U:C2'	30:0:1973:A:H5''	2.36	0.55
30:0:2718:C:H6	30:0:2718:C:H5'	1.71	0.55
30:0:2887:G:H2'	30:0:2888:U:O4'	2.07	0.55
12:L:30:ARG:HD3	30:0:164:G:H4'	1.87	0.55
30:0:1361:C:H2'	30:0:1362:U:H6	1.72	0.55
30:0:12:U:H2'	30:0:13:G:H5'	1.88	0.55
22:V:4:HIS:HB3	38:V:6622:HOH:O	2.06	0.55
26:Z:81:CYS:O	26:Z:85:ASP:HA	2.05	0.55
30:0:136:C:H2'	30:0:137:U:O4'	2.07	0.55
30:0:1809:G:H1'	38:0:7682:HOH:O	2.06	0.55
30:0:1913:C:H2'	30:0:1914:C:C6	2.41	0.55
30:0:536:A:H3'	38:0:5040:HOH:O	2.06	0.55
30:0:699:C:C2	30:0:744:G:C2	2.95	0.55
29:3:2:GLN:HA	29:3:89:GLU:O	2.07	0.55
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.32	0.55
13:M:82:ARG:H	13:M:82:ARG:HD3	1.72	0.55
23:W:38:THR:HG22	23:W:39:ASP:H	1.72	0.55
30:0:1342:C:O2'	30:0:1343:C:H5'	2.06	0.55
29:3:48:ASN:O	30:0:170:U:H4'	2.07	0.55
30:0:1762:C:H2'	30:0:1763:C:H6	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2451:G:H8	38:0:5174:HOH:O	1.90	0.55
30:0:2812:A:C2	30:0:2814:A:N6	2.71	0.55
1:A:54:PRO:HG2	1:A:160:ALA:HB3	1.89	0.55
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.88	0.55
13:M:164:THR:HG22	13:M:166:ALA:H	1.71	0.55
14:N:17:ARG:NH1	14:N:17:ARG:HB3	2.21	0.55
30:0:2480:G:H3'	38:0:4182:HOH:O	2.07	0.55
30:0:876:A:N3	30:0:876:A:H2'	2.22	0.55
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.89	0.55
8:H:29:SER:HA	8:H:62:HIS:CD2	2.41	0.55
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.89	0.55
30:0:1174:A:C5	30:0:1201:C:H4'	2.41	0.55
30:0:1202:A:C8	30:0:1203:G:C8	2.95	0.55
30:0:1204:C:H2'	30:0:1205:U:O4'	2.06	0.55
30:0:1236:A:O2'	30:0:1237:U:H5'	2.07	0.55
30:0:1667:A:C8	30:0:1667:A:H5'	2.34	0.55
30:0:2240:U:O2'	30:0:2241:C:H5'	2.06	0.55
6:F:59:ILE:CD1	30:0:263:U:C2	2.90	0.55
30:0:945:U:H2'	30:0:946:C:C6	2.42	0.55
18:R:114:VAL:HA	18:R:144:GLU:O	2.06	0.55
30:0:154:C:H2'	30:0:155:C:H6	1.72	0.55
30:0:2416:G:H2'	30:0:2417:C:C6	2.42	0.55
31:9:59:C:H4'	38:9:9127:HOH:O	2.06	0.55
19:S:57:THR:HG22	19:S:58:MET:N	2.21	0.55
25:Y:182:PHE:HD2	25:Y:200:THR:O	1.89	0.55
30:0:2102:G:N3	30:0:2103:A:C6	2.75	0.55
30:0:807:A:H2'	30:0:808:A:C8	2.41	0.55
1:A:192:VAL:HG12	38:A:9012:HOH:O	2.06	0.55
2:B:41:PHE:HA	2:B:79:MET:HE2	1.89	0.55
22:V:64:GLY:O	22:V:65:ASP:HB2	2.07	0.55
30:0:1377:C:H5'	30:0:1377:C:C6	2.42	0.54
30:0:204:A:H2'	30:0:205:U:H5'	1.89	0.54
30:0:2869:G:H2'	30:0:2870:C:H6	1.73	0.54
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.54
1:A:237:GLY:O	30:0:1939:U:H5''	2.06	0.54
3:C:188:ARG:HD3	38:C:8571:HOH:O	2.07	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.37	0.54
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.90	0.54
30:0:1878:G:C4'	38:0:6104:HOH:O	2.55	0.54
3:C:233:THR:HG22	3:C:234:VAL:N	2.21	0.54
26:Z:46:SER:O	26:Z:50:VAL:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:N3	30:0:1184:C:N4	2.55	0.54
30:0:1334:C:O2'	30:0:1335:C:H5'	2.07	0.54
30:0:2372:A:H2'	30:0:2373:U:C6	2.43	0.54
30:0:2872:U:H2'	30:0:2873:C:H6	1.73	0.54
30:0:963:C:O2	30:0:1005:A:N1	2.39	0.54
18:R:150:PRO:CG	18:R:150:PRO:CB	2.85	0.54
30:0:1188:A:C5	30:0:1189:A:C2	2.95	0.54
30:0:1902:G:N2	30:0:1936:C:C2	2.75	0.54
30:0:561:G:H2'	30:0:562:A:H8	1.73	0.54
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.88	0.54
25:Y:169:ARG:NE	33:Y:8820:CL:CL	2.73	0.54
30:0:1969:A:O2'	30:0:1970:G:H5'	2.08	0.54
20:T:52:ARG:HD2	30:0:317:A:H5''	1.90	0.54
30:0:951:A:C2'	30:0:952:G:H5'	2.37	0.54
25:Y:216:ARG:HD2	38:Y:8874:HOH:O	2.06	0.54
30:0:2102:G:C2	30:0:2103:A:C6	2.95	0.54
30:0:314:G:N2	30:0:317:A:C8	2.75	0.54
30:0:703:G:O2'	30:0:704:C:H5'	2.07	0.54
1:A:199:HIS:HD2	1:A:201:PHE:H	1.55	0.54
4:D:76:ARG:NE	31:9:44:A:O4'	2.41	0.54
14:N:43:VAL:CG1	14:N:118:ILE:HD11	2.38	0.54
14:N:5:ARG:HB2	14:N:5:ARG:NH1	2.21	0.54
18:R:80:TYR:O	30:0:2050:G:H5''	2.08	0.54
30:0:2321:A:H2'	30:0:2321:A:N3	2.22	0.54
29:3:79:LEU:HD13	30:0:2457:U:H1'	1.88	0.54
30:0:255:A:C5	30:0:256:C:C5	2.96	0.54
27:1:42:SER:HB2	38:1:354:HOH:O	2.08	0.54
31:9:55:U:H4'	31:9:56:A:H8	1.73	0.54
1:A:211:LYS:HG2	38:0:7019:HOH:O	2.08	0.54
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.06	0.54
7:G:20:VAL:O	7:G:24:VAL:HG23	2.07	0.54
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.89	0.54
16:P:115:SER:H	16:P:118:GLN:NE2	1.92	0.54
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.36	0.54
30:0:120:A:H2'	30:0:120:A:N3	2.22	0.54
30:0:535:G:C5	30:0:2063:U:C4	2.95	0.54
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.54
27:1:1:THR:HA	38:0:9360:HOH:O	2.07	0.54
12:L:41:HIS:CD2	12:L:41:HIS:H	2.25	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.54
30:0:1202:A:O2'	30:0:1203:G:H5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD2	30:0:1884:G:O6	2.08	0.54
30:0:2326:C:H4'	30:0:2412:G:C4'	2.38	0.54
30:0:2589:U:H2'	30:0:2590:U:C6	2.42	0.54
30:0:2638:G:H5'	38:0:4923:HOH:O	2.07	0.54
1:A:176:HIS:CD2	30:0:857:A:H4'	2.43	0.54
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.54
23:W:26:ILE:HB	38:W:5420:HOH:O	2.06	0.54
30:0:1176:C:H5	38:0:5727:HOH:O	1.91	0.54
30:0:1163:G:H1	30:0:1184:C:N4	2.06	0.54
30:0:1714:C:O2'	30:0:1715:C:H5'	2.08	0.54
30:0:2344:G:H8	38:0:6641:HOH:O	1.91	0.54
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.89	0.54
2:B:98:THR:HG22	2:B:99:GLU:H	1.73	0.54
3:C:237:GLU:HA	38:C:8643:HOH:O	2.08	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.22	0.54
14:N:147:ILE:HD11	31:9:49:G:O3'	2.07	0.54
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.89	0.54
30:0:1706:G:C6	30:0:1707:G:C6	2.96	0.53
30:0:2335:C:H2'	30:0:2336:G:C8	2.43	0.53
29:3:33:MET:SD	30:0:2450:C:H4'	2.48	0.53
3:C:135:GLU:HB3	38:C:8586:HOH:O	2.08	0.53
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.53
6:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.60	0.53
14:N:67:ALA:HA	14:N:71:TRP:CB	2.37	0.53
21:U:33:SER:O	21:U:37:GLU:HG3	2.08	0.53
30:0:1379:A:H1'	38:0:9690:HOH:O	2.08	0.53
30:0:1506:U:H6	30:0:1506:U:H5'	1.73	0.53
29:3:48:ASN:HB3	30:0:170:U:H5'	1.91	0.53
30:0:2347:C:H2'	30:0:2348:C:H6	1.73	0.53
30:0:2712:G:H1'	38:0:5829:HOH:O	2.08	0.53
30:0:480:C:H4'	38:0:7715:HOH:O	2.08	0.53
30:0:962:C:H5''	38:0:4907:HOH:O	2.06	0.53
21:U:51:TRP:HA	21:U:56:ARG:HE	1.72	0.53
30:0:2546:U:H4'	38:0:6160:HOH:O	2.09	0.53
30:0:311:C:H2'	30:0:312:U:C6	2.43	0.53
1:A:36:ASP:HB2	1:A:85:SER:H	1.73	0.53
3:C:180:SER:HB2	38:C:8656:HOH:O	2.06	0.53
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.74	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:88:THR:HG22	23:W:89:ASP:H	1.74	0.53
30:0:185:G:H4'	30:0:186:A:OP1	2.08	0.53
31:9:117:G:H2'	31:9:118:C:C6	2.44	0.53
31:9:13:A:O2'	31:9:14:G:H5''	2.09	0.53
31:9:39:U:H3'	31:9:40:C:C5'	2.39	0.53
31:9:60:C:O2'	31:9:61:C:H5'	2.08	0.53
1:A:109:GLU:HG2	1:A:116:GLY:N	2.23	0.53
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.72	0.53
14:N:55:ASP:OD2	31:9:7:G:H4'	2.08	0.53
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.91	0.53
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.89	0.53
30:0:1205:U:H2'	30:0:1206:U:H5''	1.88	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.43	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
13:M:164:THR:HG22	13:M:166:ALA:N	2.23	0.53
30:0:1269:G:H2'	30:0:1270:U:C6	2.44	0.53
30:0:1523:G:C6	30:0:1524:U:O4	2.62	0.53
30:0:1553:C:H2'	30:0:1554:C:H6	1.74	0.53
30:0:2112:A:C8	38:0:6930:HOH:O	2.54	0.53
30:0:363:C:O2'	30:0:364:U:H5'	2.09	0.53
30:0:517:U:H2'	30:0:518:G:H5'	1.90	0.53
30:0:1014:A:H5''	31:9:101:G:O2'	2.09	0.53
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.09	0.53
13:M:68:ARG:HG3	30:0:1469:C:OP1	2.09	0.53
30:0:2371:G:H5'	38:0:5000:HOH:O	2.07	0.53
30:0:10:U:O4	30:0:532:A:OP2	2.27	0.53
18:R:39:THR:HB	18:R:42:GLU:HG3	1.91	0.53
30:0:2578:G:C8	30:0:2578:G:H5'	2.40	0.53
30:0:734:U:O2'	30:0:736:A:N7	2.35	0.53
31:9:39:U:H3	31:9:42:C:H5''	1.72	0.53
31:9:76:G:H3'	31:9:77:A:C5'	2.23	0.53
2:B:102:THR:HG21	2:B:182:VAL:O	2.09	0.53
16:P:134:VAL:O	16:P:137:LEU:HB3	2.09	0.53
30:0:1224:G:H2'	30:0:1225:C:C6	2.43	0.53
30:0:1940:C:H4'	38:0:7336:HOH:O	2.08	0.53
30:0:312:U:C2	30:0:320:G:N2	2.77	0.53
30:0:454:U:C2	38:0:9033:HOH:O	2.53	0.53
14:N:132:ASN:O	14:N:135:VAL:HG12	2.09	0.53
30:0:10:U:C4	30:0:532:A:C8	2.97	0.53
30:0:1515:A:H2'	30:0:1516:U:C6	2.43	0.53
30:0:279:C:O2'	30:0:280:C:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:821:U:H2'	30:0:822:C:H6	1.73	0.53
29:3:70:ARG:HA	29:3:77:ALA:HB2	1.91	0.53
14:N:160:SER:CB	31:9:51:A:H5'	2.39	0.53
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.74	0.53
2:B:62:ARG:HA	2:B:65:MET:CE	2.39	0.53
14:N:42:HIS:HB3	14:N:62:HIS:HE1	1.73	0.53
23:W:13:MET:HE1	23:W:18:GLN:HA	1.90	0.53
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	1.91	0.53
30:0:2438:G:H2'	30:0:2439:C:O4'	2.09	0.52
30:0:72:C:H5'	38:0:5876:HOH:O	2.10	0.52
30:0:853:C:H3'	38:0:4548:HOH:O	2.08	0.52
1:A:51:ARG:NH2	1:A:53:ALA:HB3	2.25	0.52
2:B:211:THR:HG23	30:0:2840:A:OP1	2.08	0.52
26:Z:61:HIS:HB3	38:Z:8710:HOH:O	2.07	0.52
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.74	0.52
30:0:1180:U:H2'	30:0:1181:A:O4'	2.10	0.52
30:0:1201:C:H6	38:0:5738:HOH:O	1.93	0.52
30:0:2506:A:N6	30:0:2511:A:O2'	2.42	0.52
30:0:2748:G:H5'	38:0:7534:HOH:O	2.08	0.52
27:1:2:GLY:O	27:1:6:PRO:HG2	2.09	0.52
1:A:33:GLU:O	1:A:34:ASP:HB2	2.09	0.52
3:C:94:THR:HG22	38:C:8687:HOH:O	2.09	0.52
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.52
24:X:30:MET:HE1	24:X:55:ASN:HA	1.91	0.52
30:0:1311:G:C2	30:0:1312:G:C8	2.96	0.52
30:0:1441:G:O2'	30:0:1442:A:H5'	2.09	0.52
30:0:2499:U:H2'	30:0:2500:C:C6	2.44	0.52
30:0:705:C:H2'	30:0:705:C:O2	2.08	0.52
30:0:960:G:H2'	30:0:960:G:N3	2.23	0.52
2:B:298:LYS:HD3	38:B:9095:HOH:O	2.08	0.52
12:L:145:LEU:O	12:L:148:GLU:HG3	2.09	0.52
14:N:32:PRO:HD2	14:N:99:GLU:O	2.10	0.52
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.74	0.52
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.91	0.52
30:0:1928:C:H2'	30:0:1929:G:O4'	2.09	0.52
30:0:2295:G:N3	30:0:2361:A:C2	2.77	0.52
30:0:2864:U:O2'	30:0:2865:G:H5'	2.09	0.52
30:0:324:G:O2'	30:0:325:U:H5'	2.09	0.52
30:0:506:G:N2	30:0:509:A:C5'	2.66	0.52
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.06	0.52
13:M:73:ARG:HD2	13:M:73:ARG:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.10	0.52
30:0:107:U:H2'	30:0:108:U:H5'	1.92	0.52
30:0:1375:A:C2'	30:0:1376:G:H5'	2.39	0.52
30:0:2032:U:H2'	30:0:2033:G:H5'	1.91	0.52
30:0:2831:C:O2'	30:0:2832:C:H5'	2.10	0.52
31:9:56:A:C3'	31:9:57:A:H5''	2.39	0.52
1:A:94:LEU:N	1:A:94:LEU:HD23	2.24	0.52
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.40	0.52
5:E:80:TRP:O	5:E:134:SER:HA	2.10	0.52
20:T:28:SER:O	20:T:32:ARG:HG3	2.10	0.52
23:W:38:THR:O	23:W:42:ARG:HB2	2.09	0.52
30:0:297:U:H2'	30:0:298:C:C6	2.43	0.52
5:E:118:ILE:HG23	5:E:144:THR:HG21	1.92	0.52
21:U:6:CYS:SG	21:U:13:ILE:HD12	2.49	0.52
23:W:52:VAL:HG22	23:W:53:ALA:H	1.75	0.52
30:0:1183:C:O2	30:0:1183:C:H2'	2.08	0.52
30:0:1182:C:H1'	30:0:1192:A:H8	1.74	0.52
30:0:1269:G:H2'	30:0:1270:U:H6	1.75	0.52
3:C:70:VAL:HG21	30:0:1361:C:H5'	1.91	0.52
30:0:1667:A:H2'	30:0:1668:U:C6	2.44	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.91	0.52
30:0:64:G:H2'	30:0:65:C:O4'	2.10	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52
2:B:49:THR:HG21	2:B:331:SER:O	2.10	0.52
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.10	0.52
13:M:77:HIS:CE1	13:M:86:GLN:HG3	2.44	0.52
13:M:91:ILE:HG12	38:0:7539:HOH:O	2.10	0.52
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.40	0.52
30:0:101:C:H2'	30:0:102:A:C8	2.45	0.52
30:0:1845:A:O2'	30:0:1846:U:H5'	2.10	0.52
30:0:1972:U:H2'	30:0:1973:A:H5''	1.90	0.52
30:0:1992:U:H2'	30:0:1994:A:OP2	2.10	0.52
30:0:2111:G:H1'	38:0:9051:HOH:O	2.09	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.25	0.52
30:0:2420:G:C2'	30:0:2421:G:H5'	2.39	0.52
30:0:2584:G:H4'	38:0:7109:HOH:O	2.08	0.52
30:0:2689:A:C2'	30:0:2690:U:H5'	2.40	0.52
30:0:506:G:N2	30:0:508:A:H3'	2.25	0.52
13:M:46:LEU:HG	38:M:8918:HOH:O	2.08	0.52
13:M:89:THR:HA	38:M:8851:HOH:O	2.10	0.52
30:0:208:C:H3'	38:0:6388:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2549:C:O2'	30:0:2550:U:H5'	2.09	0.52
30:0:553:G:O4'	30:0:1325:G:H5'	2.10	0.52
29:3:51:LYS:HA	29:3:54:LYS:HD2	1.92	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:293:A:C4	30:0:360:A:C2	2.98	0.52
30:0:365:G:C6	30:0:366:U:C4	2.98	0.52
30:0:541:C:C2'	30:0:542:A:C5'	2.75	0.52
31:9:18:U:H2'	31:9:19:G:H8	1.74	0.52
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.92	0.52
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.91	0.52
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.91	0.52
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.24	0.52
14:N:119:GLN:O	14:N:123:ILE:HG13	2.10	0.52
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.31	0.52
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.91	0.52
23:W:4:LEU:O	23:W:32:CYS:HA	2.10	0.52
30:0:1189:A:H1'	30:0:1209:C:H1'	1.92	0.51
30:0:1495:C:H1'	30:0:1573:A:H1'	1.93	0.51
30:0:2526:C:O2'	30:0:2527:U:H5'	2.10	0.51
30:0:523:C:H2'	30:0:524:A:C8	2.45	0.51
30:0:960:G:N3	30:0:960:G:C2'	2.73	0.51
29:3:64:LYS:HD2	30:0:2459:G:OP2	2.11	0.51
2:B:214:PRO:HD2	38:0:9078:HOH:O	2.10	0.51
26:Z:42:TYR:HA	30:0:1829:A:H61	1.74	0.51
14:N:4:PRO:CB	30:0:1010:C:H4'	2.40	0.51
3:C:226:GLY:HA3	30:0:1308:A:O4'	2.10	0.51
30:0:1682:A:O2'	30:0:1683:G:H5''	2.10	0.51
17:Q:45:PRO:O	30:0:2365:G:H4'	2.10	0.51
29:3:42:ARG:NH1	30:0:396:U:H5'	2.25	0.51
31:9:22:G:H5'	31:9:23:U:OP1	2.10	0.51
30:0:1185:U:H5'	38:0:7461:HOH:O	2.10	0.51
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.51
30:0:2004:U:H4'	38:0:5299:HOH:O	2.09	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.24	0.51
11:K:41:LYS:HA	30:0:2582:G:O3'	2.11	0.51
30:0:78:G:C6	30:0:79:G:C6	2.99	0.51
5:E:22:VAL:O	5:E:76:VAL:HG11	2.10	0.51
14:N:102:LEU:HD13	14:N:119:GLN:HB2	1.92	0.51
22:V:44:GLY:O	22:V:48:GLU:HG2	2.10	0.51
30:0:2239:C:H2'	30:0:2240:U:C6	2.46	0.51
30:0:2269:C:O2'	30:0:2270:G:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:255:A:C4	30:0:256:C:C6	2.98	0.51
30:0:2769:C:C2'	30:0:2770:G:C5'	2.88	0.51
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.26	0.51
30:0:282:C:C2'	30:0:283:U:H5'	2.40	0.51
30:0:2088:C:H1'	30:0:2841:A:N1	2.25	0.51
13:M:81:ARG:HG2	38:M:8926:HOH:O	2.11	0.51
15:O:105:ASN:HD21	15:O:109:SER:H	1.58	0.51
30:0:1361:C:H2'	30:0:1362:U:C6	2.45	0.51
30:0:1563:G:H4'	38:0:4227:HOH:O	2.10	0.51
30:0:1788:U:C2	30:0:1805:G:N2	2.79	0.51
30:0:2269:C:H2'	30:0:2270:G:O4'	2.09	0.51
28:2:2:LYS:HG3	30:0:1486:A:C5	2.45	0.51
3:C:150:THR:HA	3:C:203:ALA:O	2.11	0.51
8:H:141:CYS:HB2	38:H:8991:HOH:O	2.10	0.51
30:0:1304:U:H2'	30:0:1305:C:C6	2.46	0.51
30:0:1061:C:H1'	30:0:2283:G:O6	2.10	0.51
30:0:2851:G:O2'	30:0:2852:A:H5'	2.11	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.11	0.51
30:0:466:A:H2'	30:0:467:G:O4'	2.10	0.51
30:0:646:G:H2'	30:0:647:U:C6	2.46	0.51
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.26	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
26:Z:37:ARG:HB2	30:0:819:A:H4'	1.92	0.51
30:0:1855:G:H4'	30:0:1856:C:O5'	2.10	0.51
30:0:1878:G:H1'	38:0:6104:HOH:O	2.11	0.51
30:0:2099:A:H2	38:0:3918:HOH:O	1.93	0.51
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.74	0.51
30:0:2507:G:H2'	30:0:2510:C:H42	1.75	0.51
30:0:2899:A:O2'	30:0:2900:G:H5'	2.10	0.51
30:0:42:C:H1'	38:0:4670:HOH:O	2.09	0.51
31:9:117:G:H2'	31:9:118:C:H6	1.75	0.51
31:9:3:A:OP2	31:9:25:G:N2	2.43	0.51
31:9:45:A:C5	31:9:46:C:C5	2.98	0.51
3:C:21:VAL:HG13	38:C:8606:HOH:O	2.09	0.51
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.58	0.51
14:N:163:PHE:HB3	38:N:8829:HOH:O	2.11	0.51
21:U:47:ARG:HG3	38:U:4381:HOH:O	2.10	0.51
22:V:56:ILE:O	22:V:60:GLN:HG3	2.10	0.51
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.24	0.51
30:0:1020:A:H1'	38:0:7218:HOH:O	2.11	0.51
30:0:1056:U:H2'	30:0:1057:A:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:124:C:H3'	38:0:7649:HOH:O	2.10	0.51
30:0:1581:A:C5	30:0:1582:C:C5	2.99	0.51
30:0:1626:A:O2'	30:0:1627:G:H5'	2.10	0.51
30:0:2354:A:H5'	30:0:2355:G:N7	2.26	0.51
30:0:2842:G:H2'	30:0:2843:A:H5'	1.92	0.51
30:0:703:G:H2'	30:0:704:C:H6	1.76	0.51
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.75	0.51
5:E:137:ASP:O	5:E:141:VAL:HG23	2.10	0.51
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.93	0.51
6:F:39:SER:OG	6:F:45:ALA:HB2	2.11	0.51
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.46	0.51
14:N:114:LYS:O	14:N:118:ILE:HG13	2.10	0.51
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.51
30:0:1562:C:O2	30:0:1562:C:C2'	2.59	0.51
30:0:1701:A:H5''	30:0:1702:U:H3'	1.93	0.51
29:3:10:TYR:HD1	30:0:2408:A:HO2'	1.52	0.51
30:0:615:G:H2'	30:0:616:U:C6	2.46	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.46	0.51
1:A:132:ASP:CG	1:A:133:ARG:H	2.14	0.51
1:A:223:ARG:HG3	38:A:9021:HOH:O	2.11	0.51
3:C:76:ARG:NH2	30:0:1363:G:OP1	2.44	0.51
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.11	0.51
30:0:1202:A:H2'	30:0:1203:G:H5'	1.92	0.51
30:0:1218:U:H2'	30:0:1219:U:C6	2.46	0.51
30:0:168:C:O5'	30:0:168:C:H6	1.92	0.51
30:0:1972:U:C2'	30:0:1973:A:C5'	2.89	0.51
30:0:2345:A:H3'	30:0:2346:C:C6	2.45	0.51
30:0:255:A:C5	30:0:256:C:C4	2.99	0.51
1:A:207:GLN:HA	38:A:8981:HOH:O	2.10	0.51
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.92	0.51
17:Q:28:ARG:HG2	38:9:9082:HOH:O	2.11	0.51
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.38	0.51
30:0:1626:A:C2'	30:0:1627:G:H5'	2.41	0.50
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.50
30:0:407:A:H5'	38:0:6009:HOH:O	2.11	0.50
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.93	0.50
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.11	0.50
17:Q:11:ARG:HH22	30:0:2363:G:C5'	2.24	0.50
20:T:72:ILE:HD13	20:T:93:THR:HG22	1.92	0.50
26:Z:80:GLN:CG	26:Z:81:CYS:H	2.22	0.50
30:0:1213:C:C2'	30:0:1214:G:H5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:151:A:H2'	30:0:152:A:O4'	2.11	0.50
30:0:2506:A:O2'	30:0:2507:G:C8	2.49	0.50
33:0:8812:CL:CL	38:0:5117:HOH:O	2.57	0.50
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.50
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.20	0.50
2:B:72:THR:HB	38:B:9075:HOH:O	2.10	0.50
3:C:46:TYR:CE1	30:0:450:C:H4'	2.45	0.50
30:0:1589:G:H4'	38:0:6843:HOH:O	2.10	0.50
30:0:1934:A:C8	30:0:1935:C:C5	3.00	0.50
30:0:2758:G:H2'	30:0:2759:C:H6	1.76	0.50
30:0:396:U:O2'	30:0:397:A:P	2.70	0.50
2:B:238:ASN:HD22	2:B:240:GLY:N	2.10	0.50
30:0:1189:A:O2'	30:0:1208:C:H2'	2.12	0.50
25:Y:115:ARG:HH22	30:0:1266:U:H4'	1.72	0.50
38:C:8676:HOH:O	30:0:2100:A:H5'	2.12	0.50
30:0:2533:C:C6	30:0:2533:C:H5'	2.42	0.50
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.26	0.50
30:0:549:A:O2'	30:0:550:C:H5'	2.11	0.50
30:0:99:A:C8	30:0:100:C:C5	2.99	0.50
1:A:162:GLY:N	26:Z:91:GLY:HA2	2.26	0.50
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.93	0.50
5:E:81:GLU:O	5:E:172:PRO:HD3	2.12	0.50
13:M:139:PRO:HA	13:M:142:GLN:HB2	1.93	0.50
21:U:9:CYS:HB2	38:U:6796:HOH:O	2.12	0.50
23:W:5:VAL:HG22	23:W:32:CYS:HB2	1.94	0.50
30:0:1118:A:H8	30:0:1119:G:H5'	1.75	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.44	0.50
30:0:693:A:H2'	30:0:694:A:C8	2.46	0.50
30:0:920:C:H4'	30:0:921:G:C2	2.46	0.50
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.94	0.50
30:0:1180:U:O2'	30:0:1181:A:H5'	2.11	0.50
30:0:1183:C:N3	30:0:1184:C:C5	2.79	0.50
30:0:1759:A:N3	30:0:1818:C:H2'	2.27	0.50
30:0:2072:G:C6	30:0:2533:C:H1'	2.47	0.50
30:0:216:A:O2'	30:0:217:C:H5'	2.12	0.50
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.50
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.94	0.50
3:C:197:SER:HB3	38:C:8583:HOH:O	2.12	0.50
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.93	0.50
13:M:72:ALA:HB3	38:M:8944:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:41:ARG:HH22	30:0:1500:U:P	2.34	0.50
30:0:1158:G:H2'	30:0:1159:G:H5'	1.93	0.50
30:0:1395:C:H2'	30:0:1396:C:H6	1.77	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1819:G:H2'	30:0:1820:G:C4'	2.42	0.50
30:0:2416:G:H2'	30:0:2417:C:H6	1.76	0.50
30:0:2781:U:C2'	30:0:2782:G:C5'	2.89	0.50
30:0:39:G:C2	30:0:444:C:C2	3.00	0.50
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.50
30:0:820:G:H5'	30:0:821:U:C5'	2.41	0.50
2:B:158:LYS:HB2	38:0:4101:HOH:O	2.11	0.50
5:E:11:VAL:HG12	5:E:12:ASP:N	2.27	0.50
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.94	0.50
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.50
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.50
30:0:1610:G:H2'	30:0:1611:G:O4'	2.12	0.50
30:0:1765:G:H1'	30:0:1780:G:N2	2.26	0.50
30:0:204:A:C2'	30:0:205:U:H5'	2.41	0.50
30:0:2354:A:H5'	30:0:2355:G:C5	2.46	0.50
30:0:2598:U:O2	30:0:2600:A:H8	1.95	0.50
30:0:441:A:C2	30:0:442:A:N6	2.80	0.50
30:0:523:C:H2'	30:0:524:A:H8	1.77	0.50
31:9:61:C:H2'	31:9:62:A:H8	1.76	0.50
10:J:82:THR:HG23	30:0:1242:A:C5'	2.17	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.94	0.50
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.50
14:N:160:SER:HB3	31:9:51:A:H5'	1.93	0.50
23:W:121:PRO:CA	23:W:153:MET:HG2	2.42	0.50
30:0:1160:G:H5'	30:0:1161:A:H5'	0.83	0.50
30:0:1226:G:H5'	38:0:4526:HOH:O	2.11	0.50
30:0:1398:G:H2'	30:0:1399:A:C8	2.47	0.50
30:0:1947:G:H2'	30:0:1948:G:H8	1.77	0.50
30:0:2269:C:H2'	30:0:2270:G:C5'	2.42	0.50
30:0:2330:U:H4'	30:0:2331:C:OP1	2.11	0.50
30:0:932:U:H2'	30:0:933:C:C6	2.47	0.50
27:I:28:HIS:HE1	30:0:776:A:OP1	1.95	0.50
31:9:58:G:C8	31:9:59:C:C5	3.00	0.50
10:J:22:VAL:O	10:J:26:VAL:HG23	2.12	0.50
10:J:76:ASP:HA	38:J:8863:HOH:O	2.11	0.50
14:N:169:PRO:O	14:N:172:PHE:HB3	2.12	0.50
30:0:1365:C:H4'	38:0:4606:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1541:G:O2'	30:0:1542:G:H5'	2.11	0.49
30:0:1791:U:O2'	30:0:1792:C:H5'	2.12	0.49
30:0:2502:C:O2'	30:0:2503:A:H5'	2.12	0.49
30:0:299:U:N3	30:0:300:U:C5	2.80	0.49
30:0:88:G:H5'	30:0:88:G:H8	1.76	0.49
27:1:28:HIS:HD2	27:1:30:LYS:H	1.58	0.49
30:0:1188:A:C6	30:0:1189:A:C6	3.00	0.49
13:M:94:ARG:HD2	30:0:158:A:OP2	2.11	0.49
30:0:1964:U:O2	30:0:1964:U:H2'	2.10	0.49
30:0:249:G:N2	30:0:250:C:C2	2.80	0.49
30:0:2705:U:H2'	30:0:2706:A:H8	1.73	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.12	0.49
31:9:114:G:H2'	31:9:115:C:H6	1.76	0.49
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.77	0.49
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.41	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.12	0.49
18:R:117:HIS:HD2	30:0:20:G:H21	1.61	0.49
30:0:2002:C:H2'	30:0:2003:U:H5'	1.94	0.49
30:0:699:C:O2'	30:0:744:G:H1'	2.12	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.75	0.49
31:9:20:G:H3'	38:9:9055:HOH:O	2.12	0.49
4:D:76:ARG:NH1	31:9:42:C:O2	2.45	0.49
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.49
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.94	0.49
5:E:15:GLN:HG2	5:E:16:ASP:N	2.28	0.49
11:K:8:VAL:HG12	11:K:9:THR:N	2.26	0.49
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.94	0.49
30:0:1191:A:H2'	30:0:1193:A:H5'	1.95	0.49
30:0:1453:G:H2'	30:0:1454:U:O4'	2.13	0.49
30:0:2316:G:H8	38:0:5642:HOH:O	1.95	0.49
30:0:816:G:H5'	30:0:1598:A:H4'	1.94	0.49
23:W:11:VAL:HG11	30:0:1086:A:C6	2.48	0.49
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.49
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.94	0.49
26:Z:38:PHE:HB3	26:Z:42:TYR:HD1	1.78	0.49
30:0:1206:U:C6	30:0:1206:U:H5'	2.31	0.49
30:0:1526:A:H4'	30:0:1527:A:H5'	1.95	0.49
30:0:1942:A:O2'	30:0:1943:C:H5'	2.11	0.49
30:0:2612:A:H4'	38:0:3666:HOH:O	2.13	0.49
30:0:445:U:O2'	30:0:446:G:H5'	2.12	0.49
30:0:514:G:OP1	30:0:514:G:H2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:38:ARG:CB	29:3:42:ARG:HH12	2.25	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.94	0.49
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.95	0.49
11:K:22:ASP:HB2	38:K:5264:HOH:O	2.13	0.49
14:N:18:THR:HG21	38:9:9099:HOH:O	2.12	0.49
15:O:25:VAL:HG23	15:O:26:TRP:N	2.27	0.49
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.96	0.49
30:0:1159:G:H2'	30:0:1160:G:O4'	2.11	0.49
30:0:1375:A:H2'	30:0:1376:G:H5'	1.95	0.49
30:0:314:G:C2	30:0:317:A:C8	3.01	0.49
30:0:352:A:H2'	30:0:353:G:C8	2.48	0.49
31:9:7:G:H5'	38:9:9099:HOH:O	2.11	0.49
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.48	0.49
2:B:28:SER:HB2	30:0:2807:U:OP2	2.13	0.49
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.94	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.27	0.49
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.49
30:0:128:A:C8	30:0:128:A:H3'	2.47	0.49
30:0:2135:A:O4'	30:0:2243:C:N4	2.45	0.49
30:0:2265:U:H2'	30:0:2266:A:H8	1.77	0.49
30:0:2820:A:H2'	30:0:2821:C:C6	2.46	0.49
27:1:16:HIS:HD2	30:0:470:U:O2'	1.95	0.49
29:3:48:ASN:ND2	30:0:169:A:H1'	2.27	0.49
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.13	0.49
30:0:1181:A:C2	30:0:1192:A:C8	3.00	0.49
30:0:1209:C:H2'	30:0:1210:G:C8	2.42	0.49
30:0:1572:A:H3'	38:0:4098:HOH:O	2.13	0.49
30:0:1765:G:O2'	30:0:1766:U:H5'	2.12	0.49
30:0:1976:G:H1'	30:0:2005:G:N2	2.28	0.49
30:0:2237:G:H1'	30:0:2238:A:H8	1.77	0.49
30:0:2707:C:H2'	30:0:2707:C:O2	2.13	0.49
30:0:2805:A:C8	30:0:2806:C:C5	3.01	0.49
30:0:661:G:C5	30:0:686:A:C2	3.01	0.49
31:9:52:A:H2'	31:9:53:G:H8	1.76	0.49
7:G:16:LYS:O	7:G:20:VAL:HG23	2.13	0.49
21:U:9:CYS:HA	21:U:52:THR:HG22	1.94	0.49
30:0:1521:C:H2'	30:0:1522:A:H8	1.78	0.49
38:L:9036:HOH:O	30:0:196:G:H2'	2.12	0.49
30:0:2254:G:H1'	38:0:5527:HOH:O	2.12	0.49
30:0:2359:G:H3'	38:0:5674:HOH:O	2.13	0.49
30:0:2635:A:C2'	30:0:2636:C:H5'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:264:G:H1'	30:0:265:U:H5	1.78	0.49
13:M:133:LEU:O	13:M:134:ILE:HD13	2.13	0.49
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.49
30:0:1118:A:N6	30:0:1244:U:H3	1.95	0.49
30:0:1566:C:O2'	30:0:1567:G:H5'	2.12	0.49
30:0:1586:G:O2'	30:0:1587:U:H5'	2.13	0.49
30:0:1913:C:H2'	30:0:1914:C:H6	1.76	0.49
30:0:2289:G:O2'	30:0:2291:A:N6	2.45	0.49
30:0:2911:C:H2'	30:0:2912:C:C6	2.48	0.49
30:0:526:U:H2'	30:0:527:U:C6	2.48	0.49
30:0:727:G:H3'	30:0:728:C:H6	1.78	0.49
29:3:68:LYS:HE3	30:0:2435:U:O2'	2.12	0.49
10:J:19:MET:HE1	10:J:132:LEU:HD21	1.93	0.49
14:N:132:ASN:HD22	30:0:2413:A:C4'	2.25	0.49
19:S:49:VAL:HG13	19:S:66:VAL:HG13	1.95	0.49
26:Z:64:PRO:HB2	26:Z:86:TYR:HE2	1.78	0.49
30:0:10:U:O4	30:0:532:A:H8	1.96	0.48
30:0:146:U:O2'	30:0:147:G:H5'	2.12	0.48
30:0:2269:C:H2'	30:0:2270:G:H5'	1.95	0.48
30:0:59:A:H5'	38:0:4330:HOH:O	2.13	0.48
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.48
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.95	0.48
6:F:91:VAL:HG12	6:F:92:GLY:N	2.22	0.48
17:Q:11:ARG:HH22	30:0:2363:G:H5''	1.78	0.48
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.94	0.48
30:0:1447:U:H3'	30:0:1506:U:O2	2.12	0.48
30:0:1641:A:O2'	30:0:1642:A:H5'	2.13	0.48
30:0:2061:C:C2'	30:0:2062:A:H5'	2.43	0.48
30:0:2073:G:C6	30:0:2489:G:H4'	2.48	0.48
30:0:2710:U:O2'	30:0:2711:U:H5'	2.13	0.48
29:3:5:ARG:O	29:3:21:GLU:HA	2.12	0.48
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.95	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
16:P:64:GLU:HG2	38:P:169:HOH:O	2.13	0.48
21:U:50:GLU:O	21:U:56:ARG:HG2	2.13	0.48
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.65	0.48
30:0:1461:U:H2'	30:0:1462:C:C6	2.48	0.48
30:0:1566:C:H2'	30:0:1567:G:H8	1.78	0.48
30:0:1922:A:N1	30:0:2449:G:O2'	2.46	0.48
30:0:2509:A:H2'	30:0:2510:C:O4'	2.13	0.48
30:0:2512:U:H4'	30:0:2514:U:O4	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2616:G:H1'	38:0:9428:HOH:O	2.12	0.48
30:0:311:C:H2'	30:0:312:U:H6	1.77	0.48
30:0:305:A:C5	30:0:329:A:C2	3.02	0.48
30:0:344:C:H2'	30:0:345:G:O4'	2.12	0.48
30:0:598:C:H2'	30:0:599:G:H8	1.77	0.48
30:0:682:A:H2'	30:0:683:G:O4'	2.13	0.48
1:A:212:PRO:HB2	38:A:8985:HOH:O	2.13	0.48
2:B:49:THR:HG22	2:B:50:HIS:H	1.79	0.48
11:K:74:VAL:HG21	11:K:96:VAL:HG23	1.95	0.48
13:M:164:THR:CG2	13:M:165:GLY:N	2.75	0.48
13:M:70:GLY:HA3	13:M:73:ARG:CZ	2.42	0.48
20:T:8:ARG:NH1	30:0:31:C:OP2	2.46	0.48
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.13	0.48
30:0:1706:G:C6	30:0:1707:G:N1	2.81	0.48
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.48
30:0:370:G:O2'	30:0:371:U:H5'	2.14	0.48
12:L:143:THR:HG22	12:L:144:ASP:N	2.28	0.48
30:0:1188:A:H5'	38:0:7418:HOH:O	2.12	0.48
30:0:1626:A:H2'	30:0:1627:G:H5'	1.96	0.48
