



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:25 AM UTC

PDB ID : 2OTL / pdb_00002otl
Title : Girodazole bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
Resolution : 2.70 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

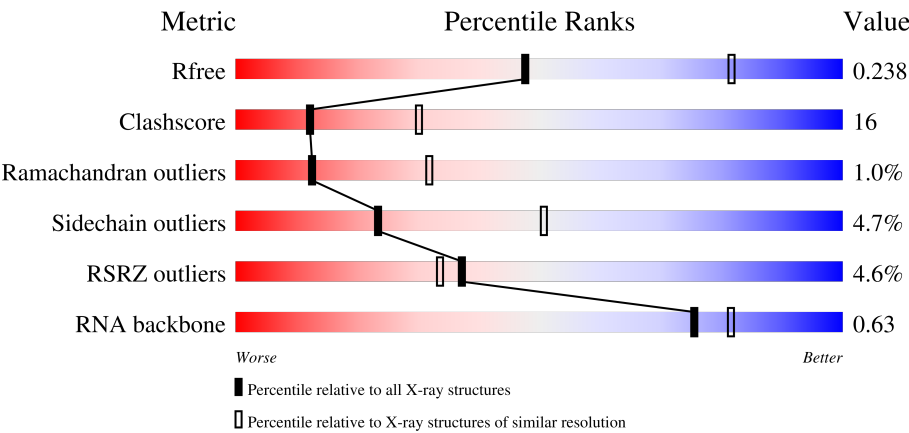
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



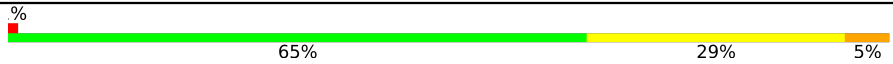
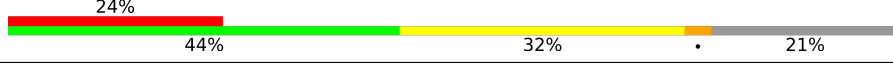
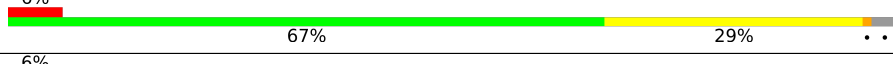
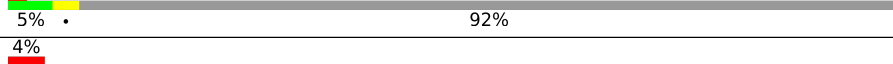
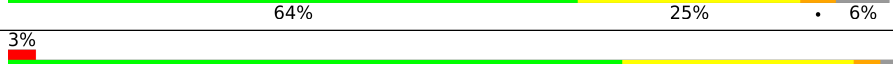
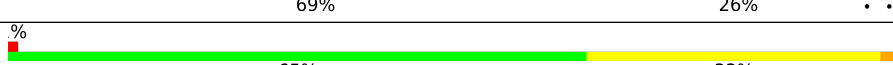
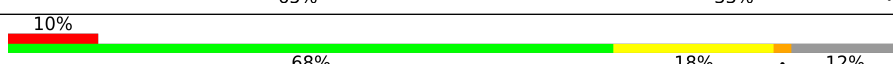
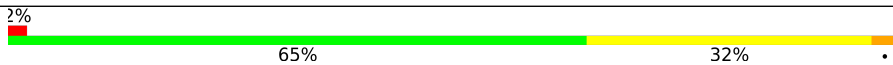
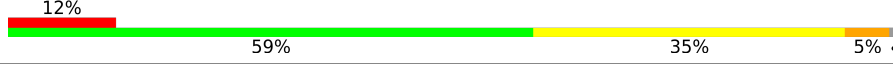
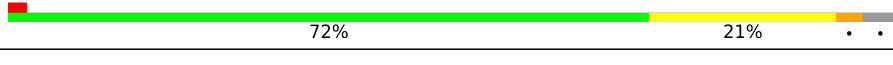
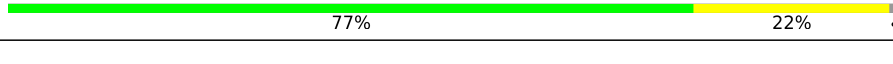
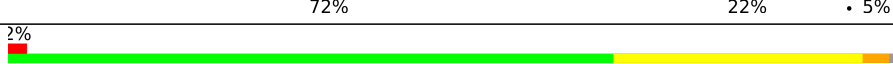
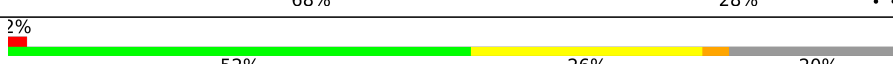
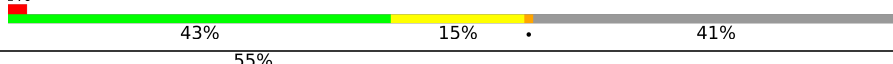
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	2% 49%39%6%6%
2	9	122	4% 43%43%12%.
3	A	239	4% 67%28%. .
4	B	337	% 58%36%5%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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
36	CL	0	8713	-	-	X	-
36	CL	J	8701	-	-	X	-
36	CL	M	8718	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

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

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	-	insertion	UNP P60617
H	166	SER	-	insertion	UNP P60617
H	167	PRO	-	insertion	UNP P60617
H	168	ALA	-	insertion	UNP P60617
H	169	GLY	-	insertion	UNP P60617
H	170	ASN	-	insertion	UNP P60617
H	171	ALA	-	insertion	UNP P60617

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	-	insertion	UNP P60618

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	insertion	UNP P60619

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

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

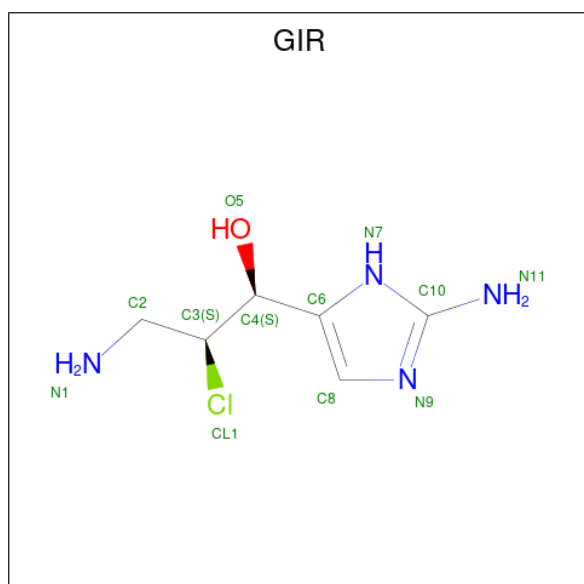
- Molecule 30 is a protein called 50S ribosomal protein L44E.

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

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is GIRODAZOLE (CCD ID: GIR) (formula: C₆H₁₁ClN₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	0	0
			12	6	1	4	1		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	9	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	S	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5893	Total O 5893 5893	0	0
38	9	145	Total O 145 145	0	0
38	A	118	Total O 118 118	0	0
38	B	147	Total O 147 147	0	0
38	C	163	Total O 163 163	0	0
38	D	48	Total O 48 48	0	0
38	E	46	Total O 46 46	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	69	Total O 69 69	0	0
38	J	58	Total O 58 58	0	0
38	K	58	Total O 58 58	0	0
38	L	81	Total O 81 81	0	0
38	M	115	Total O 115 115	0	0
38	N	58	Total O 58 58	0	0

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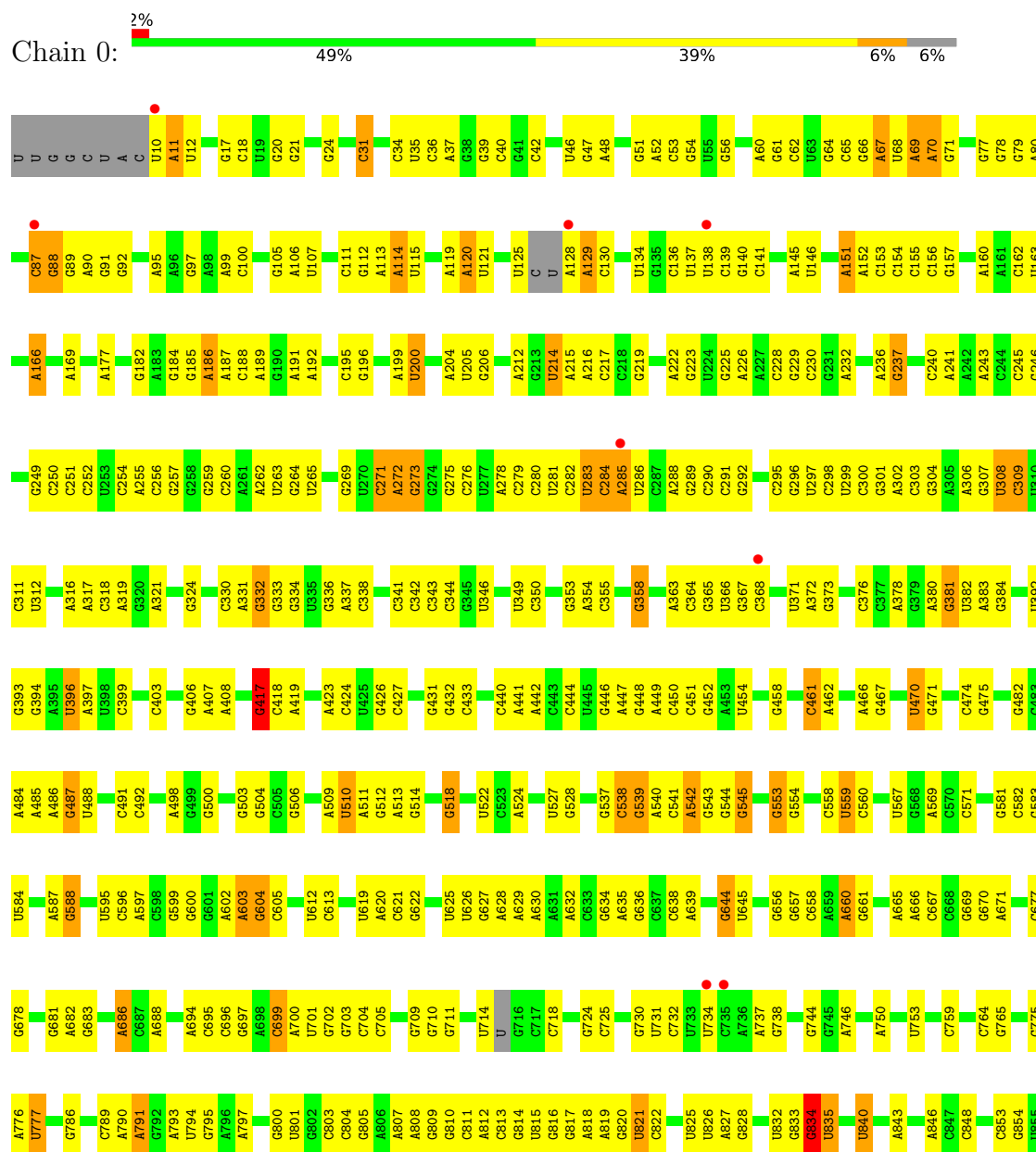
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	61	Total 61	O 61	0	0
38	Q	55	Total 55	O 55	0	0
38	R	81	Total 81	O 81	0	0
38	S	37	Total 37	O 37	0	0
38	T	39	Total 39	O 39	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	70	Total 70	O 70	0	0
38	X	26	Total 26	O 26	0	0
38	Y	99	Total 99	O 99	0	0
38	Z	32	Total 32	O 32	0	0
38	1	56	Total 56	O 56	0	0
38	2	40	Total 40	O 40	0	0
38	3	66	Total 66	O 66	0	0
38	I	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