30:0:1835:U:H3'	38:0:5569:HOH:O	2.12	0.48
30:0:2511:A:H2'	30:0:2512:U:C6	2.47	0.48
30:0:2626:C:H2'	30:0:2627:G:C8	2.49	0.48
30:0:2651:C:H2'	30:0:2652:U:O4'	2.13	0.48
30:0:2673:U:C4	30:0:2674:G:C6	3.01	0.48
30:0:645:U:O2	30:0:761:A:H2	1.97	0.48
30:0:809:G:H2'	30:0:810:G:H8	1.78	0.48
30:0:816:G:C6	30:0:817:G:N1	2.82	0.48
26:Z:37:ARG:HB2	30:0:819:A:O4'	2.14	0.48
29:3:64:LYS:HA	29:3:84:ARG:CA	2.38	0.48
13:M:48:LYS:HE3	13:M:52:GLN:HE21	1.78	0.48
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.95	0.48
30:0:1187:U:O2'	30:0:1188:A:C8	2.64	0.48
30:0:1684:A:O2'	30:0:1685:A:H5''	2.14	0.48
30:0:1905:U:H2'	30:0:1906:C:H6	1.79	0.48
30:0:2713:G:O2'	30:0:2714:U:H5'	2.13	0.48
30:0:421:C:H4'	30:0:1919:A:C6	2.49	0.48
29:3:64:LYS:HD3	29:3:82:GLY:O	2.13	0.48
11:K:130:MET:SD	21:U:25:ASP:O	2.71	0.48
13:M:74:LYS:O	13:M:88:VAL:HG13	2.13	0.48
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.43	0.48
20:T:48:VAL:HG12	20:T:49:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.36	0.48
26:Z:74:GLN:HG2	26:Z:80:GLN:HB2	1.95	0.48
30:0:1343:C:H2'	30:0:1344:G:O5'	2.12	0.48
30:0:154:C:H2'	30:0:155:C:C6	2.49	0.48
30:0:2608:C:H2'	38:0:3561:HOH:O	2.13	0.48
30:0:696:C:HO2'	30:0:697:G:H5'	1.78	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.49	0.48
31:9:23:U:H2'	31:9:23:U:O2	2.14	0.48
2:B:74:ILE:HG13	38:B:9075:HOH:O	2.13	0.48
5:E:101:GLU:HB2	5:E:116:THR:O	2.13	0.48
12:L:65:ASP:HA	12:L:109:LEU:O	2.14	0.48
18:R:33:ARG:NH1	38:R:8944:HOH:O	2.47	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.14	0.48
1:A:72:GLU:HG2	26:Z:100:GLY:CA	2.40	0.48
30:0:1168:C:H5	38:0:7488:HOH:O	1.96	0.48
30:0:1422:U:H2'	30:0:1423:C:C6	2.49	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.44	0.48
30:0:228:C:C2'	30:0:229:G:H5'	2.44	0.48
30:0:2524:G:N2	30:0:2526:C:N4	2.57	0.48
30:0:284:C:H4'	30:0:285:A:H8	1.79	0.48
30:0:533:U:H3'	38:0:3736:HOH:O	2.13	0.48
30:0:589:U:H2'	30:0:590:A:C8	2.47	0.48
2:B:84:LEU:HD23	2:B:142:LEU:HD23	1.96	0.48
10:J:135:ILE:O	10:J:139:LEU:HG	2.14	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.96	0.48
13:M:73:ARG:HH22	30:0:2263:G:H5''	1.77	0.48
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.75	0.48
23:W:107:LEU:O	23:W:112:LEU:HB2	2.13	0.48
38:2:3526:HOH:O	30:0:1413:A:H5''	2.14	0.48
30:0:1795:G:H2'	30:0:1796:A:O4'	2.13	0.48
30:0:1965:C:H2'	30:0:1966:U:C6	2.49	0.48
30:0:2614:C:O2'	30:0:2615:U:H5'	2.13	0.48
30:0:581:G:O2'	30:0:582:U:H5'	2.13	0.48
31:9:38:A:H2	31:9:43:G:H5''	1.77	0.48
30:0:113:A:C8	30:0:114:A:C8	3.02	0.48
30:0:138:U:OP2	30:0:139:C:C5	2.67	0.48
30:0:1592:G:C4	30:0:1593:C:C5	3.02	0.48
30:0:1706:G:C5	30:0:1707:G:C6	3.02	0.48
30:0:1790:C:H2'	30:0:1791:U:H6	1.79	0.48
30:0:2296:C:H2'	30:0:2297:U:H6	1.79	0.48
4:D:52:THR:HG21	30:0:2346:C:O2'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2842:G:C2'	30:0:2843:A:H5'	2.44	0.48
30:0:542:A:H2'	30:0:543:G:O4'	2.14	0.48
31:9:5:G:C2'	31:9:6:C:H5'	2.43	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.40	0.48
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.44	0.48
3:C:206:ASN:HB2	30:0:329:A:OP2	2.13	0.48
13:M:40:ILE:HG21	13:M:64:ARG:NH2	2.29	0.48
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.49	0.48
20:T:38:ARG:NH1	38:0:6667:HOH:O	2.47	0.48
23:W:134:GLU:OE2	31:9:97:U:H1'	2.14	0.48
24:X:85:VAL:HG12	24:X:86:GLU:N	2.29	0.48
30:0:1735:C:H2'	30:0:1736:A:C8	2.49	0.47
30:0:1878:G:C1'	38:0:6104:HOH:O	2.62	0.47
30:0:2074:A:H2'	38:0:3520:HOH:O	2.13	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.47
1:A:42:VAL:HG21	1:A:74:VAL:CG1	2.44	0.47
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.96	0.47
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.14	0.47
14:N:22:GLN:O	14:N:26:LEU:HB2	2.14	0.47
18:R:39:THR:HB	18:R:42:GLU:CG	2.44	0.47
23:W:11:VAL:O	23:W:12:ASN:HB2	2.14	0.47
30:0:2864:U:C2'	30:0:2865:G:H5'	2.44	0.47
30:0:45:A:N6	30:0:147:G:C4	2.83	0.47
30:0:24:G:H22	30:0:518:G:H1'	1.79	0.47
30:0:844:A:C6	30:0:882:A:C6	3.02	0.47
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.79	0.47
10:J:107:ASN:ND2	10:J:109:TYR:H	2.11	0.47
16:P:102:ARG:NH2	30:0:1596:U:C5	2.82	0.47
30:0:1205:U:C2'	30:0:1206:U:H5''	2.44	0.47
30:0:1787:C:H4'	30:0:2883:A:O4'	2.14	0.47
30:0:2241:C:O2'	30:0:2242:U:H5'	2.14	0.47
30:0:2890:A:H2'	30:0:2890:A:N3	2.29	0.47
30:0:301:C:H2'	30:0:302:A:H8	1.79	0.47
30:0:703:G:H2'	30:0:704:C:C6	2.49	0.47
27:1:20:ARG:HG2	30:0:111:C:O2'	2.14	0.47
28:2:29:THR:HG22	30:0:86:A:O4'	2.14	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.13	0.47
2:B:41:PHE:HB3	2:B:190:MET:CE	2.44	0.47
2:B:54:VAL:HB	38:B:9084:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.96	0.47
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.96	0.47
26:Z:65:ASN:HD22	26:Z:84:CYS:HB2	1.80	0.47
30:0:1561:U:H5'	38:0:7421:HOH:O	2.13	0.47
30:0:1603:A:H5''	30:0:1604:G:H3'	1.96	0.47
30:0:2032:U:C2'	30:0:2033:G:C5'	2.93	0.47
29:3:10:TYR:HE2	30:0:2382:A:H1'	1.80	0.47
30:0:2784:A:H8	30:0:2784:A:O5'	1.98	0.47
30:0:95:A:H5''	30:0:97:G:O4'	2.14	0.47
31:9:108:C:H2'	31:9:109:G:H8	1.79	0.47
2:B:305:ASP:O	2:B:306:LYS:HB2	2.15	0.47
3:C:153:VAL:O	3:C:157:LEU:HG	2.15	0.47
16:P:55:LYS:HG3	16:P:56:GLY:N	2.29	0.47
20:T:48:VAL:HG13	20:T:97:ARG:O	2.14	0.47
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	1.96	0.47
30:0:1217:G:C2	30:0:1218:U:C2	3.03	0.47
30:0:1942:A:H3'	38:0:7336:HOH:O	2.14	0.47
30:0:2336:G:C2'	38:0:6280:HOH:O	2.60	0.47
30:0:2697:A:H2'	30:0:2698:G:O4'	2.15	0.47
30:0:2908:A:O5'	30:0:2908:A:H8	1.97	0.47
30:0:292:G:H2'	30:0:358:G:N2	2.30	0.47
30:0:599:G:H2'	30:0:600:G:H8	1.79	0.47
30:0:810:G:H2'	30:0:811:C:C6	2.49	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.95	0.47
13:M:75:ARG:HB2	38:M:8905:HOH:O	2.14	0.47
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.96	0.47
1:A:45:ILE:HG22	26:Z:78:ILE:HG12	1.96	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47
30:0:1318:A:H4'	30:0:1343:C:H4'	1.96	0.47
30:0:1359:U:C5	30:0:2101:A:C8	3.03	0.47
30:0:2510:C:H5'	30:0:2511:A:OP2	2.13	0.47
30:0:371:U:H2'	30:0:372:A:C8	2.49	0.47
30:0:960:G:H3'	30:0:960:G:N3	2.30	0.47
29:3:46:ILE:HG12	38:0:3138:HOH:O	2.14	0.47
29:3:79:LEU:HB2	38:0:6581:HOH:O	2.14	0.47
1:A:186:TRP:CG	1:A:187:PRO:HA	2.50	0.47
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.47	0.47
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.47
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.97	0.47
10:J:131:THR:HG22	10:J:133:GLY:H	1.79	0.47
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:91:ILE:HD11	38:M:8830:HOH:O	2.15	0.47
23:W:120:PRO:HG2	30:0:1095:U:O2	2.14	0.47
23:W:119:HIS:HD2	23:W:120:PRO:O	1.97	0.47
30:0:1042:U:O2'	30:0:1043:C:H5'	2.15	0.47
30:0:1523:G:C6	30:0:1524:U:C4	3.03	0.47
30:0:2686:C:C2	30:0:2709:G:N2	2.82	0.47
2:B:98:THR:HG23	30:0:2820:A:OP1	2.15	0.47
30:0:484:A:N1	30:0:506:G:H4'	2.30	0.47
30:0:512:G:O3'	30:0:513:A:H8	1.97	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.14	0.47
18:R:68:HIS:CD2	18:R:76:ASP:HB2	2.50	0.47
23:W:121:PRO:HA	23:W:153:MET:HG2	1.96	0.47
23:W:88:THR:HB	38:W:6679:HOH:O	2.14	0.47
30:0:1173:A:H4'	30:0:1174:A:C8	2.49	0.47
30:0:1769:C:O2'	30:0:1770:U:H5'	2.15	0.47
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.47
30:0:1864:C:H2'	30:0:1865:A:O4'	2.14	0.47
30:0:1882:C:H2'	30:0:1883:U:H6	1.80	0.47
30:0:2598:U:O2	30:0:2600:A:C8	2.68	0.47
30:0:282:C:H1'	30:0:368:C:H41	1.78	0.47
29:3:50:GLY:HA3	38:0:9164:HOH:O	2.14	0.47
30:0:1183:C:C2	30:0:1184:C:C5	3.03	0.47
30:0:1187:U:O2'	30:0:1189:A:H2	1.98	0.47
30:0:1377:C:C5'	30:0:1377:C:H6	2.28	0.47
30:0:2134:G:N2	30:0:2242:U:C2	2.83	0.47
30:0:2253:G:H2'	30:0:2254:G:H8	1.80	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.14	0.47
30:0:2383:G:C6	30:0:2384:U:C4	3.03	0.47
30:0:2752:C:O2'	30:0:2753:G:H5'	2.15	0.47
30:0:304:G:H8	30:0:304:G:O5'	1.98	0.47
29:3:24:LYS:HE3	29:3:90:PHE:CE1	2.50	0.47
1:A:121:ALA:O	1:A:124:VAL:HG22	2.14	0.47
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.80	0.47
17:Q:14:LEU:HD21	17:Q:43:ILE:HD12	1.97	0.47
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.63	0.47
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.47
23:W:29:VAL:O	23:W:30:ASN:HB2	2.13	0.47
8:H:91:ARG:HB2	30:0:1003:U:OP1	2.15	0.47
30:0:1966:U:O5'	30:0:1966:U:H6	1.98	0.47
30:0:2096:A:H2'	30:0:2539:U:O4'	2.14	0.47
30:0:2769:C:H2'	30:0:2770:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:36:C:C2	30:0:447:A:C2	3.03	0.47
30:0:371:U:H2'	30:0:372:A:H8	1.80	0.47
30:0:447:A:O2'	30:0:448:G:H5'	2.15	0.47
25:Y:137:LYS:HD2	30:0:521:A:H5''	1.97	0.47
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.47
30:0:1878:G:O2'	30:0:1879:U:C5	2.66	0.47
30:0:2604:A:H5'	38:0:5775:HOH:O	2.14	0.47
30:0:613:C:H2'	30:0:614:U:C6	2.46	0.47
30:0:805:G:N2	30:0:807:A:H3'	2.30	0.47
3:C:103:ASN:ND2	30:0:663:C:H5''	2.29	0.47
13:M:111:ASN:HB2	38:M:8849:HOH:O	2.14	0.47
17:Q:11:ARG:CZ	30:0:2363:G:H4'	2.44	0.47
18:R:82:GLU:HG3	18:R:83:LYS:N	2.29	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:1350:U:H4'	38:0:5115:HOH:O	2.15	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:1477:C:H4'	30:0:1868:G:OP1	2.15	0.46
30:0:1969:A:C2'	30:0:1970:G:H5'	2.45	0.46
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.44	0.46
5:E:93:MET:HE1	5:E:165:GLY:H	1.79	0.46
5:E:7:ILE:HG23	5:E:45:ASP:O	2.15	0.46
30:0:1163:G:N1	30:0:1184:C:N4	2.64	0.46
30:0:1116:U:C2	30:0:1246:A:N6	2.83	0.46
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.14	0.46
30:0:1634:G:H2'	38:0:3889:HOH:O	2.15	0.46
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.46
30:0:1949:G:H22	30:0:1964:U:H1'	1.79	0.46
30:0:1838:U:O2'	30:0:2644:C:H5'	2.15	0.46
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.46
30:0:735:C:H3'	30:0:736:A:C8	2.50	0.46
30:0:877:G:C5'	30:0:878:G:OP1	2.62	0.46
30:0:921:G:H4'	30:0:924:G:N1	2.30	0.46
29:3:69:TYR:O	29:3:77:ALA:HA	2.15	0.46
2:B:79:MET:HE1	38:B:9096:HOH:O	2.15	0.46
11:K:34:VAL:HB	38:K:7169:HOH:O	2.15	0.46
30:0:1197:G:H1'	30:0:1203:G:C2	2.51	0.46
30:0:130:C:O2'	30:0:131:A:N7	2.46	0.46
30:0:1545:C:H1'	30:0:1641:A:N6	2.29	0.46
30:0:1617:C:C5	30:0:1643:C:H4'	2.50	0.46
30:0:1797:A:O3'	30:0:1798:C:C6	2.69	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2102:G:C2	30:0:2103:A:N6	2.83	0.46
30:0:2256:G:H2'	30:0:2257:G:C5'	2.46	0.46
30:0:2347:C:H2'	30:0:2348:C:C6	2.50	0.46
30:0:2526:C:H5'	30:0:2526:C:C6	2.50	0.46
30:0:530:C:H4'	30:0:612:U:H4'	1.97	0.46
30:0:790:A:H2'	30:0:791:A:O4'	2.16	0.46
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.77	0.46
7:G:63:ARG:N	38:G:2569:HOH:O	2.48	0.46
16:P:87:ARG:HG2	38:P:186:HOH:O	2.15	0.46
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.46
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.13	0.46
22:V:27:LEU:HA	22:V:49:LEU:HD13	1.98	0.46
29:3:47:GLY:HA2	30:0:2121:G:H4'	1.97	0.46
30:0:2297:U:H1'	38:0:5172:HOH:O	2.16	0.46
30:0:2438:G:H2'	30:0:2439:C:C6	2.50	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:238:C:H4'	30:0:287:C:OP1	2.16	0.46
30:0:834:G:C4'	30:0:835:U:OP2	2.61	0.46
27:1:25:LYS:O	27:1:25:LYS:HG2	2.16	0.46
4:D:29:HIS:N	4:D:29:HIS:ND1	2.61	0.46
5:E:84:MET:HG2	5:E:168:ILE:HA	1.98	0.46
21:U:13:ILE:HG13	38:U:3194:HOH:O	2.15	0.46
30:0:2434:A:H2'	30:0:2435:U:O4'	2.15	0.46
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.46
6:F:111:ILE:O	6:F:115:VAL:HG23	2.15	0.46
10:J:80:LYS:HE3	10:J:101:VAL:O	2.14	0.46
12:L:10:SER:O	12:L:11:ARG:HB3	2.16	0.46
13:M:102:GLU:CD	13:M:164:THR:HG21	2.36	0.46
21:U:56:ARG:HD2	30:0:2890:A:C1'	2.46	0.46
30:0:100:C:H2'	30:0:101:C:H6	1.80	0.46
30:0:101:C:H2'	30:0:102:A:H8	1.80	0.46
30:0:1154:A:H2'	30:0:1155:G:C8	2.50	0.46
30:0:1434:A:H2'	30:0:1436:C:C5	2.51	0.46
30:0:461:C:N3	30:0:479:G:H5'	2.31	0.46
30:0:660:A:N6	30:0:746:A:O4'	2.49	0.46
29:3:1:MET:HG2	29:3:87:ARG:O	2.16	0.46
31:9:14:G:H8	31:9:14:G:C5'	2.16	0.46
30:0:134:U:C2	30:0:145:A:C2	3.04	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.46
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:17:G:H2'	30:0:18:C:C6	2.51	0.46
30:0:1878:G:O2'	30:0:1879:U:OP2	2.33	0.46
30:0:365:G:C5	30:0:366:U:C5	3.04	0.46
30:0:517:U:C2'	30:0:518:G:H5'	2.46	0.46
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.46
27:1:16:HIS:HE1	30:0:775:G:OP1	1.97	0.46
2:B:144:THR:HG22	2:B:145:HIS:N	2.31	0.46
8:H:48:VAL:HA	8:H:170:ARG:O	2.15	0.46
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.50	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.48	0.46
16:P:115:SER:OG	16:P:118:GLN:HG3	2.16	0.46
30:0:1526:A:H4'	30:0:1527:A:C5'	2.45	0.46
30:0:1764:C:O2'	30:0:1765:G:H5'	2.15	0.46
30:0:1845:A:C2'	30:0:1846:U:H5'	2.45	0.46
30:0:1871:U:O4'	30:0:1873:G:C8	2.69	0.46
30:0:1894:C:N4	30:0:1939:U:H2'	2.30	0.46
30:0:241:A:C2	30:0:378:A:H4'	2.51	0.46
30:0:2537:G:H5''	30:0:2538:A:H5''	1.98	0.46
30:0:2812:A:N7	38:0:7508:HOH:O	2.36	0.46
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.81	0.46
29:3:30:GLN:HB3	38:3:9051:HOH:O	2.16	0.46
31:9:3:A:H2	31:9:21:G:N3	2.14	0.46
31:9:47:A:C2	31:9:48:C:C2	3.04	0.46
2:B:232:TRP:CZ3	30:0:2614:C:H5''	2.51	0.46
2:B:85:ARG:NH1	38:B:9106:HOH:O	2.47	0.46
12:L:34:GLY:HA2	38:L:9017:HOH:O	2.16	0.46
13:M:47:ASP:CG	13:M:48:LYS:N	2.70	0.46
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.16	0.46
20:T:16:LEU:HB2	30:0:100:C:H4'	1.98	0.46
30:0:1021:G:O2'	30:0:1022:A:H5'	2.16	0.46
30:0:1132:A:H61	30:0:1229:C:H2'	1.80	0.46
30:0:1294:A:H2'	30:0:1295:G:O4'	2.16	0.46
30:0:1346:U:H2'	30:0:1347:U:C6	2.50	0.46
30:0:1634:G:C4	30:0:1635:U:C5	3.03	0.46
14:N:22:GLN:HG3	30:0:2415:A:C2	2.51	0.46
30:0:2624:A:H1'	38:0:9764:HOH:O	2.14	0.46
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.46
30:0:594:C:C2'	30:0:595:U:H5'	2.46	0.46
1:A:230:SER:HB2	30:0:1852:A:H4'	1.97	0.46
3:C:43:LYS:HG2	30:0:449:A:N7	2.31	0.46
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1012:A:O5'	30:0:1012:A:H8	1.99	0.46
30:0:1166:A:C6	30:0:1181:A:C2	3.04	0.46
30:0:1588:G:C6	30:0:1589:G:N1	2.84	0.46
30:0:1615:A:H4'	38:0:5868:HOH:O	2.16	0.46
30:0:1615:A:H5'	38:0:4181:HOH:O	2.15	0.46
30:0:2017:U:O2'	30:0:2018:A:C8	2.66	0.46
30:0:2276:U:H2'	30:0:2277:U:C6	2.51	0.46
30:0:2488:A:H1'	38:0:9096:HOH:O	2.16	0.46
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.46
30:0:483:C:C4	30:0:484:A:C6	3.04	0.46
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.46
31:9:65:A:C2'	31:9:66:G:OP2	2.64	0.46
13:M:169:ARG:HD2	38:M:8885:HOH:O	2.16	0.46
38:C:8575:HOH:O	20:T:2:LYS:HE2	2.15	0.46
30:0:1052:G:H2'	30:0:1052:G:N3	2.31	0.45
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
30:0:1029:U:O2'	30:0:1273:C:OP1	2.31	0.45
30:0:1409:G:C2	30:0:1410:G:C8	3.04	0.45
30:0:1520:G:C6	30:0:1521:C:C4	3.05	0.45
30:0:1756:G:H1'	38:0:6244:HOH:O	2.15	0.45
30:0:1890:U:H4'	30:0:2010:A:C6	2.51	0.45
30:0:255:A:C4	30:0:256:C:C5	3.05	0.45
30:0:2740:G:H2'	30:0:2741:A:O4'	2.15	0.45
30:0:71:G:H8	38:0:3908:HOH:O	1.98	0.45
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.98	0.45
30:0:1625:U:H4'	38:0:4661:HOH:O	2.15	0.45
30:0:1768:C:H2'	30:0:1769:C:O4'	2.16	0.45
30:0:2057:U:O5'	30:0:2057:U:H6	1.98	0.45
30:0:2717:C:C2'	30:0:2718:C:C5'	2.84	0.45
30:0:293:A:C5	30:0:360:A:C2	3.04	0.45
30:0:633:C:O2'	30:0:634:G:H5'	2.15	0.45
30:0:810:G:H2'	30:0:811:C:H6	1.81	0.45
28:2:28:LYS:O	30:0:87:C:H2'	2.17	0.45
14:N:37:ARG:NH1	31:9:6:C:OP1	2.48	0.45
30:0:1131:G:C6	30:0:1230:A:C4	3.04	0.45
30:0:1310:U:C2'	30:0:1311:G:O5'	2.64	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.04	0.45
30:0:1730:G:H4'	30:0:1731:C:H6	1.82	0.45
30:0:1856:C:H1'	38:0:5858:HOH:O	2.17	0.45
30:0:1882:C:H2'	30:0:1883:U:C6	2.51	0.45
30:0:1902:G:O2'	30:0:1903:U:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2298:C:O2'	30:0:2299:G:H5'	2.17	0.45
30:0:612:U:H2'	30:0:613:C:C6	2.52	0.45
27:1:11:LYS:HG2	30:0:777:U:O2'	2.17	0.45
29:3:70:ARG:NH2	29:3:77:ALA:HB3	2.31	0.45
31:9:28:U:O2	31:9:57:A:N6	2.50	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.65	0.45
30:0:1342:C:H2'	30:0:1343:C:H5'	1.99	0.45
18:R:128:ARG:NH2	30:0:2054:A:C2	2.84	0.45
30:0:2438:G:H2'	30:0:2439:C:H6	1.81	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45
26:Z:34:SER:HA	30:0:797:A:C4'	2.46	0.45
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.99	0.45
2:B:275:GLY:O	2:B:291:ASP:HA	2.16	0.45
12:L:142:LEU:HG	12:L:146:GLY:HA3	1.99	0.45
13:M:88:VAL:HG13	38:M:8902:HOH:O	2.16	0.45
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.45
30:0:1187:U:C2	30:0:1189:A:OP2	2.70	0.45
30:0:1540:G:C4	30:0:1541:G:C8	3.05	0.45
30:0:1613:C:H2'	30:0:1614:G:O4'	2.15	0.45
30:0:169:A:HO2'	30:0:170:U:H6	1.63	0.45
30:0:1758:U:O2'	30:0:1759:A:H5'	2.15	0.45
30:0:2032:U:C2'	30:0:2033:G:H5''	2.46	0.45
30:0:2315:C:H4'	30:0:2425:A:C6	2.51	0.45
29:3:9:THR:HG23	29:3:20:HIS:ND1	2.32	0.45
14:N:40:ASN:HD22	31:9:28:U:H5''	1.82	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.17	0.45
11:K:115:ARG:HG3	11:K:116:GLU:N	2.32	0.45
30:0:1016:U:H2'	30:0:1017:U:O4'	2.17	0.45
30:0:1278:A:H4'	30:0:1279:U:C5	2.49	0.45
30:0:1535:G:H2'	30:0:1536:C:C6	2.52	0.45
30:0:1603:A:H5''	30:0:1605:G:C5'	2.39	0.45
30:0:2104:C:O2	30:0:2485:A:N1	2.49	0.45
30:0:2505:G:H3'	38:0:5626:HOH:O	2.17	0.45
30:0:2591:C:H2'	30:0:2592:G:O4'	2.16	0.45
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.52	0.45
8:H:123:ILE:HD12	8:H:123:ILE:N	2.32	0.45
8:H:165:ARG:HD2	38:H:9029:HOH:O	2.16	0.45
8:H:170:ARG:HD2	38:H:8987:HOH:O	2.15	0.45
10:J:42:GLU:HG2	10:J:43:ARG:HG3	1.98	0.45
12:L:75:LEU:HD21	38:O:7543:HOH:O	2.17	0.45
15:O:87:THR:O	15:O:91:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:14:GLU:O	21:U:17:THR:HB	2.16	0.45
25:Y:142:SER:HB2	38:Y:8903:HOH:O	2.16	0.45
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.50	0.45
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.45
30:0:212:A:O4'	30:0:214:U:C6	2.70	0.45
30:0:2321:A:C4	30:0:2323:G:C8	3.05	0.45
30:0:2778:A:C2	30:0:2797:C:O2	2.70	0.45
30:0:352:A:H2'	30:0:353:G:H8	1.79	0.45
2:B:254:GLN:HG2	2:B:255:GLY:N	2.31	0.45
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.47	0.45
21:U:6:CYS:SG	21:U:13:ILE:HB	2.57	0.45
30:0:1151:G:H2'	38:0:5008:HOH:O	2.17	0.45
30:0:1346:U:H2'	30:0:1347:U:H6	1.82	0.45
1:A:47:HIS:HD2	30:0:1654:U:C2'	2.30	0.45
30:0:2071:C:H5'	38:0:9532:HOH:O	2.17	0.45
30:0:213:G:N2	30:0:225:G:H2'	2.31	0.45
30:0:226:A:H1'	30:0:393:G:C5	2.51	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
30:0:644:G:H1'	38:0:6390:HOH:O	2.16	0.45
30:0:727:G:C2	30:0:728:C:C2	3.05	0.45
30:0:867:A:H2	30:0:880:C:O2	2.00	0.45
30:0:921:G:H4'	30:0:924:G:C6	2.52	0.45
31:9:26:C:H5''	38:9:9049:HOH:O	2.17	0.45
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.47	0.45
3:C:170:ASP:OD2	30:0:330:C:H5	2.00	0.45
14:N:110:THR:HB	14:N:113:SER:OG	2.17	0.45
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.99	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45
23:W:129:LYS:HE2	30:0:1098:A:O3'	2.17	0.45
30:0:113:A:H3'	30:0:114:A:H5''	1.98	0.45
30:0:1755:A:H2'	30:0:1756:G:O4'	2.16	0.45
30:0:2596:A:H2	33:0:8812:CL:CL	2.37	0.45
30:0:2650:U:O2'	30:0:2651:C:H5'	2.16	0.45
30:0:2691:A:H5'	30:0:2693:U:H1'	1.99	0.45
30:0:2735:U:H2'	30:0:2736:U:C6	2.52	0.45
30:0:282:C:H2'	30:0:283:U:O4'	2.16	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.45
30:0:559:U:H2'	30:0:560:U:O4'	2.17	0.45
30:0:941:G:C6	30:0:942:U:C4	3.05	0.45
31:9:82:U:H2'	31:9:83:G:C8	2.52	0.45
2:B:252:PRO:HD2	30:0:2548:C:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:CG	3:C:27:ARG:HH11	2.15	0.45
4:D:154:LYS:HD2	4:D:154:LYS:N	2.22	0.45
12:L:136:ALA:HB3	38:L:9035:HOH:O	2.17	0.45
13:M:68:ARG:HD3	13:M:68:ARG:C	2.37	0.45
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.45
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.17	0.45
30:0:1249:U:H2'	30:0:1250:C:H6	1.82	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.45
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.45
30:0:2010:A:C2'	38:0:5942:HOH:O	2.51	0.45
30:0:2252:A:C5	30:0:2253:G:H1'	2.51	0.45
30:0:792:G:O2'	30:0:793:A:H5'	2.16	0.45
2:B:5:ARG:HD2	2:B:8:LYS:HE2	1.99	0.45
3:C:39:GLN:O	3:C:43:LYS:HD3	2.17	0.45
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.51	0.45
1:A:76:VAL:HG23	26:Z:87:LYS:O	2.17	0.45
30:0:1209:C:C2	30:0:1210:G:C8	3.04	0.44
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.44
30:0:152:A:H2'	30:0:153:C:C6	2.52	0.44
30:0:2301:A:H5''	30:0:2302:A:H5'	1.99	0.44
30:0:2335:C:H2'	30:0:2336:G:H8	1.80	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
30:0:2837:U:H2'	38:0:6825:HOH:O	2.15	0.44
30:0:65:C:O2'	30:0:66:G:H5'	2.16	0.44
30:0:699:C:C2	30:0:744:G:N2	2.85	0.44
30:0:797:A:N6	30:0:816:G:H1'	2.32	0.44
28:2:41:HIS:H	28:2:45:ASN:ND2	2.04	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.65	0.44
13:M:72:ALA:C	13:M:74:LYS:H	2.20	0.44
15:O:98:LEU:O	15:O:102:ILE:HG13	2.17	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.16	0.44
18:R:114:VAL:HG13	18:R:114:VAL:O	2.18	0.44
30:0:1310:U:H2'	30:0:1311:G:O5'	2.17	0.44
21:U:42:LEU:O	30:0:1810:C:H5'	2.17	0.44
30:0:1949:G:N2	30:0:1964:U:H1'	2.32	0.44
30:0:2074:A:H1'	38:0:9875:HOH:O	2.16	0.44
30:0:2250:G:C2	30:0:2251:G:H1'	2.52	0.44
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.44
30:0:2734:G:O2'	30:0:2735:U:H5'	2.17	0.44
30:0:365:G:C5	30:0:366:U:C4	3.05	0.44
30:0:598:C:H2'	30:0:599:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:1:U:O3'	31:9:3:A:H5''	2.16	0.44
1:A:206:ARG:HH21	30:0:2629:C:N4	2.16	0.44
1:A:51:ARG:C	1:A:53:ALA:H	2.20	0.44
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.81	0.44
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.99	0.44
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.44
30:0:1206:U:C3'	30:0:1206:U:C6	3.01	0.44
30:0:1279:U:C5'	30:0:1280:A:OP2	2.65	0.44
30:0:1461:U:H2'	30:0:1462:C:H6	1.83	0.44
30:0:1735:C:O2'	30:0:1736:A:H5'	2.17	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.17	0.44
30:0:2410:G:O2'	30:0:2411:C:H5'	2.18	0.44
30:0:2642:G:H2'	30:0:2643:G:O4'	2.16	0.44
30:0:2777:G:O2'	30:0:2778:A:H5'	2.17	0.44
30:0:307:G:C2	30:0:309:C:C4	3.05	0.44
30:0:40:C:O5'	30:0:40:C:H6	2.01	0.44
30:0:734:U:H2'	30:0:736:A:OP2	2.17	0.44
30:0:970:U:H2'	38:0:6313:HOH:O	2.16	0.44
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.44
5:E:3:VAL:HG22	5:E:49:ILE:HB	2.00	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.65	0.44
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.82	0.44
38:B:9136:HOH:O	21:U:17:THR:HG21	2.16	0.44
23:W:24:LEU:O	23:W:26:ILE:HG22	2.18	0.44
26:Z:65:ASN:HB2	26:Z:84:CYS:SG	2.58	0.44
30:0:161:A:H2'	30:0:162:C:C6	2.52	0.44
30:0:1928:C:O2'	30:0:1929:G:H5'	2.17	0.44
13:M:73:ARG:NH2	30:0:2263:G:H5''	2.32	0.44
30:0:2663:U:N3	30:0:2664:A:N6	2.65	0.44
30:0:2755:G:H1'	38:0:4677:HOH:O	2.17	0.44
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.44
30:0:711:G:C2	30:0:718:C:O2	2.70	0.44
3:C:226:GLY:HA3	30:0:1308:A:C4'	2.48	0.44
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.44
4:D:22:VAL:HA	4:D:73:VAL:O	2.17	0.44
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.98	0.44
20:T:71:VAL:HG12	20:T:72:ILE:N	2.32	0.44
30:0:1076:G:C2	30:0:1084:C:C2	3.06	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	1.98	0.44
30:0:2245:C:H6	30:0:2245:C:O5'	2.00	0.44
31:9:82:U:H2'	31:9:83:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HD3	38:0:9221:HOH:O	2.17	0.44
3:C:162:VAL:CG2	3:C:232:LEU:HD21	2.47	0.44
4:D:159:PRO:O	4:D:163:VAL:HG23	2.17	0.44
5:E:95:VAL:HG11	5:E:131:LEU:HD11	1.99	0.44
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.44
18:R:125:ARG:HG2	38:R:8942:HOH:O	2.17	0.44
20:T:23:VAL:HG23	20:T:41:ARG:HG3	2.00	0.44
30:0:1028:U:H1'	38:0:3631:HOH:O	2.18	0.44
30:0:1067:A:H5'	38:0:4344:HOH:O	2.18	0.44
30:0:1116:U:C2'	30:0:1118:A:H2	2.28	0.44
10:J:63:ILE:CD1	30:0:1236:A:C8	3.01	0.44
30:0:2119:C:O2'	30:0:2120:U:H5'	2.18	0.44
30:0:2313:C:H4'	38:0:6558:HOH:O	2.18	0.44
30:0:2325:U:O2'	30:0:2411:C:H1'	2.18	0.44
30:0:2887:G:H2'	30:0:2888:U:H6	1.79	0.44
30:0:549:A:C2	30:0:550:C:C2	3.06	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.18	0.44
30:0:81:G:N3	30:0:98:A:C2	2.85	0.44
3:C:37:ALA:HA	3:C:100:LEU:HD12	2.00	0.44
9:I:114:TYR:N	9:I:114:TYR:CD1	2.86	0.44
12:L:129:ALA:O	12:L:133:VAL:HG23	2.17	0.44
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.18	0.44
13:M:97:ILE:HD13	13:M:127:LYS:HD2	2.00	0.44
14:N:93:GLN:HA	14:N:93:GLN:HE21	1.82	0.44
15:O:49:GLU:OE1	15:O:72:LYS:HG3	2.17	0.44
16:P:18:LYS:O	16:P:21:VAL:HG13	2.18	0.44
19:S:57:THR:CG2	19:S:58:MET:N	2.79	0.44
21:U:7:ASP:HB2	21:U:29:THR:HG23	2.00	0.44
1:A:46:GLU:C	26:Z:78:ILE:HD11	2.38	0.44
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.44
30:0:1249:U:H2'	30:0:1250:C:C6	2.53	0.44
30:0:912:A:C4	30:0:1294:A:C2	3.05	0.44
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.49	0.44
30:0:1597:A:C4	30:0:1598:A:C8	3.05	0.44
27:1:1:THR:O	30:0:1836:A:H1'	2.17	0.44
30:0:1883:U:C2'	30:0:1884:G:H5'	2.48	0.44
4:D:56:ARG:NH2	30:0:2332:A:H5'	2.32	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.44
30:0:462:A:H2'	38:0:4875:HOH:O	2.18	0.44
30:0:615:G:H2'	30:0:616:U:H6	1.83	0.44
30:0:725:C:H2'	30:0:726:C:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:62:THR:HG21	30:0:2317:C:H5'	1.98	0.44
12:L:149:ARG:O	12:L:150:GLN:HB2	2.17	0.44
13:M:171:ARG:NH2	30:0:189:A:OP1	2.50	0.44
17:Q:3:SER:O	17:Q:8:GLU:HG3	2.18	0.44
25:Y:116:LEU:HA	25:Y:116:LEU:HD23	1.80	0.44
30:0:1246:A:C4	30:0:1248:A:C8	3.06	0.44
30:0:1307:A:H2'	30:0:1308:A:C8	2.53	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.96	0.44
30:0:1730:G:H4'	30:0:1731:C:C6	2.52	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
30:0:1773:G:C2'	30:0:1774:G:H5'	2.48	0.44
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.44
30:0:2128:G:C5	30:0:2129:U:C5	3.06	0.44
30:0:2276:U:O2'	30:0:2277:U:H5'	2.18	0.44
30:0:2457:U:O2'	30:0:2458:U:H5'	2.17	0.44
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.53	0.44
30:0:2793:A:H2'	30:0:2794:G:H5'	2.00	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.48	0.44
2:B:119:HIS:O	2:B:121:PRO:HD3	2.18	0.44
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.48	0.44
15:O:21:SER:OG	15:O:106:PRO:HB2	2.18	0.44
23:W:122:ARG:NH2	23:W:154:ARG:HG2	2.33	0.44
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.33	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.53	0.44
30:0:1254:C:O2'	30:0:1255:A:H5'	2.18	0.44
13:M:95:LYS:HE2	30:0:157:G:H4'	1.99	0.44
30:0:1657:A:H2'	30:0:1658:A:C8	2.53	0.44
1:A:26:ASP:OD2	30:0:1872:C:H4'	2.18	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.48	0.44
30:0:2473:U:O2'	30:0:2474:A:H5''	2.18	0.44
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.06	0.44
30:0:416:G:H2'	38:0:9910:HOH:O	2.16	0.44
30:0:559:U:C6	30:0:559:U:C3'	3.01	0.44
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.57	0.44
3:C:27:ARG:HD2	38:O:327:HOH:O	2.17	0.44
8:H:157:TYR:HD1	8:H:157:TYR:C	2.21	0.44
14:N:147:ILE:HD11	31:9:50:G:OP1	2.18	0.44
17:Q:62:THR:O	17:Q:64:GLU:HG2	2.18	0.44
30:0:1198:U:C6	30:0:1200:A:OP2	2.71	0.43
30:0:1592:G:H1'	30:0:1593:C:C6	2.53	0.43
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.43
30:0:590:A:H2'	30:0:591:A:O4'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.52	0.43
4:D:59:GLY:HA3	38:D:4886:HOH:O	2.17	0.43
12:L:117:GLU:HB3	38:L:9018:HOH:O	2.18	0.43
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.43
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.17	0.43
20:T:48:VAL:CG1	20:T:49:GLU:N	2.81	0.43
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.00	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.17	0.43
30:0:1973:A:H2'	30:0:1974:G:O4'	2.17	0.43
17:Q:1:PRO:HA	30:0:2299:G:O6	2.18	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.52	0.43
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.43
5:E:111:LYS:HE3	30:0:2690:U:H4'	1.99	0.43
30:0:549:A:C6	30:0:550:C:C4	3.07	0.43
30:0:596:C:H2'	30:0:597:A:C8	2.53	0.43
31:9:64:C:O2'	31:9:65:A:H5'	2.18	0.43
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.83	0.43
2:B:41:PHE:HB3	2:B:190:MET:HE2	2.00	0.43
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.43
2:B:305:ASP:O	2:B:306:LYS:CB	2.66	0.43
3:C:118:THR:O	3:C:136:VAL:HG13	2.18	0.43
4:D:45:THR:HB	4:D:75:LEU:HD21	1.99	0.43