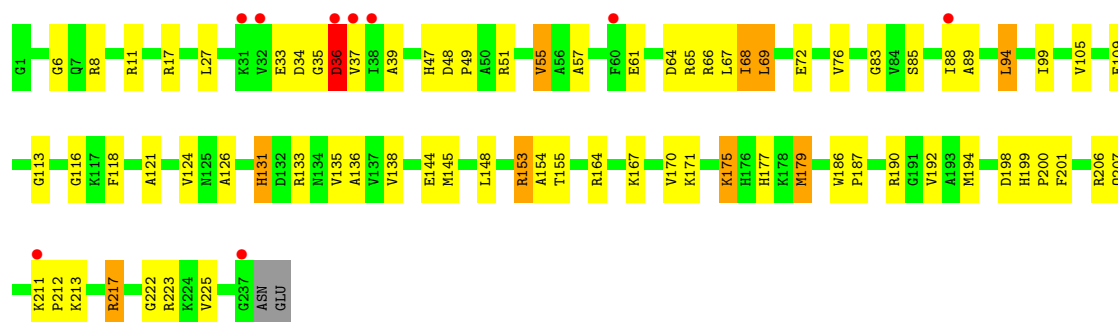
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA

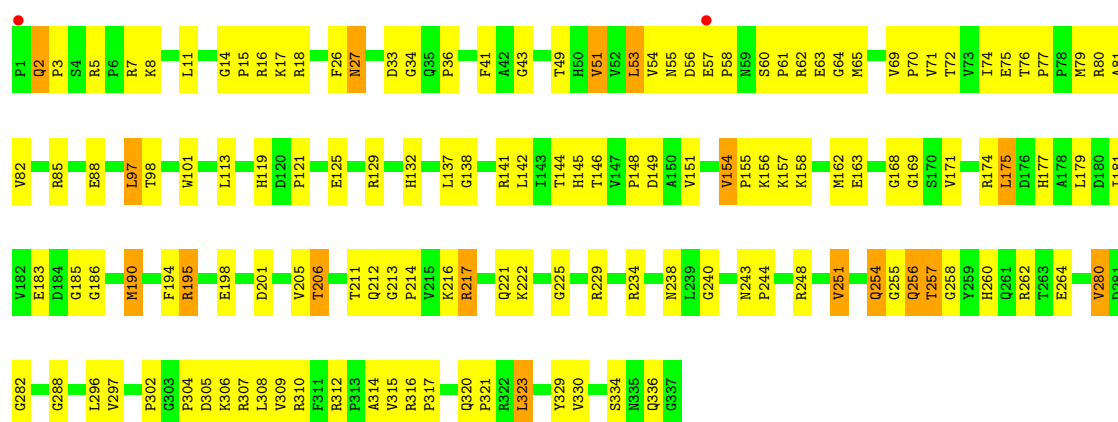




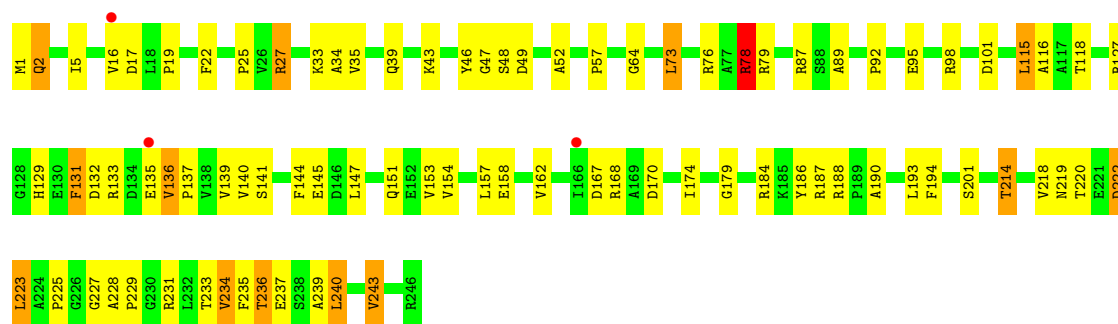




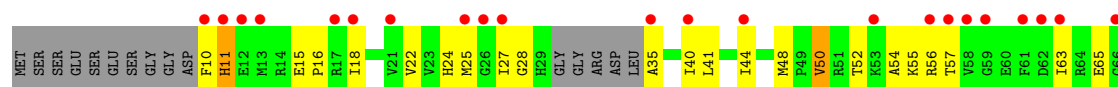
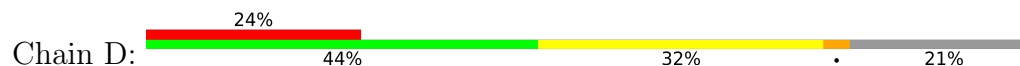
• Molecule 4: 50S ribosomal protein L3P