12:L:41:HIS:CD2	30:0:926:A:O2'	2.71	0.43
16:P:10:ALA:HA	16:P:13:VAL:HG12	2.01	0.43
19:S:50:GLU:HB3	19:S:67:ARG:NH2	2.33	0.43
20:T:38:ARG:HH11	20:T:38:ARG:HG3	1.83	0.43
30:0:107:U:C2'	30:0:108:U:H5'	2.48	0.43
30:0:1362:U:H5'	38:0:3253:HOH:O	2.18	0.43
30:0:1702:U:H5''	38:0:7207:HOH:O	2.19	0.43
30:0:2321:A:N1	30:0:2378:U:O2	2.52	0.43
1:A:211:LYS:HB2	38:A:9038:HOH:O	2.18	0.43
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.00	0.43
14:N:67:ALA:CA	14:N:71:TRP:HB3	2.44	0.43
20:T:48:VAL:HG11	20:T:96:VAL:CG1	2.46	0.43
25:Y:144:ARG:NH1	38:Y:8882:HOH:O	2.51	0.43
25:Y:148:GLY:HA3	30:0:622:G:P	2.59	0.43
30:0:1183:C:H41	30:0:1192:A:P	2.42	0.43
30:0:1878:G:O2'	30:0:1879:U:C6	2.60	0.43
30:0:2474:A:H4'	30:0:2475:C:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2834:G:H2'	30:0:2835:C:O5'	2.18	0.43
30:0:275:G:N2	30:0:376:C:C2	2.87	0.43
30:0:496:G:H3'	38:0:7658:HOH:O	2.18	0.43
30:0:853:C:H2'	30:0:854:G:O4'	2.17	0.43
30:0:920:C:H5''	30:0:921:G:O5'	2.18	0.43
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.17	0.43
2:B:199:TYR:HE1	2:B:319:ASP:HB2	1.83	0.43
2:B:42:ALA:CB	2:B:162:MET:HE3	2.48	0.43
8:H:157:TYR:C	8:H:157:TYR:CD1	2.90	0.43
14:N:154:LEU:C	14:N:156:GLU:H	2.20	0.43
22:V:50:ARG:HH12	30:0:56:G:C5'	2.30	0.43
26:Z:94:LYS:HA	38:Z:8719:HOH:O	2.18	0.43
30:0:1809:G:H2'	30:0:1811:A:OP2	2.19	0.43
30:0:2355:G:H5''	30:0:2356:A:OP2	2.19	0.43
30:0:40:C:H4'	38:0:6993:HOH:O	2.18	0.43
29:3:39:GLN:HG2	29:3:43:ASN:OD1	2.19	0.43
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.52	0.43
23:W:118:LEU:HD12	23:W:153:MET:HE3	2.00	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.99	0.43
30:0:1185:U:H2'	30:0:1186:C:C6	2.54	0.43
30:0:1471:A:H2'	30:0:1472:C:C6	2.54	0.43
30:0:2039:A:H2'	30:0:2040:C:C6	2.53	0.43
30:0:2102:G:N2	30:0:2104:C:N3	2.67	0.43
30:0:2346:C:O5'	30:0:2346:C:C6	2.72	0.43
30:0:2718:C:H5'	30:0:2718:C:C6	2.52	0.43
30:0:557:C:O2'	30:0:558:C:H5'	2.19	0.43
6:F:14:ASP:O	6:F:18:GLU:HG3	2.18	0.43
10:J:19:MET:HE2	10:J:79:PHE:HA	2.01	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.38	0.43
14:N:86:LEU:O	14:N:90:LEU:HG	2.19	0.43
20:T:43:ASN:C	20:T:45:GLY:H	2.22	0.43
22:V:49:LEU:O	22:V:53:ILE:HG13	2.18	0.43
30:0:1173:A:H4'	30:0:1174:A:H8	1.83	0.43
30:0:1427:A:C2'	30:0:1428:C:H5'	2.49	0.43
30:0:1566:C:H2'	30:0:1567:G:C8	2.54	0.43
30:0:1773:G:H4'	38:0:3505:HOH:O	2.19	0.43
30:0:878:G:H4'	30:0:1835:U:H4'	2.00	0.43
11:K:66:ARG:NH2	30:0:1994:A:OP1	2.52	0.43
30:0:2103:A:H2'	30:0:2103:A:N3	2.33	0.43
30:0:2379:G:N3	30:0:2418:G:H2'	2.34	0.43
30:0:2564:G:OP2	30:0:2565:C:H5''	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:328:U:C2	30:0:348:C:H4'	2.53	0.43
30:0:459:A:H4'	38:0:9455:HOH:O	2.17	0.43
30:0:750:A:H2'	30:0:751:U:C6	2.54	0.43
28:2:20:ARG:NH1	28:2:39:ARG:HH21	2.17	0.43
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.48	0.43
31:9:45:A:N7	31:9:46:C:C5	2.87	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
1:A:217:ARG:HG2	1:A:229:ALA:CB	2.48	0.43
1:A:51:ARG:HH21	1:A:53:ALA:HB3	1.82	0.43
10:J:107:ASN:HD22	10:J:107:ASN:C	2.22	0.43
20:T:82:THR:HG21	30:0:488:U:O2'	2.19	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.51	0.43
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	1.99	0.43
30:0:119:A:H2'	30:0:120:A:C5'	2.49	0.43
38:M:8865:HOH:O	30:0:2244:A:H1'	2.18	0.43
30:0:2681:A:H4'	30:0:2682:C:OP1	2.19	0.43
30:0:2694:A:H3'	30:0:2695:C:H6	1.84	0.43
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.83	0.43
30:0:361:C:H2'	30:0:362:G:O4'	2.19	0.43
31:9:110:G:C5	31:9:111:U:C5	3.07	0.43
31:9:110:G:C2	31:9:111:U:C6	3.07	0.43
1:A:192:VAL:O	1:A:207:GLN:HG2	2.18	0.43
3:C:132:ASP:O	3:C:133:ARG:HG3	2.19	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.17	0.43
14:N:109:PRO:HB3	30:0:2413:A:N7	2.34	0.43
14:N:49:THR:HG22	14:N:56:ASP:CB	2.49	0.43
18:R:59:PHE:O	18:R:63:ASN:HB3	2.18	0.43
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.84	0.43
26:Z:95:PRO:HD2	38:Z:8719:HOH:O	2.18	0.43
30:0:1099:G:H2'	30:0:1100:G:O4'	2.19	0.43
30:0:1156:C:O2'	30:0:1157:C:H5'	2.19	0.43
9:I:69:PRO:HA	30:0:1164:U:OP1	2.19	0.43
30:0:1592:G:HO2'	30:0:1593:C:H6	1.67	0.43
30:0:1937:U:O2'	30:0:1938:G:H5'	2.18	0.43
26:Z:40:ALA:O	30:0:2018:A:H2	2.02	0.43
30:0:2487:C:C5	38:0:4880:HOH:O	2.57	0.43
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.19	0.43
30:0:2523:U:H2'	30:0:2524:G:O4'	2.18	0.43
30:0:2581:U:H1'	38:0:4466:HOH:O	2.17	0.43
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.01	0.43
30:0:636:G:H5'	30:0:2059:U:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:802:G:H2'	30:0:803:C:C6	2.54	0.43
30:0:920:C:C5	30:0:2467:A:OP1	2.72	0.43
2:B:215:VAL:HB	38:B:9090:HOH:O	2.19	0.43
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.34	0.43
26:Z:88:PHE:N	26:Z:88:PHE:CD2	2.86	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.53	0.43
30:0:1561:U:C5'	38:0:7421:HOH:O	2.67	0.43
30:0:1758:U:H2'	30:0:1759:A:O4'	2.19	0.43
30:0:1923:G:H2'	30:0:1924:A:H8	1.83	0.43
30:0:2252:A:H2'	30:0:2253:G:O4'	2.19	0.43
30:0:236:A:OP1	30:0:236:A:H8	2.02	0.43
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.52	0.43
30:0:301:C:H2'	30:0:302:A:C8	2.54	0.43
30:0:308:U:C4	30:0:342:C:C1'	3.01	0.43
29:3:13:HIS:HD2	29:3:76:LYS:HB3	1.83	0.43
31:9:3:A:N6	31:9:22:G:H1'	2.34	0.43
1:A:230:SER:CB	30:0:1852:A:H4'	2.49	0.43
1:A:48:ASP:HB3	1:A:51:ARG:HG3	2.00	0.43
4:D:136:ARG:HA	4:D:137:PRO:HD3	1.84	0.43
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.86	0.43
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.84	0.43
16:P:129:GLY:HA2	38:P:153:HOH:O	2.18	0.43
16:P:58:SER:HB3	38:0:5616:HOH:O	2.18	0.43
23:W:122:ARG:NH2	38:0:5280:HOH:O	2.51	0.43
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.43
30:0:1095:U:H2'	30:0:1096:U:O4'	2.18	0.42
30:0:1552:G:C6	30:0:1634:G:C6	3.07	0.42
30:0:1748:U:C5	30:0:1749:U:C4	3.07	0.42
30:0:1882:C:O2'	30:0:2012:U:OP2	2.32	0.42
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.42
30:0:2499:U:H1'	38:0:9433:HOH:O	2.19	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.01	0.42
30:0:290:C:C2'	30:0:291:C:H5'	2.49	0.42
30:0:412:C:O2'	30:0:413:G:H5'	2.18	0.42
30:0:612:U:H2'	30:0:613:C:H6	1.84	0.42
31:9:65:A:N6	31:9:112:U:C6	2.86	0.42
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.19	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.34	0.42
12:L:117:GLU:HG3	12:L:117:GLU:O	2.19	0.42
12:L:150:GLN:HB3	38:L:9032:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1562:C:N4	38:0:5849:HOH:O	2.49	0.42
30:0:1878:G:H4'	38:0:6104:HOH:O	2.19	0.42
30:0:1878:G:H5''	38:0:5160:HOH:O	2.18	0.42
30:0:2061:C:H2'	30:0:2062:A:H5'	1.99	0.42
30:0:2415:A:H2'	30:0:2416:G:H5'	2.01	0.42
30:0:271:C:C2	30:0:273:G:O4'	2.73	0.42
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.42
30:0:696:C:H4'	38:0:7268:HOH:O	2.19	0.42
30:0:706:G:N2	30:0:707:C:H41	2.17	0.42
15:O:112:ARG:NH2	30:0:719:C:O2'	2.52	0.42
1:A:135:VAL:HG22	1:A:136:ALA:N	2.35	0.42
5:E:146:ALA:O	5:E:150:GLN:HG2	2.19	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.18	0.42
30:0:113:A:H3'	30:0:114:A:C5'	2.48	0.42
30:0:1206:U:H3'	30:0:1206:U:C6	2.55	0.42
30:0:128:A:C8	30:0:128:A:C3'	2.99	0.42
30:0:1345:A:H2'	30:0:1346:U:C6	2.54	0.42
30:0:1407:A:O2'	30:0:1408:U:H3'	2.20	0.42
30:0:1544:U:O2'	30:0:1545:C:H5'	2.19	0.42
13:M:84:LYS:HB2	30:0:170:U:OP1	2.18	0.42
30:0:1757:U:H6	30:0:1757:U:O5'	2.03	0.42
30:0:2035:C:H6	30:0:2035:C:O5'	2.02	0.42
30:0:276:C:O5'	30:0:276:C:H6	2.02	0.42
30:0:2787:C:H5	38:0:4627:HOH:O	2.02	0.42
27:1:25:LYS:HD2	28:2:48:ASP:HA	2.02	0.42
1:A:8:ARG:HG2	38:A:8978:HOH:O	2.20	0.42
2:B:217:ARG:HG3	2:B:257:THR:CG2	2.41	0.42
2:B:17:LYS:O	2:B:260:HIS:HD2	2.02	0.42
2:B:62:ARG:HA	2:B:65:MET:HE2	2.01	0.42
2:B:8:LYS:HG3	2:B:220:VAL:HG12	2.01	0.42
12:L:11:ARG:O	30:0:903:U:C2	2.72	0.42
16:P:105:LEU:HD21	16:P:137:LEU:HD11	2.01	0.42
17:Q:2:SER:HA	38:0:6711:HOH:O	2.19	0.42
23:W:142:ASP:HB3	23:W:145:GLY:H	1.83	0.42
30:0:1173:A:C2	30:0:1177:A:C8	3.07	0.42
30:0:1393:A:N1	30:0:1725:C:O2'	2.44	0.42
30:0:1585:C:H2'	30:0:1586:G:H8	1.84	0.42
30:0:1804:A:H2'	30:0:1805:G:C8	2.53	0.42
30:0:1902:G:C2	30:0:1936:C:C2	3.07	0.42
4:D:54:ALA:HB2	30:0:2346:C:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2709:G:N2	38:0:7613:HOH:O	2.53	0.42
30:0:2828:G:H8	30:0:2828:G:O5'	2.03	0.42
18:R:68:HIS:O	30:0:2842:G:H5'	2.19	0.42
30:0:707:C:C2	30:0:708:A:C8	3.07	0.42
29:3:3:MET:HA	29:3:4:PRO:HD2	1.86	0.42
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.34	0.42
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.73	0.42
4:D:50:VAL:HG13	31:9:41:C:O4'	2.19	0.42
5:E:126:ILE:HA	5:E:131:LEU:HD23	2.00	0.42
11:K:79:PRO:HB3	11:K:87:ARG:HB3	2.02	0.42
12:L:7:GLN:HB3	12:L:13:HIS:CE1	2.54	0.42
13:M:97:ILE:HG21	13:M:127:LYS:HD2	2.01	0.42
30:0:1321:A:H2'	30:0:1322:G:C8	2.55	0.42
30:0:1420:C:O2	30:0:1420:C:H2'	2.19	0.42
30:0:420:U:O4'	30:0:1920:C:C4	2.73	0.42
30:0:1933:G:O2'	30:0:1934:A:H5'	2.19	0.42
30:0:2480:G:O2'	30:0:2481:G:H5'	2.19	0.42
30:0:407:A:H3'	38:0:4452:HOH:O	2.19	0.42
30:0:727:G:H3'	30:0:728:C:C6	2.54	0.42
30:0:849:C:H2'	30:0:850:U:O4'	2.20	0.42
30:0:939:A:N1	30:0:1027:G:O2'	2.45	0.42
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.42
2:B:310:ARG:HB3	38:B:9121:HOH:O	2.19	0.42
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.32	0.42
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.42
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.34	0.42
16:P:103:THR:O	16:P:107:GLU:HG3	2.19	0.42
19:S:6:LYS:HD3	38:S:2519:HOH:O	2.20	0.42
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.19	0.42
30:0:1006:A:H2'	30:0:1007:A:C8	2.55	0.42
30:0:1559:A:C8	30:0:1559:A:OP2	2.70	0.42
30:0:154:C:O2'	30:0:155:C:H5'	2.18	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.53	0.42
30:0:273:G:H2'	30:0:274:G:O4'	2.20	0.42
30:0:299:U:C2	30:0:300:U:C5	3.08	0.42
30:0:571:C:H6	30:0:571:C:O5'	2.02	0.42
29:3:29:ARG:HG2	29:3:30:GLN:N	2.35	0.42
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.54	0.42
2:B:145:HIS:CD2	2:B:146:THR:O	2.63	0.42
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.00	0.42
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.19	0.42
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.85	0.42
13:M:188:ARG:NH1	30:0:154:C:H3'	2.35	0.42
30:0:1168:C:C5	30:0:1169:U:C4	3.08	0.42
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.42
30:0:1454:U:H5''	30:0:1455:C:OP2	2.19	0.42
30:0:17:G:H2'	30:0:18:C:H6	1.84	0.42
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.53	0.42
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.42
30:0:1924:A:H1'	38:0:5731:HOH:O	2.19	0.42
30:0:2274:A:H2'	30:0:2275:G:C8	2.54	0.42
8:H:117:ARG:HH12	30:0:2287:C:N4	2.17	0.42
30:0:2321:A:C5	30:0:2323:G:C8	3.07	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.02	0.42
13:M:172:GLY:HA2	38:0:9086:HOH:O	2.19	0.42
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.50	0.42
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.54	0.42
30:0:1188:A:C5	30:0:1189:A:N1	2.88	0.42
30:0:1539:U:O2'	30:0:1540:G:H5'	2.20	0.42
30:0:1576:G:H2'	30:0:1577:U:C6	2.54	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
30:0:1815:A:H2'	30:0:1816:C:O4'	2.20	0.42
30:0:2354:A:C2	30:0:2367:A:C8	3.08	0.42
30:0:2671:U:C2'	30:0:2672:C:O5'	2.68	0.42
30:0:2673:U:O2'	30:0:2674:G:H5'	2.20	0.42
30:0:2690:U:C4	30:0:2691:A:C5	3.07	0.42
30:0:644:G:N3	30:0:644:G:H5'	2.35	0.42
30:0:918:G:C2	30:0:926:A:C2	3.08	0.42
29:3:64:LYS:HB3	29:3:82:GLY:O	2.20	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.42
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.53	0.42
2:B:252:PRO:HD3	38:0:9818:HOH:O	2.18	0.42
8:H:151:GLU:HA	8:H:151:GLU:OE1	2.19	0.42
11:K:132:VAL:HG11	21:U:22:VAL:HG22	2.02	0.42
13:M:74:LYS:HB3	38:M:8944:HOH:O	2.20	0.42
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.20	0.42
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.02	0.42
22:V:39:ALA:C	22:V:41:GLU:H	2.22	0.42
24:X:70:ILE:O	24:X:70:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:42:TYR:HA	30:0:1829:A:N6	2.35	0.42
30:0:1198:U:H2'	30:0:1200:A:OP2	2.20	0.42
30:0:1200:A:H4'	38:0:7330:HOH:O	2.19	0.42
30:0:1474:C:C5'	30:0:1474:C:C6	2.89	0.42
30:0:151:A:H2'	30:0:152:A:C8	2.55	0.42
30:0:1573:A:H2'	30:0:1574:C:O4'	2.20	0.42
30:0:2332:A:H2'	38:0:5623:HOH:O	2.19	0.42
30:0:2458:U:O2'	30:0:2459:G:H5'	2.20	0.42
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.34	0.42
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
30:0:710:G:O2'	30:0:711:G:H5'	2.20	0.42
30:0:820:G:O2'	30:0:856:G:H4'	2.20	0.42
28:2:43:ARG:HH22	30:0:1684:A:C1'	2.26	0.42
8:H:10:ARG:HD2	8:H:161:THR:HG21	2.01	0.42
10:J:74:ARG:O	10:J:78:ILE:HG12	2.20	0.42
13:M:187:LEU:HD22	13:M:194:GLY:HA3	2.01	0.42
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.34	0.42
25:Y:160:LYS:HA	25:Y:160:LYS:HD3	1.87	0.42
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.23	0.42
30:0:1158:G:H2'	30:0:1159:G:C5'	2.50	0.42
30:0:1181:A:N1	30:0:1192:A:O2'	2.45	0.42
30:0:1314:U:H5''	30:0:1316:G:O4'	2.19	0.42
30:0:1538:C:O2'	30:0:1539:U:H5'	2.19	0.42
30:0:1585:C:H2'	30:0:1586:G:C8	2.54	0.42
30:0:1794:G:N2	30:0:1796:A:H3'	2.35	0.42
30:0:191:A:H2'	30:0:237:G:O6	2.20	0.42
30:0:364:U:H2'	30:0:365:G:O4'	2.20	0.42
18:R:98:ASN:ND2	30:0:500:G:H21	2.11	0.42
31:9:29:C:C5	31:9:30:C:C6	3.08	0.42
1:A:94:LEU:HD12	1:A:98:GLU:CB	2.47	0.42
10:J:52:GLN:HE21	30:0:1119:G:H5'	1.84	0.42
18:R:89:LEU:HA	18:R:89:LEU:HD23	1.82	0.42
20:T:48:VAL:CG1	20:T:96:VAL:HG13	2.50	0.42
23:W:139:GLY:O	23:W:141:HIS:CD2	2.73	0.42
24:X:10:VAL:HG11	24:X:36:HIS:HE1	1.85	0.42
30:0:1135:G:H5'	38:0:5913:HOH:O	2.19	0.41
30:0:1316:G:H5''	38:0:5311:HOH:O	2.20	0.41
30:0:1345:A:H2'	30:0:1346:U:H6	1.85	0.41
30:0:1359:U:C5	30:0:2101:A:H8	2.38	0.41
30:0:1531:U:O2	30:0:1661:A:C2	2.73	0.41
30:0:1734:C:H6	30:0:1734:C:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:HB3	30:0:1872:C:H5	1.85	0.41
30:0:299:U:H2'	30:0:300:U:H6	1.85	0.41
31:9:73:A:N1	31:9:108:C:O2	2.53	0.41
2:B:49:THR:HG22	2:B:331:SER:HB3	2.02	0.41
6:F:54:VAL:HG13	30:0:263:U:C4	2.55	0.41
9:I:91:PHE:CD2	9:I:131:GLY:HA2	2.44	0.41
10:J:42:GLU:HG2	10:J:43:ARG:N	2.34	0.41
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.48	0.41
26:Z:41:ARG:HD3	38:Z:8717:HOH:O	2.19	0.41
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.36	0.41
30:0:1333:U:H2'	30:0:1334:C:C6	2.54	0.41
30:0:1405:U:H2'	38:0:6827:HOH:O	2.20	0.41
30:0:1441:G:H1'	38:0:7755:HOH:O	2.19	0.41
30:0:1572:A:C2	30:0:1573:A:C4	3.08	0.41
30:0:1832:G:H5''	38:0:9044:HOH:O	2.19	0.41
30:0:1926:G:C4	30:0:1927:A:C8	3.08	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:1997:A:C6	30:0:1998:G:C5	3.09	0.41
30:0:257:G:N2	30:0:258:G:C4	2.88	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.45	0.41
30:0:34:C:H1'	38:0:9175:HOH:O	2.18	0.41
30:0:559:U:C4	30:0:560:U:C4	3.08	0.41
30:0:567:U:H5''	38:0:6387:HOH:O	2.19	0.41
30:0:820:G:N3	30:0:1831:U:H1'	2.35	0.41
31:9:3:A:C8	31:9:26:C:O2	2.72	0.41
1:A:135:VAL:HG11	1:A:147:ARG:HH21	1.85	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.21	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
20:T:52:ARG:O	30:0:317:A:OP1	2.37	0.41
26:Z:65:ASN:ND2	26:Z:84:CYS:SG	2.91	0.41
30:0:1116:U:C2'	30:0:1118:A:C2	3.04	0.41
30:0:1168:C:C4	30:0:1169:U:C4	3.08	0.41
30:0:1168:C:C5	30:0:1169:U:C5	3.09	0.41
30:0:2675:A:H1'	30:0:2813:A:C2	2.56	0.41
30:0:282:C:O2'	30:0:283:U:C4'	2.69	0.41
30:0:2909:G:H2'	30:0:2910:A:H8	1.85	0.41
30:0:778:C:C4	30:0:779:U:C4	3.08	0.41
30:0:818:A:C6	30:0:819:A:C2	3.07	0.41
28:2:40:ARG:HD2	28:2:47:THR:HG22	2.01	0.41
31:9:119:C:H2'	31:9:120:A:C8	2.55	0.41
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:NH2	1:A:69:LEU:HD11	2.36	0.41
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.56	0.41
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.41
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.02	0.41
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.40	0.41
30:0:1015:C:C2	30:0:1016:U:C5	3.09	0.41
30:0:1246:A:C5	30:0:1248:A:C5	3.09	0.41
30:0:1607:A:C4	30:0:1608:G:C8	3.08	0.41
30:0:2011:A:H5'	30:0:2013:G:H1'	2.01	0.41
30:0:2092:G:H5''	30:0:2613:G:OP1	2.21	0.41
30:0:2874:G:H3'	38:0:9578:HOH:O	2.21	0.41
30:0:271:C:N4	30:0:378:A:C2	2.76	0.41
30:0:546:C:O5'	30:0:546:C:H6	2.03	0.41
30:0:820:G:C5'	30:0:821:U:H5'	2.46	0.41
29:3:69:TYR:CE1	29:3:80:ARG:HB2	2.55	0.41
14:N:40:ASN:HD21	31:9:28:U:H5''	1.83	0.41
31:9:31:C:O2'	31:9:32:G:H5'	2.20	0.41
31:9:7:G:C5'	38:9:9099:HOH:O	2.68	0.41
14:N:42:HIS:CB	14:N:62:HIS:HE1	2.33	0.41
30:0:1183:C:O2	30:0:1183:C:C2'	2.68	0.41
30:0:1191:A:H3'	30:0:1191:A:H8	1.84	0.41
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.20	0.41
30:0:932:U:H1'	30:0:1296:A:H1'	2.02	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.56	0.41
30:0:1545:C:H2'	30:0:1546:G:O4'	2.20	0.41
30:0:2799:A:N6	30:0:2801:A:C2	2.89	0.41
30:0:293:A:P	30:0:358:G:H22	2.43	0.41
30:0:488:U:H2'	38:0:4003:HOH:O	2.20	0.41
30:0:652:G:H8	38:0:3003:HOH:O	2.03	0.41
29:3:46:ILE:HA	38:0:7897:HOH:O	2.20	0.41
31:9:9:C:H2'	31:9:10:C:H5'	2.03	0.41
31:9:112:U:H2'	31:9:113:C:H5'	2.02	0.41
31:9:1:U:O3'	31:9:3:A:OP1	2.39	0.41
9:I:123:VAL:O	9:I:127:CYS:SG	2.78	0.41
10:J:116:LEU:HB2	10:J:119:THR:HG21	2.02	0.41
13:M:68:ARG:CZ	13:M:73:ARG:HD3	2.51	0.41
16:P:3:LEU:HA	16:P:6:GLN:OE1	2.21	0.41
17:Q:21:ARG:HG2	17:Q:22:GLY:H	1.86	0.41
22:V:12:THR:H	22:V:15:GLU:HB2	1.85	0.41
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	2.02	0.41
30:0:1362:U:H2'	30:0:1363:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1427:A:O2'	30:0:1428:C:H5'	2.21	0.41
28:2:2:LYS:HG3	30:0:1486:A:C4	2.55	0.41
30:0:1563:G:H4'	30:0:1564:C:H5'	2.01	0.41
30:0:1757:U:H5	38:0:3211:HOH:O	2.03	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.73	0.41
30:0:1915:U:H2'	30:0:1916:C:O4'	2.21	0.41
30:0:2092:G:H2'	30:0:2613:G:OP1	2.21	0.41
30:0:2409:C:H5''	38:0:4005:HOH:O	2.20	0.41
30:0:69:A:C2'	30:0:70:A:OP2	2.69	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:822:C:C2	30:0:823:U:C5	3.08	0.41
27:1:16:HIS:CD2	30:0:470:U:O2'	2.72	0.41
29:3:73:GLU:HB3	38:3:9056:HOH:O	2.21	0.41
1:A:194:MET:CE	1:A:199:HIS:HB2	2.50	0.41
3:C:27:ARG:NH1	3:C:27:ARG:CG	2.79	0.41
7:G:71:LEU:C	7:G:73:ASP:H	2.23	0.41
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.51	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.68	0.41
13:M:77:HIS:CG	13:M:81:ARG:HB2	2.56	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.50	0.41
17:Q:16:ASN:HA	17:Q:16:ASN:HD22	1.67	0.41
18:R:17:MET:HE3	18:R:19:ARG:HH21	1.86	0.41
23:W:24:LEU:HD21	23:W:44:MET:SD	2.61	0.41
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.41
30:0:1051:C:H2'	30:0:1052:G:O4'	2.20	0.41
30:0:130:C:H2'	38:0:3150:HOH:O	2.21	0.41
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.41
30:0:186:A:H4'	30:0:186:A:OP1	2.21	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.55	0.41
30:0:2872:U:C2	30:0:2873:C:C6	3.08	0.41
30:0:2880:A:H2'	30:0:2881:C:H5'	2.02	0.41
30:0:396:U:H1'	30:0:397:A:OP1	2.20	0.41
30:0:536:A:N1	30:0:2075:G:O2'	2.50	0.41
30:0:964:G:C4	30:0:965:A:C8	3.08	0.41
31:9:70:U:H2'	31:9:71:C:O4'	2.20	0.41
4:D:84:LEU:HA	4:D:87:ALA:HB3	2.02	0.41
5:E:155:ASN:ND2	5:E:155:ASN:H	2.17	0.41
5:E:77:THR:OG1	5:E:78:GLU:N	2.52	0.41
16:P:13:VAL:HG13	16:P:14:LEU:N	2.36	0.41
23:W:38:THR:HG22	38:W:3580:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1215:A:O3'	30:0:1216:G:C4'	2.69	0.41
30:0:1337:G:C6	30:0:1338:U:C4	3.09	0.41
30:0:1682:A:H5''	38:0:9458:HOH:O	2.20	0.41
30:0:240:C:O2	30:0:240:C:H2'	2.20	0.41
30:0:2780:C:C4	30:0:2781:U:C4	3.09	0.41
30:0:2892:G:C6	30:0:2893:C:C4	3.09	0.41
30:0:397:A:H1'	30:0:417:G:H1'	2.03	0.41
30:0:706:G:O2'	30:0:707:C:H6	2.03	0.41
30:0:73:U:O2'	30:0:74:G:H5'	2.21	0.41
30:0:800:G:H2'	30:0:801:U:C6	2.56	0.41
3:C:22:PHE:HA	3:C:116:ALA:HA	2.02	0.41
30:0:99:A:C8	30:0:100:C:C6	3.09	0.41
30:0:1244:U:H4'	30:0:1246:A:O4'	2.21	0.41
30:0:1423:C:O2'	30:0:1424:A:H5'	2.20	0.41
30:0:1523:G:C5	30:0:1524:U:C4	3.08	0.41
30:0:1819:G:C2'	30:0:1820:G:H5'	2.50	0.41
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.41
30:0:210:U:O2'	30:0:211:U:H5'	2.21	0.41
30:0:2296:C:H2'	30:0:2297:U:C6	2.56	0.41
2:B:27:ASN:HD21	30:0:2807:U:P	2.43	0.41
30:0:37:A:C2	30:0:446:G:C2	3.09	0.41
30:0:565:A:N6	30:0:593:A:C8	2.88	0.41
29:3:88:LEU:HD22	33:3:8804:CL:CL	2.58	0.41
2:B:274:GLU:HA	2:B:292:GLY:O	2.21	0.41
3:C:44:GLN:HA	38:C:8614:HOH:O	2.21	0.41
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.41
11:K:75:ARG:HD2	11:K:90:PHE:CD2	2.55	0.41
14:N:48:VAL:HG11	14:N:55:ASP:HB3	2.02	0.41
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.68	0.41
26:Z:54:GLU:HB3	38:Z:8731:HOH:O	2.21	0.41
1:A:45:ILE:HD12	26:Z:89:THR:HG23	2.02	0.41
30:0:1351:G:H1'	38:0:4673:HOH:O	2.21	0.41
30:0:2345:A:H3'	30:0:2346:C:C5	2.56	0.41
30:0:2438:G:C6	30:0:2439:C:C4	3.08	0.41
12:L:53:ARG:HD2	30:0:2441:U:H4'	2.02	0.41
3:C:87:ARG:NH2	30:0:894:A:C2	2.89	0.41
31:9:75:G:H1	31:9:106:U:H3	1.69	0.41
2:B:58:PRO:HA	2:B:63:GLU:CD	2.40	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.82	0.41
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.41
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1193:A:C2	30:0:1194:A:N6	2.89	0.41
30:0:1419:U:H2'	30:0:1685:A:C2	2.56	0.41
30:0:1769:C:C2'	30:0:1770:U:H5'	2.51	0.41
30:0:2002:C:C2'	30:0:2003:U:H5'	2.50	0.41
30:0:2064:U:H5'	30:0:2652:U:O3'	2.21	0.41
13:M:193:LYS:HB3	30:0:392:U:C5'	2.51	0.41
30:0:407:A:H8	38:0:4452:HOH:O	2.04	0.41
30:0:375:G:C4	30:0:411:A:C6	3.09	0.41
30:0:39:G:C2	30:0:444:C:N3	2.89	0.41
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.41
30:0:685:C:O2	30:0:748:C:H4'	2.21	0.41
27:1:38:GLY:HA3	38:1:6935:HOH:O	2.20	0.41
4:D:53:LYS:HE3	31:9:40:C:H42	1.85	0.41
1:A:191:GLY:HA2	1:A:194:MET:HE2	2.02	0.41
1:A:33:GLU:CD	1:A:33:GLU:H	2.24	0.41
1:A:47:HIS:CD2	30:0:1654:U:C2'	3.02	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.41	0.41
2:B:244:PRO:HG3	2:B:248:ARG:NH2	2.35	0.41
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.56	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.02	0.41
14:N:22:GLN:HG3	30:0:2415:A:H2	1.85	0.41
15:O:68:GLY:HA3	30:0:745:G:O6	2.20	0.41
16:P:81:LYS:HG2	38:0:9540:HOH:O	2.20	0.41
21:U:20:MET:HG3	21:U:28:THR:HG23	2.03	0.41
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.41
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.56	0.41
30:0:1008:C:H2'	30:0:1009:U:C6	2.56	0.40
30:0:1327:G:C6	30:0:1331:G:C6	3.09	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.40
30:0:375:G:C2	30:0:411:A:C2	3.08	0.40
31:9:14:G:C8	31:9:14:G:C5'	2.95	0.40
4:D:172:VAL:HG12	4:D:173:GLU:N	2.36	0.40
8:H:12:ILE:HG12	8:H:59:GLN:HG3	2.02	0.40
10:J:47:THR:O	10:J:53:ILE:HD11	2.21	0.40
13:M:46:LEU:HD22	13:M:50:ARG:HD2	2.03	0.40
13:M:95:LYS:HA	13:M:170:ASN:HD21	1.86	0.40
19:S:42:GLU:HG2	19:S:49:VAL:HG23	2.03	0.40
26:Z:53:ILE:HG23	26:Z:93:TYR:HB3	2.02	0.40
26:Z:65:ASN:HD22	26:Z:84:CYS:CB	2.33	0.40
30:0:1398:G:H2'	30:0:1399:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1531:U:C2	30:0:1661:A:C2	3.10	0.40
30:0:1576:G:H2'	30:0:1577:U:H6	1.87	0.40
30:0:1577:U:O2'	30:0:1578:C:H5'	2.21	0.40
30:0:1589:G:C2	30:0:1605:G:N3	2.89	0.40
30:0:1497:G:H4'	30:0:1627:G:O2'	2.21	0.40
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.40
30:0:1543:G:N1	30:0:1641:A:OP2	2.41	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.89	0.40
30:0:1972:U:O2'	30:0:1973:A:H5''	2.22	0.40
30:0:2319:C:H2'	30:0:2320:U:H5'	2.03	0.40
30:0:245:C:N4	30:0:246:G:C6	2.89	0.40
30:0:2526:C:H6	30:0:2526:C:H3'	1.86	0.40
30:0:559:U:C6	30:0:559:U:H3'	2.57	0.40
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.56	0.40
1:A:47:HIS:HA	38:A:9024:HOH:O	2.20	0.40
5:E:139:GLU:OE2	30:0:2781:U:C1'	2.68	0.40
5:E:166:VAL:HB	38:E:6341:HOH:O	2.19	0.40
7:G:19:GLU:O	7:G:23:ILE:HG13	2.21	0.40
10:J:19:MET:HE3	10:J:132:LEU:HD11	2.03	0.40
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.58	0.40
11:K:74:VAL:HG12	11:K:75:ARG:HG3	2.02	0.40
12:L:73:VAL:HG23	12:L:74:THR:H	1.86	0.40
16:P:7:LYS:HD3	16:P:21:VAL:HG22	2.03	0.40
17:Q:80:LYS:HG2	17:Q:82:LYS:HE3	2.02	0.40
23:W:4:LEU:HA	23:W:4:LEU:HD23	1.88	0.40
30:0:1074:G:H4'	30:0:1260:G:C6	2.57	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
30:0:1461:U:H1'	38:0:7457:HOH:O	2.21	0.40
30:0:1749:U:O2	30:0:1751:G:C8	2.75	0.40
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.40
30:0:2867:G:H2'	30:0:2868:C:H6	1.86	0.40
30:0:372:A:H2'	30:0:373:G:H8	1.86	0.40
30:0:464:G:HO2'	30:0:465:U:P	2.44	0.40
30:0:611:U:O5'	30:0:611:U:H6	2.05	0.40
30:0:727:G:N2	30:0:728:C:H1'	2.36	0.40
31:9:2:U:OP2	31:9:2:U:H4'	2.22	0.40
2:B:148:PRO:HD2	38:B:9047:HOH:O	2.21	0.40
3:C:168:ARG:NH2	3:C:190:ALA:O	2.55	0.40
9:I:120:ALA:O	9:I:124:VAL:HG23	2.21	0.40
9:I:78:ALA:HB1	9:I:93:ALA:CB	2.51	0.40
10:J:57:TYR:O	10:J:61:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:117:GLU:HG2	38:L:9025:HOH:O	2.20	0.40
13:M:64:ARG:HD2	38:M:8879:HOH:O	2.21	0.40
13:M:74:LYS:O	13:M:88:VAL:HG22	2.21	0.40
26:Z:65:ASN:CB	26:Z:84:CYS:SG	3.08	0.40
30:0:113:A:OP2	30:0:114:A:H2'	2.21	0.40
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	0.40
30:0:1936:C:H2'	30:0:1937:U:C6	2.56	0.40
30:0:1982:C:H2'	30:0:1983:C:O4'	2.21	0.40
30:0:2248:C:H2'	30:0:2249:G:C8	2.54	0.40
8:H:8:MET:SD	30:0:2494:G:H4'	2.61	0.40
30:0:2803:C:H2'	30:0:2804:C:H6	1.86	0.40
30:0:2826:G:C6	30:0:2913:A:C6	3.10	0.40
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.22	0.40
31:9:27:C:C4	31:9:28:U:C5	3.09	0.40
1:A:105:VAL:HG13	1:A:155:THR:O	2.21	0.40
2:B:294:TYR:HE2	38:B:9123:HOH:O	2.03	0.40
8:H:91:ARG:O	30:0:1003:U:H4'	2.22	0.40
12:L:56:LYS:NZ	38:L:9036:HOH:O	2.54	0.40
12:L:67:ARG:O	12:L:71:GLU:HG3	2.22	0.40
14:N:58:LEU:HD12	14:N:58:LEU:H	1.85	0.40
16:P:89:ASN:HB3	16:P:92:GLU:HB2	2.03	0.40
30:0:1130:U:H4'	38:0:6109:HOH:O	2.21	0.40
30:0:1135:G:O2'	30:0:1136:U:H5'	2.22	0.40
30:0:1163:G:C2	30:0:1184:C:N3	2.89	0.40
30:0:1191:A:H3'	30:0:1191:A:C8	2.56	0.40
30:0:1397:C:O2'	30:0:1398:G:H5'	2.22	0.40
30:0:1589:G:H5'	38:0:6843:HOH:O	2.20	0.40
30:0:1815:A:H4'	30:0:2751:C:O4'	2.22	0.40
30:0:2321:A:H1'	30:0:2322:U:H3'	2.04	0.40
30:0:2295:G:N3	30:0:2361:A:H2	2.17	0.40
30:0:2694:A:C6	30:0:2702:A:C8	3.09	0.40
30:0:2803:C:C4	30:0:2804:C:C5	3.10	0.40
30:0:506:G:N2	30:0:509:A:H5'	2.31	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.40
30:0:763:C:O2'	30:0:764:C:H5'	2.21	0.40
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.53	0.40
1:A:88:ILE:HG22	1:A:88:ILE:O	2.20	0.40
2:B:10:SER:O	2:B:16:ARG:NH1	2.45	0.40
13:M:34:GLU:HB3	13:M:38:GLU:HG3	2.02	0.40
16:P:59:ARG:HD3	38:0:6252:HOH:O	2.22	0.40
20:T:21:LYS:HA	20:T:24:ARG:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:139:GLY:O	23:W:141:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	202 (86%)	27 (12%)	6 (3%)	6	28
2	B	335/338 (99%)	309 (92%)	17 (5%)	9 (3%)	6	27
3	C	244/246 (99%)	222 (91%)	20 (8%)	2 (1%)	22	61
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	5	24
5	E	170/178 (96%)	157 (92%)	12 (7%)	1 (1%)	28	67
6	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	4	21
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	14	48
9	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	2	9
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	25	64
11	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	22	61
12	L	141/165 (86%)	120 (85%)	21 (15%)	0	100	100
13	M	192/196 (98%)	179 (93%)	9 (5%)	4 (2%)	8	35
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	8	33
15	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	17	53
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	25	64
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	11	41
21	U	51/67 (76%)	42 (82%)	8 (16%)	1 (2%)	9	36
22	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
23	W	152/154 (99%)	140 (92%)	10 (7%)	2 (1%)	14	48
24	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	6	29
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	58 (82%)	8 (11%)	5 (7%)	1	5
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	7	31
29	3	90/92 (98%)	74 (82%)	13 (14%)	3 (3%)	4	21
All	All	3705/4472 (83%)	3359 (91%)	286 (8%)	60 (2%)	11	42