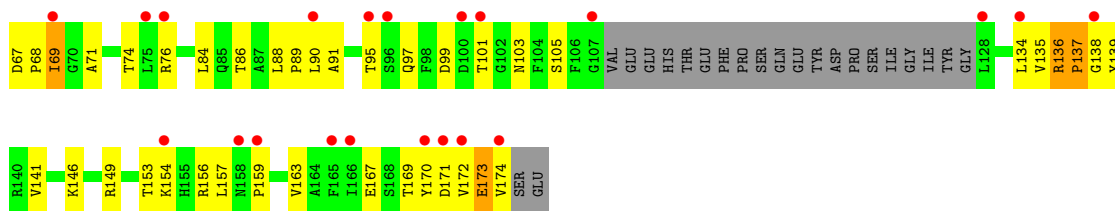


• Molecule 5: 50S ribosomal protein L4P

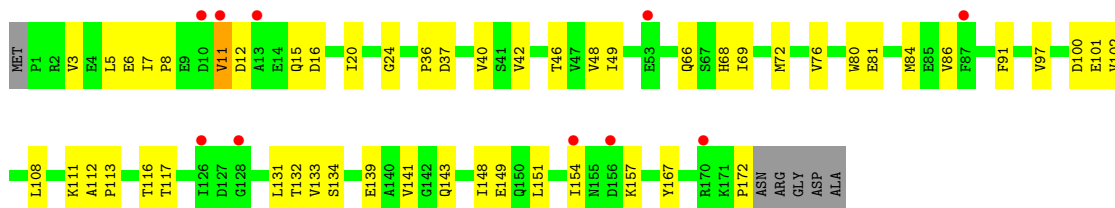


• Molecule 6: 50S ribosomal protein L5P

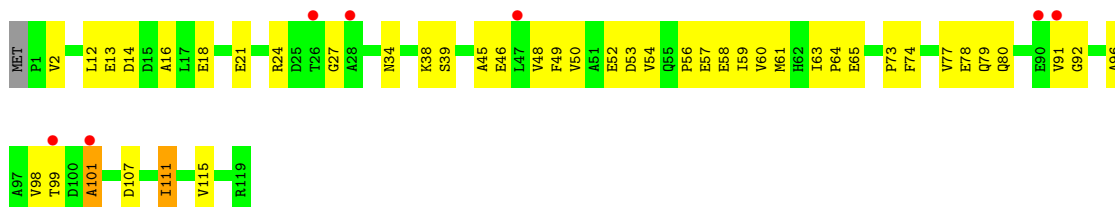




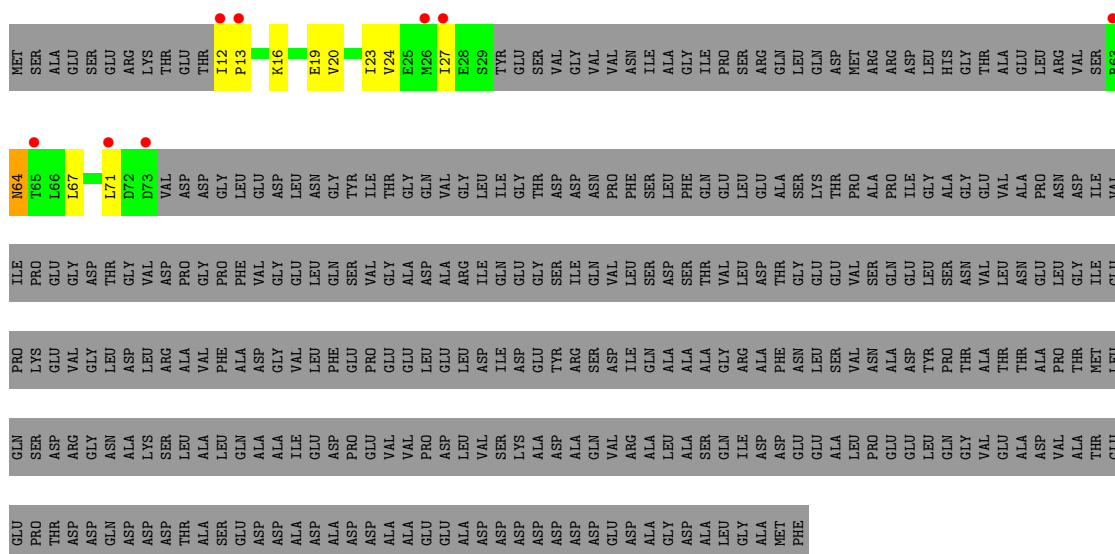
- Molecule 7: 50S ribosomal protein L6P



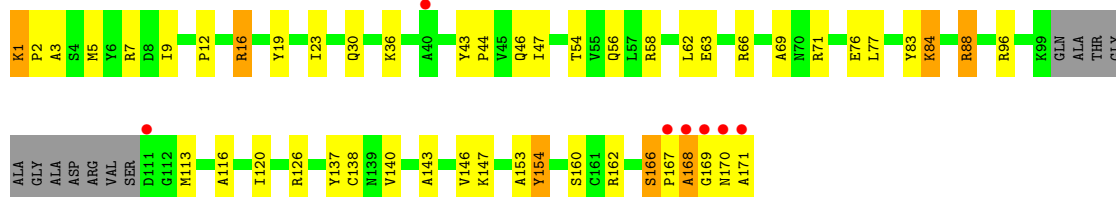
- Molecule 8: 50S ribosomal protein L7Ae



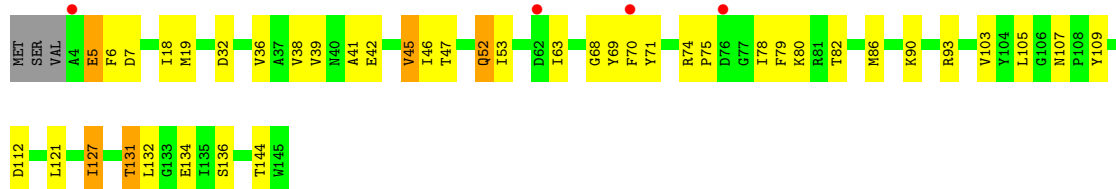
- Molecule 9: 50S ribosomal protein L10E



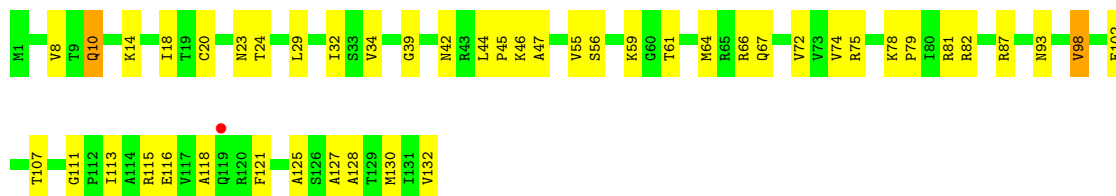
- Molecule 10: 50S ribosomal protein L10e