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	37	VAL
1	A	74	VAL
4	D	65	GLU
4	D	137	PRO
8	H	19	ARG
11	K	127	ALA
13	M	82	ARG
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
26	Z	105	ARG
29	3	64	LYS
2	B	306	LYS
6	F	61	MET
6	F	101	ALA
13	M	71	SER
21	U	51	TRP
24	X	70	ILE
26	Z	70	ARG
2	B	184	ASP
3	C	8	LEU
5	E	44	GLY

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Mol	Chain	Res	Type
6	F	27	GLY
9	I	83	GLY
20	T	44	ALA
23	W	36	PRO
23	W	49	ASN
24	X	87	ALA
26	Z	67	GLY
29	3	46	ILE
2	B	2	GLN
2	B	107	SER
4	D	56	ARG
9	I	106	GLN
13	M	86	GLN
20	T	46	ASP
26	Z	83	TYR
28	2	37	HIS
1	A	52	SER
1	A	119	ALA
2	B	206	THR
3	C	79	ARG
10	J	65	ASN
13	M	79	ALA
18	R	114	VAL
29	3	56	PRO
2	B	63	GLU
6	F	104	ALA
8	H	171	GLY
14	N	164	ASP
4	D	27	ILE
17	Q	48	PRO
2	B	34	GLY
2	B	169	GLY
26	Z	64	PRO
2	B	185	GLY
9	I	108	HIS
9	I	131	GLY
1	A	42	VAL