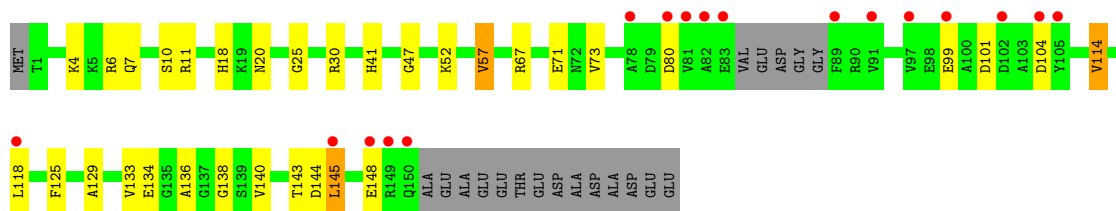
- Molecule 11: 50S ribosomal protein L13P



- Molecule 12: 50S ribosomal protein L14P



- Molecule 13: 50S ribosomal protein L15P

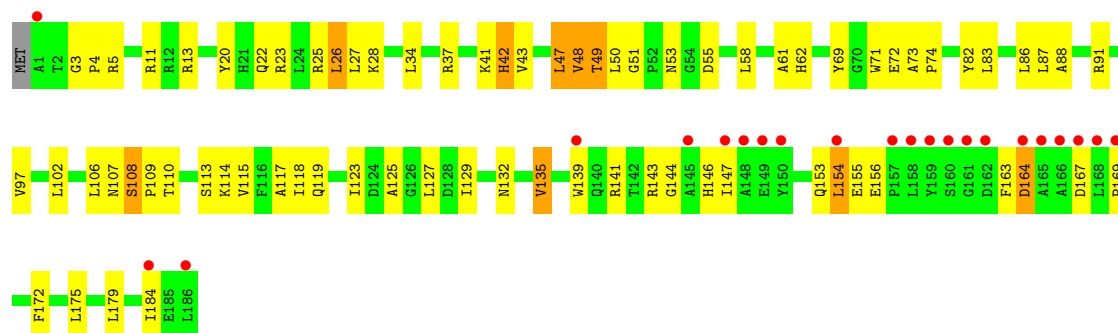


- Molecule 14: 50S ribosomal protein L15e

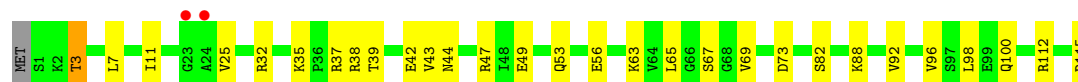
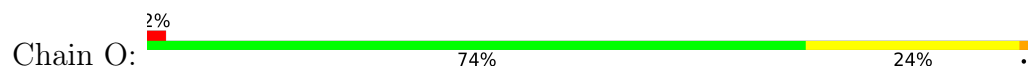




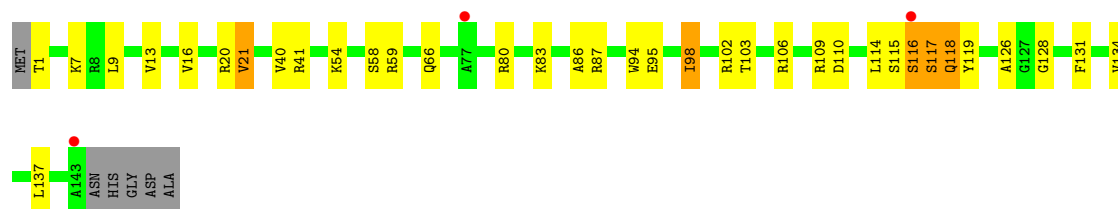
• Molecule 15: 50S ribosomal protein L18P



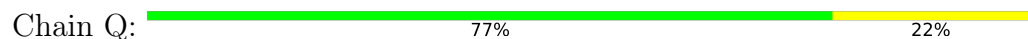
• Molecule 16: 50S ribosomal protein L18e



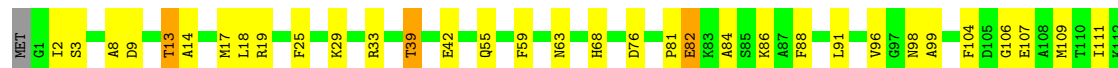
• Molecule 17: 50S ribosomal protein L19e



• Molecule 18: 50S ribosomal protein L21e

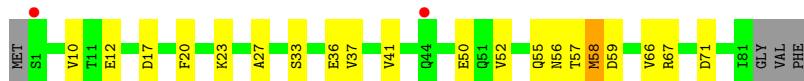


• Molecule 19: 50S ribosomal protein L22P





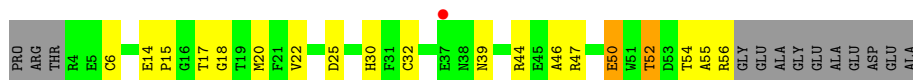
- Molecule 20: 50S ribosomal protein L23P



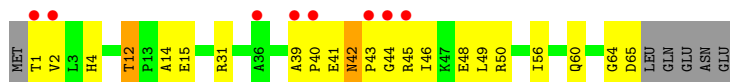
- Molecule 21: 50S ribosomal protein L24P



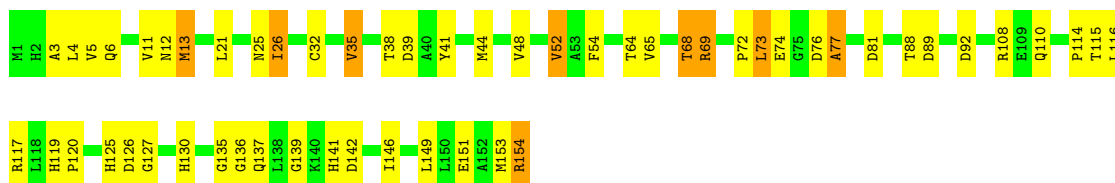
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P