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	69
2	B	282/283 (100%)	264 (94%)	18 (6%)	20	54
3	C	193/193 (100%)	182 (94%)	11 (6%)	24	59
4	D	117/148 (79%)	110 (94%)	7 (6%)	22	57
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	82
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	74
8	H	134/145 (92%)	126 (94%)	8 (6%)	22	57
9	I	58/130 (45%)	56 (97%)	2 (3%)	42	76
10	J	118/121 (98%)	113 (96%)	5 (4%)	34	71
11	K	106/106 (100%)	104 (98%)	2 (2%)	62	87
12	L	113/127 (89%)	108 (96%)	5 (4%)	33	69
13	M	158/160 (99%)	148 (94%)	10 (6%)	21	55
14	N	149/150 (99%)	144 (97%)	5 (3%)	42	76
15	O	93/94 (99%)	92 (99%)	1 (1%)	78	92
16	P	113/117 (97%)	107 (95%)	6 (5%)	26	62
17	Q	79/80 (99%)	78 (99%)	1 (1%)	73	91
18	R	117/122 (96%)	114 (97%)	3 (3%)	51	82
19	S	71/74 (96%)	70 (99%)	1 (1%)	71	90
20	T	105/106 (99%)	99 (94%)	6 (6%)	24	59
21	U	44/53 (83%)	41 (93%)	3 (7%)	18	51
22	V	51/57 (90%)	49 (96%)	2 (4%)	37	73
23	W	130/130 (100%)	124 (95%)	6 (5%)	31	68
24	X	66/74 (89%)	61 (92%)	5 (8%)	15	46
25	Y	120/196 (61%)	115 (96%)	5 (4%)	34	71
26	Z	60/94 (64%)	57 (95%)	3 (5%)	28	65
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	83
29	3	79/79 (100%)	76 (96%)	3 (4%)	38	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3095/3646 (85%)	2963 (96%)	132 (4%)	33 70

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	162	MET
2	B	191	ASN
2	B	192	ASP
2	B	195	ARG
2	B	238	ASN
2	B	248	ARG
2	B	251	VAL
2	B	254	GLN
2	B	265	LEU
2	B	277	GLU
2	B	307	ARG
3	C	2	GLN
3	C	76	ARG
3	C	88	SER
3	C	136	VAL
3	C	187	ARG
3	C	202	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL

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Mol	Chain	Res	Type
4	D	19	GLU
4	D	24	HIS
4	D	29	HIS
4	D	50	VAL
4	D	61	PHE
4	D	149	ARG
4	D	161	ASP
5	E	7	ILE
5	E	68	HIS
5	E	126	ILE
5	E	155	ASN
7	G	73	ASP
8	H	21	GLU
8	H	33	GLN
8	H	45	ASP
8	H	61	ARG
8	H	62	HIS
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
9	I	115	ASP
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	107	ASN
10	J	130	VAL
11	K	10	GLN
11	K	55	VAL
12	L	35	ARG
12	L	99	GLU
12	L	101	ASP
12	L	104	ASP
12	L	114	VAL
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	73	ARG
13	M	82	ARG
13	M	86	GLN
13	M	93	ARG
13	M	99	ARG

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Mol	Chain	Res	Type
13	M	116	ASN
13	M	125	ARG
14	N	5	ARG
14	N	17	ARG
14	N	49	THR
14	N	56	ASP
14	N	80	SER
15	O	3	THR
16	P	21	VAL
16	P	79	SER
16	P	91	LYS
16	P	94	TRP
16	P	98	ILE
16	P	120	ARG
17	Q	16	ASN
18	R	13	THR
18	R	39	THR
18	R	143	VAL
19	S	30	ASP
20	T	5	ASP
20	T	39	ASN
20	T	73	HIS
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	25	ASP
21	U	52	THR
21	U	53	ASP
22	V	12	THR
22	V	65	ASP
23	W	1	MET
23	W	4	LEU
23	W	35	VAL
23	W	88	THR
23	W	125	HIS
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
25	Y	154	ARG

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Mol	Chain	Res	Type
25	Y	189	ASN
25	Y	203	VAL
25	Y	223	ASP
25	Y	235	GLU
26	Z	37	ARG
26	Z	70	ARG
26	Z	88	PHE
28	2	18	ASN
29	3	30	GLN
29	3	56	PRO
29	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	73	GLN
3	C	103	ASN
3	C	129	HIS
4	D	103	ASN
5	E	55	ASN
5	E	90	HIS
5	E	143	GLN
5	E	150	GLN
7	G	64	ASN
8	H	59	GLN
9	I	99	GLN
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS

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Mol	Chain	Res	Type
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	29	GLN
13	M	170	ASN
14	N	40	ASN
14	N	53	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	123	GLN
19	S	7	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	38	ASN
21	U	39	ASN
22	V	34	GLN
22	V	60	GLN
23	W	2	HIS
23	W	12	ASN
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN

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Mol	Chain	Res	Type
25	Y	189	ASN
26	Z	80	GLN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	30	GLN
29	3	48	ASN
29	3	91	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	250 (9%)	21 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	269 (9%)	23 (0%)

All (269) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A

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Mol	Chain	Res	Type
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	409	U
30	0	417	G
30	0	461	C
30	0	473	A
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	699	C

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Mol	Chain	Res	Type
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	846	A
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G

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Mol	Chain	Res	Type
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1205	U
30	0	1206	U
30	0	1216	G
30	0	1234	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1562	C
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A

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Mol	Chain	Res	Type
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1710	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G

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Mol	Chain	Res	Type
30	0	2103	A
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2322	U
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C

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Mol	Chain	Res	Type
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2906	A
30	0	2912	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	396	U
30	0	603	A
30	0	644	G
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	2011	A
30	0	2321	A
30	0	2467	A
30	0	2526	C
30	0	2718	C
30	0	2726	U
30	0	2791	U
31	9	43	G
31	9	65	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
30	OMU	0	2587	30	14,22,23	0.96	1 (7%)	18,31,34	3.67	2 (11%)
30	OMG	0	2588	30	18,26,27	0.99	2 (11%)	22,38,41	2.49	4 (18%)
30	UR3	0	2619	30	14,22,23	0.75	0	16,32,35	0.65	0
30	PSU	0	2621	30	16,21,22	1.67	3 (18%)	20,30,33	6.12	5 (25%)
30	1MA	0	628	30,35	16,25,26	1.07	1 (6%)	13,37,40	1.25	1 (7%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.22	1.47	1.52
30	0	2588	OMG	C8-N7	-2.07	1.30	1.34
30	0	2621	PSU	C2-N1	2.35	1.42	1.38
30	0	2587	OMU	C4-N3	2.35	1.37	1.33
30	0	2621	PSU	C4-N3	2.59	1.37	1.33
30	0	628	1MA	C6-N6	2.87	1.34	1.27
30	0	2588	OMG	C6-N1	3.15	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.08	114.68	128.40
30	0	2621	PSU	C5-C4-N3	-12.95	114.81	125.43
30	0	2588	OMG	C5-C6-N1	-8.35	111.59	123.48
30	0	628	1MA	C2-N3-C4	-3.68	110.76	116.41
30	0	2587	OMU	C5-C4-N3	-3.51	114.75	123.12
30	0	2588	OMG	C2-N3-C4	-2.91	111.76	115.16
30	0	2588	OMG	N3-C2-N1	-2.44	123.90	127.46
30	0	2621	PSU	C5-C1'-C2'	-2.19	111.77	115.55
30	0	2621	PSU	C6-N1-C2	2.73	119.72	115.36
30	0	2588	OMG	C6-N1-C2	6.43	125.31	116.06
30	0	2621	PSU	C4-N3-C2	13.85	127.28	115.16
30	0	2587	OMU	C4-N3-C2	15.04	127.05	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2588	OMG	1	0
30	0	2621	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 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	A	237/240 (98%)	-0.14	8 (3%) 46 29	36, 71, 108, 128	0
2	B	337/338 (99%)	-0.45	0 100 100	38, 67, 98, 112	0
3	C	246/246 (100%)	-0.38	0 100 100	32, 56, 80, 91	0
4	D	140/177 (79%)	1.53	53 (37%) 0 0	89, 121, 144, 151	0
5	E	172/178 (96%)	-0.06	4 (2%) 61 41	57, 83, 104, 113	0
6	F	119/120 (99%)	0.51	15 (12%) 4 2	64, 88, 121, 131	0
7	G	29/348 (8%)	1.10	4 (13%) 3 2	92, 107, 116, 118	0
8	H	160/177 (90%)	0.89	30 (18%) 1 1	65, 89, 118, 127	0
9	I	70/162 (43%)	3.64	50 (71%) 0 0	145, 162, 177, 179	0
10	J	142/145 (97%)	-0.38	1 (0%) 87 74	47, 63, 86, 105	0
11	K	132/132 (100%)	-0.38	0 100 100	45, 63, 91, 100	0
12	L	145/165 (87%)	0.55	21 (14%) 3 1	41, 88, 131, 140	0
13	M	194/196 (98%)	0.25	20 (10%) 7 4	37, 53, 115, 122	0
14	N	186/187 (99%)	0.65	26 (13%) 3 1	70, 90, 134, 139	0
15	O	115/116 (99%)	-0.37	0 100 100	46, 64, 81, 87	0
16	P	143/149 (95%)	-0.30	0 100 100	48, 67, 85, 96	0
17	Q	95/96 (98%)	-0.17	1 (1%) 80 63	57, 69, 89, 97	0
18	R	150/155 (96%)	-0.50	0 100 100	39, 56, 79, 95	0
19	S	81/85 (95%)	-0.28	2 (2%) 58 39	52, 70, 89, 104	0
20	T	119/120 (99%)	-0.04	5 (4%) 37 23	48, 67, 95, 125	0
21	U	53/67 (79%)	4.50	49 (92%) 0 0	112, 125, 131, 134	0
22	V	65/71 (91%)	0.91	12 (18%) 1 1	51, 83, 131, 135	0
23	W	154/154 (100%)	-0.34	1 (0%) 89 77	45, 62, 79, 92	0
24	X	82/92 (89%)	0.03	4 (4%) 30 18	54, 72, 95, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.60	0 100 100	30, 53, 78, 97	0
26	Z	73/116 (62%)	7.40	59 (80%) 0 0	111, 130, 139, 142	0
27	1	56/57 (98%)	-0.51	0 100 100	30, 39, 47, 65	0
28	2	46/50 (92%)	-0.22	3 (6%) 20 11	39, 72, 104, 110	0
29	3	92/92 (100%)	8.52	91 (98%) 0 0	123, 135, 142, 148	0
30	0	2749/2923 (94%)	-0.63	10 (0%) 92 82	25, 58, 106, 183	0
31	9	122/122 (100%)	-0.81	2 (1%) 72 53	51, 90, 111, 159	0
All	All	6646/7517 (88%)	-0.00	471 (7%) 17 9	25, 66, 129, 183	0