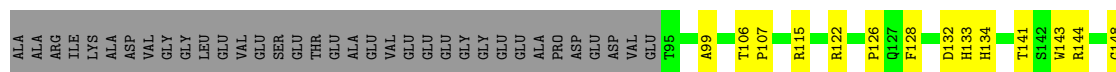
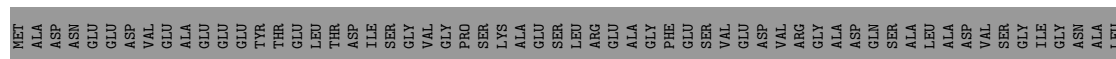
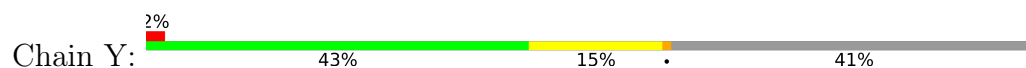


- Molecule 25: 50S ribosomal protein L31e

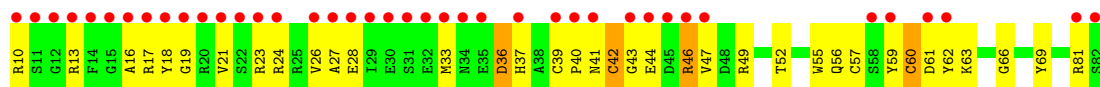




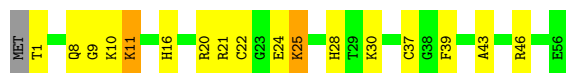
• Molecule 26: 50S ribosomal protein L32e



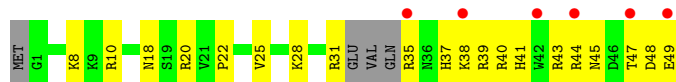
• Molecule 27: 50S ribosomal protein L37Ae



• Molecule 28: 50S ribosomal protein L37e



• Molecule 29: 50S ribosomal protein L39e

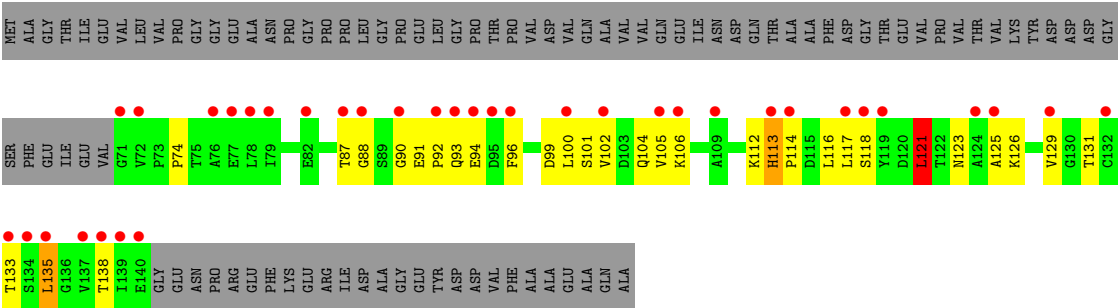


• Molecule 30: 50S ribosomal protein L44E



• Molecule 31: 50S ribosomal protein L11P





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.08Å 300.60Å 575.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 49.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.36-2.70) 90.6 (49.36-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.248 0.196 , 0.238	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99016	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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: OMG, PSU, NA, CL, K, MG, GIR, 1MA, OMU, CD, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.40	0/65959	0.62	18/102870 (0.0%)
2	9	0.38	0/2905	0.59	2/4528 (0.0%)
3	A	0.44	0/1786	1.01	7/2408 (0.3%)
4	B	0.43	0/2690	1.02	14/3652 (0.4%)
5	C	0.48	0/1884	1.03	8/2551 (0.3%)
6	D	0.40	0/1111	0.96	7/1498 (0.5%)
7	E	0.41	0/1382	0.87	2/1880 (0.1%)
8	F	0.44	0/901	0.97	2/1224 (0.2%)
9	G	0.35	0/241	0.83	0/324
10	H	0.42	0/1287	0.98	6/1725 (0.3%)
11	J	0.46	0/1136	0.98	6/1530 (0.4%)
12	K	0.44	0/1001	1.05	6/1347 (0.4%)
13	L	0.43	0/1130	1.00	6/1509 (0.4%)
14	M	0.43	0/1584	0.95	3/2119 (0.1%)
15	N	0.40	0/1474	1.05	14/1999 (0.7%)
16	O	0.45	0/874	0.91	2/1181 (0.2%)
17	P	0.41	0/1147	0.86	1/1528 (0.1%)
18	Q	0.44	0/749	1.05	4/1005 (0.4%)
19	R	0.49	0/1172	0.96	4/1578 (0.3%)
20	S	0.38	0/648	0.91	2/875 (0.2%)
21	T	0.41	0/958	0.98	4/1289 (0.3%)
22	U	0.45	0/417	0.87	1/562 (0.2%)
23	V	0.40	0/502	1.00	2/675 (0.3%)
24	W	0.53	1/1219 (0.1%)	0.98	4/1655 (0.2%)
25	X	0.47	0/664	1.04	5/895 (0.6%)
26	Y	0.46	0/1146	0.95	2/1536 (0.1%)
27	Z	0.60	0/590	1.01	2/787 (0.3%)
28	1	0.45	0/437	0.94	2/578 (0.3%)
29	2	0.47	0/401	0.77	0/529
30	3	0.45	0/771	0.87	5/1024 (0.5%)
31	I	0.41	0/526	0.97	2/716 (0.3%)
All	All	0.41	1/98692 (0.0%)	0.73	143/147577 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	52

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	W	13	MET	SD-CE	-6.17	1.64	1.79