All (471) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	58	ASN	25.8
29	3	39	GLN	21.9
29	3	41	GLU	19.9
29	3	47	GLY	19.1
29	3	35	TRP	18.9
26	Z	35	SER	18.6
26	Z	55	SER	18.5
29	3	32	GLY	18.0
26	Z	46	SER	17.6
26	Z	36	GLY	17.2
13	M	87	GLY	17.0
29	3	44	SER	16.5
29	3	42	ARG	16.0
29	3	45	GLY	15.6
29	3	36	ILE	15.5
26	Z	50	VAL	15.5
29	3	48	ASN	15.5
26	Z	39	GLY	15.0
26	Z	56	GLU	15.0
26	Z	38	PHE	14.7
26	Z	34	SER	14.6
29	3	43	ASN	14.5
26	Z	43	GLY	14.4
26	Z	59	GLU	14.1
29	3	38	ARG	13.9
29	3	33	MET	13.8
29	3	40	ARG	13.4
26	Z	69	ASP	13.3

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Mol	Chain	Res	Type	RSRZ
29	3	82	GLY	13.0
29	3	11	CYS	12.7
26	Z	42	TYR	12.7
26	Z	82	SER	12.7
13	M	80	GLY	12.7
29	3	34	LYS	12.4
29	3	37	ASP	12.3
29	3	62	THR	12.0
26	Z	44	ARG	11.9
26	Z	57	MET	11.8
29	3	56	PRO	11.8
29	3	15	ASN	11.4
26	Z	45	VAL	11.2
26	Z	54	GLU	11.2
29	3	57	GLY	11.1
29	3	20	HIS	10.8
29	3	81	GLU	10.5
26	Z	68	GLU	10.5
29	3	59	ASP	10.4
29	3	55	VAL	10.4
26	Z	53	ILE	10.2
29	3	31	THR	10.1
9	I	70	THR	9.9
29	3	51	LYS	9.9
9	I	104	ALA	9.7
29	3	83	TRP	9.5
9	I	74	ILE	9.5
29	3	30	GLN	9.4
29	3	10	TYR	9.3
29	3	71	CYS	9.2
13	M	83	SER	9.0
29	3	53	SER	9.0
21	U	40	ALA	8.9
29	3	18	GLN	8.9
29	3	27	SER	8.8
13	M	90	ARG	8.8
29	3	14	CYS	8.7
13	M	89	THR	8.7
26	Z	49	ARG	8.6
29	3	19	GLU	8.4
21	U	9	CYS	8.4
26	Z	77	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
29	3	78	HIS	8.3
26	Z	78	ILE	8.3
26	Z	71	VAL	8.3
21	U	31	PHE	8.2
26	Z	60	ASP	8.0
21	U	43	GLY	8.0
29	3	13	HIS	8.0
9	I	128	THR	7.9
29	3	61	PRO	7.9
29	3	80	ARG	7.9
26	Z	48	ARG	7.8
29	3	12	PRO	7.8
29	3	46	ILE	7.7
29	3	16	GLU	7.7
26	Z	81	CYS	7.7
29	3	9	THR	7.7
13	M	82	ARG	7.7
21	U	36	CYS	7.7
29	3	1	MET	7.5
21	U	52	THR	7.5
21	U	38	ASN	7.5
26	Z	37	ARG	7.5
29	3	58	GLY	7.4
29	3	17	HIS	7.4
9	I	106	GLN	7.3
21	U	54	THR	7.3
9	I	66	GLY	7.2
4	D	57	THR	7.1
29	3	8	ASN	7.0
26	Z	52	GLU	7.0
26	Z	79	TRP	7.0
29	3	69	TYR	6.9
21	U	41	ASP	6.9
26	Z	61	HIS	6.9
22	V	1	THR	6.9
22	V	39	ALA	6.9
21	U	51	TRP	6.9
29	3	91	GLN	6.9
29	3	52	PHE	6.8
9	I	71	ALA	6.8
29	3	77	ALA	6.7
29	3	74	CYS	6.7

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Mol	Chain	Res	Type	RSRZ
29	3	22	VAL	6.7
13	M	70	GLY	6.7
12	L	60	GLU	6.6
26	Z	67	GLY	6.6
21	U	46	ALA	6.6
26	Z	62	ALA	6.5
13	M	81	ARG	6.4
26	Z	47	ARG	6.4
26	Z	63	CYS	6.4
29	3	28	GLY	6.3
26	Z	51	ALA	6.2
14	N	166	ALA	6.2
9	I	113	SER	6.2
9	I	97	VAL	6.1
29	3	29	ARG	6.1
9	I	103	ILE	6.1
29	3	49	ASP	6.0
13	M	74	LYS	6.0
4	D	69	ILE	6.0
29	3	92	GLU	6.0
26	Z	40	ALA	6.0
29	3	66	ASP	6.0
13	M	78	LYS	5.9
21	U	30	HIS	5.9
26	Z	65	ASN	5.8
9	I	132	VAL	5.8
21	U	12	ASP	5.7
29	3	90	PHE	5.7
4	D	18	ILE	5.7
9	I	100	VAL	5.7
21	U	19	THR	5.7
29	3	76	LYS	5.6
26	Z	74	GLN	5.6
26	Z	66	CYS	5.5
29	3	84	ARG	5.5
29	3	3	MET	5.5
4	D	63	ILE	5.5
21	U	53	ASP	5.5
26	Z	93	TYR	5.5
21	U	33	SER	5.5
9	I	111	LEU	5.4
26	Z	76	THR	5.4