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1979	G	C2'-C3'-O3'	9.87	124.31	109.50
21	T	52	ARG	N-CA-C	8.61	124.63	113.18
18	Q	17	LYS	N-CA-C	-8.00	99.67	109.83
17	P	118	GLN	N-CA-C	-7.87	102.01	111.69
3	A	222	GLY	N-CA-C	-7.83	105.16	114.48
11	J	68	GLY	N-CA-C	7.81	121.04	112.29
14	M	70	GLY	N-CA-C	7.79	122.90	111.76
13	L	47	GLY	N-CA-C	7.77	119.92	112.08
10	H	160	SER	N-CA-C	-7.57	99.31	110.52
6	D	136	ARG	CA-C-N	7.55	129.28	119.84
6	D	136	ARG	C-N-CA	7.55	129.28	119.84
7	E	11	VAL	N-CA-C	7.15	119.39	109.45
13	L	80	ASP	N-CA-C	6.96	120.47	110.24
4	B	157	LYS	N-CA-C	-6.93	105.44	114.04
12	K	8	VAL	N-CA-C	6.91	117.79	108.11
4	B	222	LYS	N-CA-C	-6.89	99.74	110.42
4	B	323	LEU	N-CA-C	6.85	119.14	110.24
12	K	111	GLY	CA-C-N	6.80	126.74	120.21
12	K	111	GLY	C-N-CA	6.80	126.74	120.21
25	X	79	GLU	N-CA-C	6.75	119.47	111.71
28	1	43	ALA	N-CA-C	-6.70	104.06	111.36
31	I	121	LEU	N-CA-C	-6.63	105.01	113.23
6	D	170	TYR	N-CA-C	6.57	120.59	112.58
15	N	102	LEU	N-CA-C	6.44	118.65	108.67
15	N	3	GLY	CA-C-N	6.44	126.20	119.05
15	N	3	GLY	C-N-CA	6.44	126.20	119.05
5	C	89	ALA	N-CA-C	6.43	118.87	111.02
25	X	77	PHE	N-CA-C	6.43	116.35	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	11	LYS	N-CA-C	6.41	119.58	109.39
15	N	13	ARG	N-CA-C	-6.39	105.14	113.12
13	L	145	LEU	N-CA-C	-6.38	104.40	111.36
8	F	79	GLN	N-CA-C	6.35	119.30	109.07
13	L	20	ASN	N-CA-C	6.29	120.78	111.04
6	D	15	GLU	CA-C-N	6.26	127.67	119.84
6	D	15	GLU	C-N-CA	6.26	127.67	119.84
11	J	71	TYR	CA-C-N	6.25	126.21	119.78
11	J	71	TYR	C-N-CA	6.25	126.21	119.78
13	L	57	VAL	N-CA-C	-6.22	107.19	113.47
8	F	111	ILE	N-CA-C	-6.19	104.47	110.72
10	H	116	ALA	N-CA-C	6.18	120.66	113.18
10	H	88	ARG	N-CA-C	6.13	120.02	112.54
4	B	154	VAL	CA-C-N	6.12	125.84	119.05
4	B	154	VAL	C-N-CA	6.12	125.84	119.05
1	0	2291	A	N9-C1'-C2'	6.11	121.16	112.00
1	0	1592	G	N9-C1'-C2'	6.11	121.16	112.00
15	N	51	GLY	CA-C-N	6.09	126.27	119.32
15	N	51	GLY	C-N-CA	6.09	126.27	119.32
15	N	153	GLN	N-CA-C	-6.02	101.37	110.70
3	A	68	ILE	N-CA-C	6.01	117.02	108.42
1	0	1559	A	C2'-C3'-O3'	6.00	122.71	113.70
3	A	133	ARG	N-CA-C	-5.98	106.12	113.41
19	R	141	VAL	N-CA-C	5.97	117.08	108.48
25	X	60	ALA	N-CA-C	5.93	118.22	111.11
21	T	16	LEU	N-CA-C	5.92	118.21	111.11
18	Q	49	ASN	N-CA-C	5.92	118.16	110.53
15	N	42	HIS	N-CA-C	5.89	117.16	108.86
24	W	69	ARG	N-CA-C	5.86	121.15	113.30
30	3	60	LYS	N-CA-C	-5.84	102.71	110.07
1	0	920	C	C2'-C3'-O3'	-5.77	105.05	113.70
10	H	7	ARG	N-CA-C	5.76	119.57	112.54
27	Z	21	VAL	N-CA-C	5.75	116.40	110.36
3	A	148	LEU	N-CA-C	5.74	118.57	109.50
11	J	47	THR	N-CA-C	5.67	117.65	110.33
1	0	874	A	C4'-C3'-O3'	-5.67	104.50	113.00
15	N	48	VAL	N-CA-C	5.67	117.75	108.97
14	M	193	LYS	N-CA-C	5.66	120.52	111.81
19	R	122	GLN	N-CA-C	-5.65	99.92	108.67
16	O	69	VAL	N-CA-C	5.63	116.69	108.53
1	0	1819	G	C5'-C4'-C3'	5.63	124.44	116.00
5	C	219	ASN	N-CA-C	5.63	117.79	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	V	42	ASN	CA-C-N	5.62	126.87	119.84
23	V	42	ASN	C-N-CA	5.62	126.87	119.84
2	9	3039	U	N1-C1'-C2'	5.59	120.38	112.00
24	W	25	ASN	N-CA-C	5.58	119.67	112.86
6	D	11	HIS	N-CA-C	5.58	117.04	111.07
25	X	51	ASP	CA-C-N	5.58	126.81	119.84
25	X	51	ASP	C-N-CA	5.58	126.81	119.84
12	K	46	LYS	N-CA-C	5.57	118.89	109.76
26	Y	143	TRP	N-CA-C	5.57	118.39	110.10
15	N	20	TYR	N-CA-C	5.57	118.28	111.82
22	U	50	GLU	N-CA-C	5.56	117.34	111.28
31	I	135	LEU	N-CA-C	-5.55	108.29	114.62
6	D	171	ASP	N-CA-C	5.54	115.70	107.88
4	B	175	LEU	N-CA-C	-5.53	105.17	111.14
27	Z	46	ARG	N-CA-C	5.53	117.52	110.61