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Mol	Chain	Res	Type	RSRZ
26	Z	88	PHE	5.3
29	3	68	LYS	5.3
26	Z	41	ARG	5.3
21	U	42	LEU	5.3
4	D	135	VAL	5.3
26	Z	70	ARG	5.3
9	I	117	THR	5.3
21	U	29	THR	5.3
9	I	73	LEU	5.2
29	3	88	LEU	5.2
29	3	60	LYS	5.2
9	I	102	GLN	5.2
29	3	85	ALA	5.2
19	S	81	ILE	5.1
29	3	7	PHE	5.1
31	9	1	U	5.1
29	3	86	GLY	5.1
9	I	109	PRO	5.1
21	U	24	LYS	5.1
29	3	5	ARG	5.1
13	M	86	GLN	5.1
21	U	55	ALA	5.1
26	Z	89	THR	5.0
4	D	75	LEU	5.0
21	U	32	CYS	5.0
29	3	4	PRO	5.0
14	N	179	LEU	5.0
13	M	79	ALA	5.0
26	Z	85	ASP	5.0
29	3	23	GLU	5.0
9	I	72	GLU	4.9
13	M	71	SER	4.9
26	Z	80	GLN	4.9
21	U	39	ASN	4.9
22	V	43	PRO	4.8
29	3	6	ARG	4.8
29	3	70	ARG	4.8
29	3	25	VAL	4.8
9	I	108	HIS	4.8
4	D	27	ILE	4.8
29	3	2	GLN	4.8
21	U	45	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
9	I	105	GLU	4.7
21	U	47	ARG	4.7
20	T	119	ALA	4.7
29	3	50	GLY	4.7
29	3	64	LYS	4.6
21	U	11	THR	4.6
9	I	116	LEU	4.6
29	3	54	LYS	4.6
29	3	72	GLY	4.6
4	D	25	MET	4.5
9	I	118	ASN	4.5
21	U	48	ASN	4.5
21	U	25	ASP	4.5
9	I	78	ALA	4.5
13	M	76	ARG	4.5
9	I	110	ASP	4.5
22	V	38	GLY	4.5
4	D	40	ILE	4.5
4	D	90	LEU	4.4
4	D	166	ILE	4.4
29	3	75	GLY	4.4
21	U	6	CYS	4.4
21	U	28	THR	4.4
21	U	8	TYR	4.3
26	Z	92	SER	4.3
29	3	89	GLU	4.3
21	U	13	ILE	4.3
9	I	69	PRO	4.2
22	V	40	PRO	4.2
29	3	67	LEU	4.2
29	3	65	THR	4.2
26	Z	86	TYR	4.2
22	V	37	GLY	4.2
21	U	4	ARG	4.2
29	3	73	GLU	4.2
9	I	94	ASP	4.1
7	G	27	ILE	4.1
29	3	21	GLU	4.1
12	L	106	VAL	4.1
26	Z	83	TYR	4.1
21	U	10	GLY	4.1
9	I	67	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	88	LEU	4.1
13	M	75	ARG	4.0
21	U	23	HIS	4.0
4	D	26	GLY	4.0
13	M	73	ARG	4.0
13	M	88	VAL	4.0
24	X	10	VAL	3.9
26	Z	72	ASP	3.9
30	0	970	U	3.9
22	V	44	GLY	3.9
4	D	134	LEU	3.8
9	I	93	ALA	3.8
4	D	84	LEU	3.8
29	3	87	ARG	3.8
8	H	84	GLY	3.8
9	I	98	ASP	3.8
4	D	87	ALA	3.7
9	I	91	PHE	3.7
21	U	37	GLU	3.7
8	H	39	LYS	3.7
9	I	112	LEU	3.7
1	A	237	GLY	3.7
29	3	24	LYS	3.7
4	D	44	ILE	3.7
9	I	75	LYS	3.6
8	H	82	GLU	3.6
7	G	23	ILE	3.6
21	U	5	GLU	3.6
30	0	735	C	3.6
9	I	92	VAL	3.6
9	I	80	PHE	3.6
6	F	17	LEU	3.6
12	L	105	TYR	3.6
9	I	119	ALA	3.6
6	F	75	ILE	3.5
8	H	66	GLU	3.5
29	3	26	ARG	3.5
8	H	133	GLY	3.5
8	H	40	GLN	3.5
9	I	95	LEU	3.5
26	Z	73	ARG	3.5
1	A	64	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
6	F	106	ALA	3.5
8	H	77	ILE	3.5
26	Z	103	VAL	3.5
4	D	11	HIS	3.4
12	L	48	LYS	3.4
29	3	63	LYS	3.4
30	0	1198	U	3.4
12	L	120	LEU	3.4
9	I	82	THR	3.4
4	D	130	VAL	3.4
9	I	68	PRO	3.3
8	H	86	TYR	3.3
13	M	77	HIS	3.3
4	D	41	LEU	3.2
9	I	88	GLN	3.2
22	V	2	VAL	3.2
8	H	69	ARG	3.2
1	A	37	VAL	3.2
4	D	157	LEU	3.2
4	D	129	ASP	3.2
28	2	49	GLU	3.1
4	D	93	LEU	3.1
9	I	83	GLY	3.1
26	Z	84	CYS	3.1
8	H	81	GLY	3.1
4	D	128	LEU	3.1
8	H	36	MET	3.1
9	I	76	ASP	3.1
28	2	48	ASP	3.1
8	H	35	LYS	3.1
9	I	124	VAL	3.0
9	I	127	CYS	3.0
4	D	165	PHE	3.0
14	N	155	GLU	3.0
13	M	84	LYS	3.0
30	0	1172	G	3.0
1	A	65	ARG	3.0
30	0	1177	A	3.0
8	H	38	ARG	3.0
9	I	121	LYS	3.0
4	D	104	PHE	3.0
8	H	76	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
12	L	123	ASP	3.0
4	D	10	PHE	2.9
4	D	16	PRO	2.9
6	F	99	THR	2.9
12	L	96	VAL	2.9
8	H	149	VAL	2.9
14	N	78	MET	2.9
21	U	22	VAL	2.9
6	F	49	PHE	2.8
4	D	92	GLU	2.8
4	D	17	ARG	2.8
30	0	1199	A	2.8
8	H	89	THR	2.8
4	D	58	VAL	2.8
12	L	142	LEU	2.8
6	F	108	VAL	2.8
8	H	88	MET	2.7
4	D	67	ASP	2.7
12	L	79	ASP	2.7
14	N	142	THR	2.7
4	D	70	GLY	2.7
9	I	101	LYS	2.7
14	N	178	THR	2.7
14	N	95	ALA	2.7
24	X	88	GLU	2.7
14	N	159	TYR	2.7
21	U	20	MET	2.7
4	D	23	VAL	2.7
21	U	44	ARG	2.7
22	V	3	LEU	2.7
4	D	56	ARG	2.7
24	X	71	ARG	2.7
6	F	44	SER	2.6
22	V	41	GLU	2.6
4	D	83	PHE	2.6
21	U	49	LEU	2.6
8	H	141	CYS	2.6
14	N	145	ALA	2.6
12	L	125	PHE	2.6
21	U	21	PHE	2.6
14	N	185	GLU	2.6
12	L	80	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
12	L	130	ARG	2.6
22	V	8	ILE	2.6
14	N	97	VAL	2.6
4	D	80	ALA	2.6
6	F	119	ARG	2.6
21	U	56	ARG	2.6
6	F	20	LEU	2.5
4	D	28	GLY	2.5
9	I	79	GLY	2.5
5	E	5	LEU	2.5
22	V	36	ALA	2.5
8	H	31	ILE	2.5
4	D	106	PHE	2.5
12	L	124	ASP	2.5
9	I	122	GLU	2.5
4	D	89	PRO	2.5
12	L	91	VAL	2.5
26	Z	104	ARG	2.5
21	U	35	LYS	2.5
4	D	73	VAL	2.4
12	L	76	LEU	2.4
19	S	45	TYR	2.4
9	I	123	VAL	2.4
12	L	114	VAL	2.4
14	N	181	ASP	2.4
14	N	83	LEU	2.4
14	N	180	LEU	2.4
14	N	75	THR	2.4
20	T	116	ASP	2.4
4	D	51	ARG	2.4
6	F	19	ALA	2.4
7	G	63	ARG	2.4
8	H	73	ASN	2.4
4	D	101	THR	2.4
8	H	145	ASP	2.4
14	N	84	THR	2.4
6	F	28	ALA	2.4
12	L	75	LEU	2.4
12	L	89	PHE	2.4
8	H	126	THR	2.4
9	I	99	GLN	2.4
20	T	42	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	171	ASP	2.3
12	L	118	LEU	2.3
7	G	25	GLU	2.3
8	H	85	ASP	2.3
13	M	72	ALA	2.3
5	E	118	ILE	2.3
6	F	37	THR	2.3
26	Z	64	PRO	2.3
30	0	1170	U	2.3
10	J	70	PHE	2.3
8	H	79	GLU	2.3
4	D	61	PHE	2.3
14	N	153	GLN	2.3
8	H	132	ALA	2.3
4	D	64	ARG	2.3
31	9	24	U	2.3
9	I	120	ALA	2.3
14	N	92	ALA	2.3
30	0	1163	G	2.3
4	D	172	VAL	2.2
1	A	52	SER	2.2
8	H	98	LEU	2.2
5	E	100	ASP	2.2
1	A	145	MET	2.2
30	0	282	C	2.2
20	T	118	SER	2.2
14	N	156	GLU	2.2
5	E	87	PHE	2.2
6	F	97	ALA	2.2
14	N	172	PHE	2.2
23	W	45	VAL	2.2
12	L	62	ALA	2.2
4	D	19	GLU	2.2
4	D	24	HIS	2.2
14	N	182	GLY	2.1
4	D	62	ASP	2.1
17	Q	20	ASP	2.1
21	U	27	ALA	2.1
8	H	169	GLU	2.1
21	U	15	PRO	2.1
8	H	29	SER	2.1
21	U	26	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
14	N	163	PHE	2.1
1	A	133	ARG	2.1
14	N	81	ALA	2.1
21	U	18	GLY	2.1
4	D	158	ASN	2.1
24	X	7	GLU	2.1
6	F	16	ALA	2.1
4	D	43	GLU	2.1
28	2	39	ARG	2.1
14	N	149	GLU	2.1
20	T	112	LEU	2.1
21	U	50	GLU	2.1
30	0	1000	C	2.1
8	H	74	ARG	2.1
6	F	115	VAL	2.1
12	L	141	GLU	2.1
26	Z	96	GLU	2.1
14	N	7	LYS	2.0
14	N	69	TYR	2.0
8	H	64	SER	2.0
21	U	7	ASP	2.0
1	A	82	VAL	2.0
4	D	48	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	PSU	0	2621	20/21	0.98	0.18	-	39,41,53,53	0
30	OMG	0	2588	24/25	0.98	0.12	-	41,43,46,50	0
30	1MA	0	628	23/24	0.98	0.14	-	38,44,47,47	0
30	UR3	0	2619	21/22	0.98	0.13	-	47,49,51,54	0
30	OMU	0	2587	21/22	0.98	0.11	-	43,47,50,51	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8565	1/1	0.91	1.07	93.90	78,78,78,78	0
35	NA	0	8547	1/1	0.93	0.99	61.90	67,67,67,67	0
35	NA	0	8562	1/1	0.83	0.97	46.93	82,82,82,82	0
35	NA	0	8564	1/1	0.95	0.43	40.53	69,69,69,69	0
34	SR	L	8969	1/1	0.92	0.30	21.44	200,200,200,200	0
34	SR	0	8986	1/1	0.98	1.04	20.37	200,200,200,200	0
35	NA	0	8521	1/1	0.93	0.46	19.54	64,64,64,64	0
35	NA	0	8542	1/1	0.93	0.53	17.94	58,58,58,58	0
34	SR	B	8987	1/1	0.93	0.62	16.03	200,200,200,200	0
35	NA	0	8528	1/1	0.51	0.66	15.81	76,76,76,76	0
35	NA	0	8546	1/1	0.94	0.74	14.85	94,94,94,94	0
35	NA	0	8530	1/1	0.93	0.43	12.64	74,74,74,74	0
36	K	0	8401	1/1	0.92	0.64	11.84	139,139,139,139	0
35	NA	0	8556	1/1	0.98	0.81	10.04	71,71,71,71	0
35	NA	9	8572	1/1	0.95	0.27	9.29	88,88,88,88	0
35	NA	0	8507	1/1	0.99	0.24	8.58	43,43,43,43	0
35	NA	0	8535	1/1	0.83	0.29	8.43	67,67,67,67	0
35	NA	0	8513	1/1	0.96	0.41	8.23	68,68,68,68	0
35	NA	0	8555	1/1	0.87	0.42	8.12	52,52,52,52	0
35	NA	0	8527	1/1	0.94	0.28	6.49	72,72,72,72	0
34	SR	0	8903	1/1	1.00	0.19	6.37	57,57,57,57	0
35	NA	0	8559	1/1	0.98	0.17	5.92	77,77,77,77	0
32	MG	0	8085	1/1	0.96	0.17	5.59	76,76,76,76	0
35	NA	0	8568	1/1	0.94	0.34	5.51	54,54,54,54	0
32	MG	0	8047	1/1	0.97	0.30	5.30	66,66,66,66	0
35	NA	0	8575	1/1	0.99	0.23	5.23	103,103,103,103	0
33	CL	0	8816	1/1	0.96	0.43	5.10	85,85,85,85	0
35	NA	B	8552	1/1	0.78	0.28	4.99	89,89,89,89	0
34	SR	0	8926	1/1	0.98	0.14	4.63	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8553	1/1	0.93	0.28	4.46	89,89,89,89	0
34	SR	0	8992	1/1	0.84	0.22	3.96	159,159,159,159	0
32	MG	0	8009	1/1	0.99	0.24	3.93	34,34,34,34	0
32	MG	0	8079	1/1	0.97	0.20	3.76	66,66,66,66	0
33	CL	B	8819	1/1	0.93	0.21	3.45	69,69,69,69	0
34	SR	R	8912	1/1	0.98	0.19	3.30	95,95,95,95	0
34	SR	0	8904	1/1	1.00	0.20	2.81	57,57,57,57	0
34	SR	0	8975	1/1	0.90	0.14	2.65	149,149,149,149	0
34	SR	0	8943	1/1	0.95	0.13	2.26	84,84,84,84	0
35	NA	0	8569	1/1	0.94	0.18	2.14	50,50,50,50	0
32	MG	0	8011	1/1	0.99	0.22	1.81	25,25,25,25	0
34	SR	0	8949	1/1	0.98	0.15	1.73	117,117,117,117	0
32	MG	0	8003	1/1	0.97	0.17	1.56	38,38,38,38	0
32	MG	0	8014	1/1	0.99	0.17	1.50	37,37,37,37	0
32	MG	0	8028	1/1	0.94	0.17	1.48	34,34,34,34	0
32	MG	0	8080	1/1	0.90	0.76	1.15	83,83,83,83	0
35	NA	0	8537	1/1	0.95	0.16	1.14	50,50,50,50	0
32	MG	0	8016	1/1	0.99	0.17	1.00	40,40,40,40	0
32	MG	A	8051	1/1	0.76	0.26	0.93	94,94,94,94	0
34	SR	0	8964	1/1	0.99	0.12	0.73	134,134,134,134	0
35	NA	M	8539	1/1	0.97	0.14	0.70	42,42,42,42	0
32	MG	0	8084	1/1	0.99	0.14	0.60	35,35,35,35	0
32	MG	0	8008	1/1	0.99	0.13	0.59	31,31,31,31	0
32	MG	0	8041	1/1	0.97	0.16	0.55	36,36,36,36	0
32	MG	0	8043	1/1	0.98	0.13	0.39	52,52,52,52	0
34	SR	0	8922	1/1	0.94	0.17	0.20	168,168,168,168	0
34	SR	0	8923	1/1	1.00	0.13	0.12	109,109,109,109	0
32	MG	0	8006	1/1	0.94	0.12	0.02	44,44,44,44	0
32	MG	0	8062	1/1	0.97	0.17	-0.04	56,56,56,56	0
34	SR	0	8918	1/1	0.99	0.12	-0.06	85,85,85,85	0
32	MG	0	8012	1/1	0.98	0.16	-0.07	25,25,25,25	0
34	SR	0	8935	1/1	0.99	0.11	-0.10	103,103,103,103	0
35	NA	C	8503	1/1	0.95	0.17	-0.15	46,46,46,46	0
34	SR	0	8902	1/1	0.99	0.15	-0.15	68,68,68,68	0
35	NA	0	8515	1/1	0.96	0.15	-0.22	32,32,32,32	0
35	NA	0	8523	1/1	0.98	0.13	-0.29	54,54,54,54	0
36	K	M	8402	1/1	0.92	0.19	-0.34	87,87,87,87	0
34	SR	A	8930	1/1	0.93	0.15	-0.46	142,142,142,142	0
35	NA	J	8538	1/1	0.58	0.15	-0.48	78,78,78,78	0
32	MG	0	8045	1/1	0.97	0.10	-0.53	31,31,31,31	0
35	NA	0	8520	1/1	0.97	0.10	-0.54	56,56,56,56	0
33	CL	O	8808	1/1	0.92	0.17	-0.57	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	A	8929	1/1	0.95	0.11	-0.58	139,139,139,139	0
35	NA	R	8532	1/1	0.98	0.11	-0.59	50,50,50,50	0
35	NA	Q	8540	1/1	0.86	0.11	-0.67	79,79,79,79	0
34	SR	0	8936	1/1	0.99	0.11	-0.70	95,95,95,95	0
34	SR	H	8972	1/1	0.92	0.11	-0.78	164,164,164,164	0
37	CD	Z	8703	1/1	0.78	0.46	-0.78	200,200,200,200	0
37	CD	U	8701	1/1	0.95	0.45	-0.87	200,200,200,200	0
35	NA	0	8504	1/1	1.00	0.12	-1.07	40,40,40,40	0
37	CD	3	8704	1/1	0.78	0.67	-1.14	200,200,200,200	0
32	MG	0	8058	1/1	0.97	0.06	-1.16	18,18,18,18	0
35	NA	0	8563	1/1	0.59	0.12	-1.21	117,117,117,117	0
33	CL	J	8821	1/1	0.96	0.10	-1.34	77,77,77,77	0
34	SR	F	9005	1/1	0.98	0.07	-1.35	147,147,147,147	0
35	NA	0	8534	1/1	0.98	0.12	-1.41	50,50,50,50	0
35	NA	0	8519	1/1	0.95	0.15	-1.50	52,52,52,52	0
35	NA	0	8533	1/1	0.95	0.09	-1.66	70,70,70,70	0
37	CD	1	8702	1/1	1.00	0.10	-1.69	61,61,61,61	0
34	SR	0	8985	1/1	0.86	0.06	-1.74	164,164,164,164	0
32	MG	0	8004	1/1	0.99	0.12	-1.75	29,29,29,29	0
34	SR	0	8910	1/1	0.98	0.09	-1.84	108,108,108,108	0
32	MG	0	8052	1/1	0.96	0.08	-2.05	44,44,44,44	0
32	MG	0	8025	1/1	0.98	0.10	-2.06	37,37,37,37	0
35	NA	0	8557	1/1	0.94	0.06	-2.47	65,65,65,65	0
32	MG	T	8057	1/1	0.98	0.07	-2.48	65,65,65,65	0
32	MG	Y	8086	1/1	0.95	0.08	-2.50	50,50,50,50	0
32	MG	0	8021	1/1	0.95	0.09	-3.00	33,33,33,33	0
33	CL	0	8812	1/1	0.98	0.05	-3.02	61,61,61,61	0
32	MG	A	8050	1/1	0.94	0.06	-3.05	64,64,64,64	0
32	MG	0	8001	1/1	0.98	0.11	-3.33	36,36,36,36	0
32	MG	0	8088	1/1	0.99	0.10	-3.33	35,35,35,35	0
32	MG	0	8044	1/1	0.94	0.05	-3.35	58,58,58,58	0
32	MG	0	8059	1/1	0.93	0.09	-3.35	51,51,51,51	0
32	MG	0	8002	1/1	0.97	0.10	-3.61	40,40,40,40	0
32	MG	0	8076	1/1	0.98	0.06	-3.72	40,40,40,40	0
32	MG	0	8034	1/1	1.00	0.07	-3.82	50,50,50,50	0
33	CL	M	8818	1/1	0.99	0.05	-3.95	49,49,49,49	0
32	MG	0	8075	1/1	0.85	0.05	-4.42	55,55,55,55	0
35	NA	0	8517	1/1	0.96	0.09	-4.54	38,38,38,38	0
34	SR	9	8978	1/1	0.93	0.06	-4.55	157,157,157,157	0
32	MG	0	8013	1/1	0.99	0.06	-5.07	28,28,28,28	0
34	SR	0	8970	1/1	0.96	0.05	-5.52	125,125,125,125	0
32	MG	0	8065	1/1	0.97	0.05	-6.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	1	8913	1/1	0.99	0.06	-10.48	95,95,95,95	0
34	SR	0	8945	1/1	0.98	0.09	-	105,105,105,105	0
35	NA	0	8529	1/1	0.95	0.12	-	48,48,48,48	0
34	SR	B	8950	1/1	0.96	0.16	-	130,130,130,130	0
32	MG	0	8068	1/1	0.96	0.10	-	56,56,56,56	0
32	MG	0	8046	1/1	1.00	0.10	-	45,45,45,45	0
34	SR	0	8995	1/1	0.98	0.19	-	150,150,150,150	0
32	MG	0	8030	1/1	0.90	0.48	-	90,90,90,90	0
33	CL	0	8811	1/1	0.99	0.20	-	81,81,81,81	0
32	MG	0	8070	1/1	0.99	0.17	-	66,66,66,66	0
35	NA	0	8531	1/1	0.99	0.06	-	39,39,39,39	0
34	SR	0	8957	1/1	0.86	0.34	-	200,200,200,200	0
32	MG	0	8038	1/1	0.98	0.08	-	74,74,74,74	0
34	SR	0	8959	1/1	0.81	0.28	-	200,200,200,200	0
34	SR	0	8947	1/1	0.95	0.26	-	200,200,200,200	0
34	SR	0	8967	1/1	0.97	0.04	-	131,131,131,131	0
37	CD	O	8705	1/1	0.99	0.08	-	100,100,100,100	0
34	SR	0	8934	1/1	0.99	0.13	-	133,133,133,133	0
33	CL	0	8813	1/1	0.99	0.07	-	60,60,60,60	0
35	NA	0	8522	1/1	0.91	0.14	-	82,82,82,82	0
34	SR	0	8998	1/1	0.99	0.18	-	178,178,178,178	0
35	NA	0	8536	1/1	0.90	0.17	-	64,64,64,64	0
32	MG	0	8039	1/1	0.96	0.20	-	84,84,84,84	0
34	SR	0	8982	1/1	0.67	1.93	-	200,200,200,200	0
34	SR	0	8979	1/1	0.54	0.19	-	196,196,196,196	0
34	SR	0	8973	1/1	0.99	0.16	-	146,146,146,146	0
32	MG	0	8072	1/1	0.98	0.06	-	59,59,59,59	0
34	SR	0	8901	1/1	0.99	0.18	-	66,66,66,66	0
35	NA	0	8549	1/1	0.98	0.84	-	56,56,56,56	0
35	NA	9	8543	1/1	0.91	0.21	-	61,61,61,61	0
32	MG	0	8061	1/1	0.94	0.17	-	36,36,36,36	0
32	MG	0	8060	1/1	0.94	0.06	-	53,53,53,53	0
32	MG	0	8081	1/1	0.85	0.16	-	88,88,88,88	0
32	MG	0	8024	1/1	0.99	0.17	-	62,62,62,62	0
34	SR	0	8951	1/1	0.85	0.10	-	155,155,155,155	0
35	NA	0	8514	1/1	0.96	0.29	-	55,55,55,55	0
33	CL	0	8803	1/1	0.98	0.09	-	60,60,60,60	0
34	SR	0	8981	1/1	0.99	0.13	-	161,161,161,161	0
32	MG	0	8031	1/1	0.92	0.40	-	83,83,83,83	0
35	NA	0	8509	1/1	0.83	0.13	-	69,69,69,69	0
32	MG	0	8010	1/1	0.96	0.13	-	72,72,72,72	0
32	MG	0	8048	1/1	0.99	0.24	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	CL	0	8817	1/1	0.98	0.14	-	72,72,72,72	0
34	SR	0	8920	1/1	0.95	0.05	-	127,127,127,127	0
32	MG	0	8090	1/1	0.95	0.17	-	97,97,97,97	0
32	MG	0	8055	1/1	0.94	0.07	-	62,62,62,62	0
32	MG	0	8017	1/1	0.99	0.17	-	40,40,40,40	0
34	SR	0	8940	1/1	0.99	0.09	-	93,93,93,93	0
33	CL	R	8806	1/1	0.99	0.14	-	58,58,58,58	0
32	MG	0	8067	1/1	0.89	0.11	-	35,35,35,35	0
34	SR	S	8961	1/1	0.95	0.09	-	128,128,128,128	0
34	SR	0	8962	1/1	0.84	0.09	-	172,172,172,172	0
32	MG	0	8063	1/1	0.93	0.30	-	116,116,116,116	0
34	SR	0	8991	1/1	0.66	0.08	-	180,180,180,180	0
34	SR	0	9006	1/1	0.56	0.98	-	200,200,200,200	0
33	CL	N	8807	1/1	0.94	0.22	-	87,87,87,87	0
35	NA	0	8558	1/1	0.93	0.20	-	58,58,58,58	0
35	NA	0	8566	1/1	0.92	0.30	-	63,63,63,63	0
35	NA	0	8525	1/1	0.77	0.16	-	75,75,75,75	0
32	MG	0	8027	1/1	0.98	0.12	-	47,47,47,47	0
32	MG	0	8023	1/1	0.99	0.17	-	28,28,28,28	0
34	SR	0	9000	1/1	0.95	0.08	-	183,183,183,183	0
35	NA	0	8505	1/1	0.98	0.66	-	53,53,53,53	0
34	SR	0	8906	1/1	1.00	0.21	-	67,67,67,67	0
35	NA	0	8573	1/1	0.94	0.12	-	73,73,73,73	0
34	SR	0	8905	1/1	0.99	0.25	-	72,72,72,72	0
34	SR	0	8939	1/1	0.94	0.04	-	144,144,144,144	0
35	NA	0	8550	1/1	0.94	0.26	-	71,71,71,71	0
32	MG	0	8069	1/1	0.98	0.09	-	102,102,102,102	0
34	SR	0	8911	1/1	0.98	0.12	-	88,88,88,88	0
34	SR	0	8927	1/1	0.96	0.06	-	181,181,181,181	0
35	NA	0	8567	1/1	0.93	0.24	-	78,78,78,78	0
34	SR	0	8993	1/1	0.89	0.08	-	167,167,167,167	0
35	NA	0	8544	1/1	0.90	0.20	-	79,79,79,79	0
34	SR	0	8971	1/1	0.92	0.06	-	192,192,192,192	0
34	SR	0	8944	1/1	0.90	0.07	-	172,172,172,172	0
35	NA	0	8541	1/1	0.98	0.22	-	64,64,64,64	0
32	MG	0	8071	1/1	0.84	0.12	-	60,60,60,60	0
34	SR	0	8996	1/1	0.92	0.51	-	200,200,200,200	0
34	SR	0	8924	1/1	0.99	0.20	-	124,124,124,124	0
32	MG	9	8074	1/1	0.89	0.07	-	87,87,87,87	0
35	NA	0	8554	1/1	0.97	0.85	-	69,69,69,69	0
32	MG	0	8018	1/1	0.99	0.24	-	33,33,33,33	0
34	SR	0	8997	1/1	0.93	0.15	-	189,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8545	1/1	0.88	0.81	-	58,58,58,58	0
32	MG	0	8053	1/1	0.93	0.05	-	63,63,63,63	0
34	SR	0	8965	1/1	0.95	0.06	-	134,134,134,134	0
34	SR	0	8955	1/1	0.96	0.07	-	200,200,200,200	0
34	SR	0	8954	1/1	0.91	0.12	-	108,108,108,108	0
35	NA	0	8524	1/1	0.97	0.69	-	73,73,73,73	0
34	SR	3	8932	1/1	0.90	0.24	-	178,178,178,178	0
32	MG	0	8019	1/1	0.94	0.19	-	29,29,29,29	0
35	NA	H	8518	1/1	0.86	0.42	-	91,91,91,91	0
33	CL	A	8809	1/1	0.99	0.15	-	104,104,104,104	0
32	MG	0	8020	1/1	0.95	0.16	-	41,41,41,41	0
33	CL	L	8810	1/1	0.96	0.05	-	64,64,64,64	0
34	SR	0	8988	1/1	0.62	0.08	-	173,173,173,173	0
35	NA	0	8571	1/1	0.94	0.12	-	79,79,79,79	0
35	NA	S	8510	1/1	0.93	0.03	-	44,44,44,44	0
34	SR	0	8919	1/1	0.87	0.09	-	168,168,168,168	0
34	SR	0	8974	1/1	0.97	0.07	-	166,166,166,166	0
32	MG	0	8078	1/1	0.98	0.25	-	65,65,65,65	0
34	SR	0	9007	1/1	0.79	1.78	-	200,200,200,200	0
34	SR	0	8908	1/1	0.96	0.11	-	85,85,85,85	0
33	CL	0	8815	1/1	0.93	0.22	-	89,89,89,89	0
34	SR	0	8968	1/1	0.94	0.06	-	177,177,177,177	0
34	SR	0	8953	1/1	0.86	0.54	-	200,200,200,200	0
33	CL	0	8814	1/1	0.97	0.16	-	79,79,79,79	0
34	SR	0	8914	1/1	0.98	0.27	-	133,133,133,133	0
32	MG	0	8007	1/1	0.99	0.18	-	36,36,36,36	0
32	MG	0	8033	1/1	0.96	0.06	-	63,63,63,63	0
34	SR	0	8983	1/1	0.91	0.34	-	197,197,197,197	0
32	MG	0	8089	1/1	0.81	0.24	-	65,65,65,65	0
32	MG	0	8066	1/1	0.94	0.17	-	69,69,69,69	0
32	MG	0	8073	1/1	0.96	0.08	-	72,72,72,72	0
32	MG	0	8056	1/1	0.89	0.06	-	57,57,57,57	0
35	NA	0	8548	1/1	0.88	0.12	-	56,56,56,56	0
34	SR	0	9004	1/1	0.71	0.84	-	200,200,200,200	0
33	CL	Y	8820	1/1	0.95	0.07	-	52,52,52,52	0
34	SR	0	8917	1/1	0.94	0.16	-	114,114,114,114	0
33	CL	0	8805	1/1	0.93	0.17	-	98,98,98,98	0
32	MG	K	8054	1/1	0.99	0.17	-	57,57,57,57	0
34	SR	0	8938	1/1	0.80	0.08	-	183,183,183,183	0
35	NA	0	8502	1/1	0.86	0.12	-	69,69,69,69	0
32	MG	0	8029	1/1	1.00	0.13	-	59,59,59,59	0
34	SR	9	9003	1/1	0.89	0.10	-	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8049	1/1	0.99	0.23	-	64,64,64,64	0
35	NA	0	8551	1/1	0.90	0.46	-	63,63,63,63	0
33	CL	J	8801	1/1	0.84	0.12	-	95,95,95,95	0
35	NA	0	8511	1/1	0.68	0.08	-	81,81,81,81	0
32	MG	0	8015	1/1	1.00	0.13	-	45,45,45,45	0
34	SR	0	8976	1/1	0.90	0.29	-	193,193,193,193	0
34	SR	0	8909	1/1	1.00	0.14	-	93,93,93,93	0
34	SR	0	9002	1/1	0.82	0.12	-	193,193,193,193	0
35	NA	0	8560	1/1	0.86	0.55	-	118,118,118,118	0
34	SR	0	8942	1/1	0.97	0.09	-	124,124,124,124	0
32	MG	0	8091	1/1	0.95	0.12	-	56,56,56,56	0
34	SR	0	8921	1/1	0.99	0.13	-	83,83,83,83	0
34	SR	0	8966	1/1	0.96	0.09	-	105,105,105,105	0
34	SR	0	8990	1/1	0.99	0.14	-	137,137,137,137	0
34	SR	3	8999	1/1	0.84	0.28	-	187,187,187,187	0
32	MG	0	8092	1/1	0.95	0.08	-	76,76,76,76	0
34	SR	0	8937	1/1	0.96	0.15	-	113,113,113,113	0
34	SR	0	8994	1/1	0.86	0.48	-	200,200,200,200	0
34	SR	0	8946	1/1	0.91	0.20	-	137,137,137,137	0
32	MG	0	8040	1/1	0.59	0.39	-	86,86,86,86	0
32	MG	0	8093	1/1	0.96	0.06	-	36,36,36,36	0
32	MG	0	8087	1/1	0.96	0.09	-	38,38,38,38	0
34	SR	0	8984	1/1	0.97	0.09	-	119,119,119,119	0
32	MG	0	8005	1/1	0.98	0.21	-	42,42,42,42	0
32	MG	0	8036	1/1	0.95	0.10	-	48,48,48,48	0
35	NA	0	8526	1/1	0.93	0.14	-	46,46,46,46	0
34	SR	0	8915	1/1	0.93	0.09	-	126,126,126,126	0
35	NA	0	8561	1/1	0.96	0.31	-	65,65,65,65	0
34	SR	0	9008	1/1	0.98	0.14	-	92,92,92,92	0
34	SR	0	8960	1/1	0.96	0.02	-	151,151,151,151	0
34	SR	0	9001	1/1	0.75	0.13	-	177,177,177,177	0
32	MG	0	8064	1/1	0.96	0.18	-	45,45,45,45	0
32	MG	0	8022	1/1	0.99	0.20	-	33,33,33,33	0
32	MG	0	8077	1/1	0.98	0.08	-	48,48,48,48	0
34	SR	0	8963	1/1	0.95	0.06	-	133,133,133,133	0
35	NA	0	8506	1/1	0.72	0.20	-	83,83,83,83	0
32	MG	B	8042	1/1	0.97	0.07	-	69,69,69,69	0
34	SR	0	8916	1/1	0.99	0.05	-	105,105,105,105	0
34	SR	1	8952	1/1	1.00	0.15	-	90,90,90,90	0
33	CL	3	8804	1/1	0.24	0.20	-	128,128,128,128	0
34	SR	0	8989	1/1	0.89	0.20	-	178,178,178,178	0
34	SR	0	8958	1/1	0.97	0.07	-	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8977	1/1	0.79	0.07	-	200,200,200,200	0
33	CL	0	8822	1/1	0.97	0.43	-	88,88,88,88	0
34	SR	0	8941	1/1	0.97	0.11	-	114,114,114,114	0
35	NA	0	8516	1/1	0.99	0.19	-	39,39,39,39	0
32	MG	0	8037	1/1	0.99	0.21	-	77,77,77,77	0
32	MG	0	8032	1/1	0.98	0.04	-	52,52,52,52	0
35	NA	0	8508	1/1	0.89	0.48	-	52,52,52,52	0
34	SR	9	8980	1/1	0.87	0.15	-	183,183,183,183	0
32	MG	0	8082	1/1	0.94	0.23	-	76,76,76,76	0
34	SR	0	8931	1/1	0.97	0.10	-	111,111,111,111	0
34	SR	0	8928	1/1	0.85	0.04	-	137,137,137,137	0
34	SR	0	8907	1/1	0.99	0.13	-	63,63,63,63	0
34	SR	0	8925	1/1	0.99	0.13	-	98,98,98,98	0
34	SR	0	8956	1/1	0.95	0.12	-	169,169,169,169	0
34	SR	0	8933	1/1	0.96	0.05	-	135,135,135,135	0
32	MG	0	8026	1/1	0.95	0.08	-	50,50,50,50	0
35	NA	0	8574	1/1	0.95	0.58	-	60,60,60,60	0
32	MG	0	8083	1/1	0.95	0.10	-	55,55,55,55	0
33	CL	J	8802	1/1	0.93	0.06	-	67,67,67,67	0
32	MG	0	8035	1/1	0.98	0.10	-	66,66,66,66	0
35	NA	0	8570	1/1	0.66	0.09	-	61,61,61,61	0
34	SR	0	8948	1/1	0.99	0.10	-	115,115,115,115	0
35	NA	0	8512	1/1	0.98	0.15	-	56,56,56,56	0
35	NA	0	8501	1/1	0.99	0.16	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.