5	C	186	TYR	N-CA-C	5.53	118.98	110.42
4	B	158	LYS	CA-C-N	5.52	125.44	119.76
4	B	158	LYS	C-N-CA	5.52	125.44	119.76
20	S	27	ALA	N-CA-C	-5.51	99.74	108.73
4	B	213	GLY	CA-C-N	5.51	125.16	119.05
4	B	213	GLY	C-N-CA	5.51	125.16	119.05
21	T	3	GLN	CA-C-N	5.50	126.71	119.84
21	T	3	GLN	C-N-CA	5.50	126.71	119.84
30	3	67	LEU	N-CA-C	5.49	118.64	110.52
1	0	834	G	C2'-C3'-O3'	-5.43	105.55	113.70
26	Y	203	VAL	N-CA-C	5.43	116.40	108.53
5	C	78	ARG	N-CA-C	5.42	116.22	108.74
1	0	1504	A	N9-C1'-C2'	5.41	120.12	112.00
4	B	217	ARG	N-CA-C	5.39	117.24	111.36
5	C	167	ASP	N-CA-C	-5.39	105.97	112.54
24	W	68	THR	N-CA-C	5.37	118.29	111.69
13	L	7	GLN	N-CA-C	5.36	118.04	111.82
4	B	113	LEU	N-CA-C	5.35	118.01	110.14
1	0	206	G	C5'-C4'-C3'	-5.35	107.98	116.00
1	0	2664	A	N9-C1'-C2'	5.33	120.00	112.00
30	3	42	ARG	N-CA-C	5.31	116.76	110.97
12	K	61	THR	CA-C-N	5.30	126.47	119.84
12	K	61	THR	C-N-CA	5.30	126.47	119.84
14	M	74	LYS	N-CA-C	5.30	118.44	109.76
1	0	877	G	C2'-C3'-O3'	-5.29	105.76	113.70
3	A	198	ASP	N-CA-C	5.29	119.83	112.90
4	B	151	VAL	CA-C-N	5.29	124.92	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	151	VAL	C-N-CA	5.29	124.92	119.05
19	R	3	SER	N-CA-C	-5.26	101.30	109.24
3	A	213	LYS	N-CA-C	5.25	118.94	112.54
3	A	118	PHE	N-CA-C	5.23	118.21	110.48
5	C	179	GLY	N-CA-C	-5.22	106.33	113.27
18	Q	13	LYS	N-CA-C	5.20	118.41	111.75
30	3	11	CYS	CA-C-N	5.20	124.86	119.56
30	3	11	CYS	C-N-CA	5.20	124.86	119.56
1	0	2726	U	N1-C1'-C2'	5.18	119.77	112.00
10	H	1	LYS	CA-C-N	5.17	125.08	119.85
10	H	1	LYS	C-N-CA	5.17	125.08	119.85
2	9	3065	A	N9-C1'-C2'	5.17	119.75	112.00
19	R	137	ASN	N-CA-C	5.17	118.43	110.42
5	C	64	GLY	N-CA-C	5.14	120.60	114.48
15	N	117	ALA	N-CA-C	-5.14	105.57	111.07
5	C	144	PHE	N-CA-C	-5.13	105.77	111.36
1	0	2071	C	C2'-C3'-O3'	-5.12	106.02	113.70
1	0	2313	C	C5'-C4'-C3'	5.09	123.63	116.00
18	Q	84	ILE	N-CA-C	5.07	115.15	107.75
11	J	112	ASP	N-CA-C	-5.07	102.19	110.20
1	0	2301	A	N9-C1'-C2'	5.06	119.59	112.00
20	S	20	PHE	N-CA-C	5.06	119.72	113.50
16	O	82	SER	N-CA-C	-5.06	103.37	110.50
7	E	37	ASP	N-CA-C	5.05	119.39	113.23
11	J	36	VAL	N-CA-C	5.04	115.73	108.48
1	0	2526	C	N1-C1'-C2'	5.03	119.54	112.00
15	N	28	LYS	N-CA-C	5.02	117.48	111.71
24	W	35	VAL	N-CA-C	5.02	113.36	107.89
1	0	1878	G	N9-C1'-C2'	-5.01	104.49	112.00
15	N	108	SER	CA-C-N	5.00	126.10	119.84
15	N	108	SER	C-N-CA	5.00	126.10	119.84

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1316	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1376	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1681	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	2101	A	Sidechain
1	0	214	U	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2524	G	Sidechain
1	0	2526	C	Sidechain
1	0	2551	C	Sidechain
1	0	2564	G	Sidechain
1	0	2597	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	332	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	458	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	686	A	Sidechain
1	0	791	A	Sidechain
1	0	857	A	Sidechain
1	0	888	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	1368	0
2	9	2600	0	1326	96	0
3	A	1753	0	1766	77	0
4	B	2625	0	2533	111	0
5	C	1859	0	1816	71	0
6	D	1094	0	1085	48	0
7	E	1357	0	1266	39	0
8	F	890	0	843	36	0
9	G	240	0	231	9	0
10	H	1266	0	1268	44	0
11	J	1120	0	1098	42	0
12	K	992	0	1031	40	0
13	L	1118	0	1076	25	0
14	M	1560	0	1568	57	0
15	N	1445	0	1401	63	0
16	O	865	0	873	22	0
17	P	1136	0	1123	35	0
18	Q	735	0	729	13	0
19	R	1149	0	1122	42	0
20	S	641	0	605	12	0
21	T	950	0	923	38	0
22	U	410	0	364	17	0
23	V	499	0	511	20	0
24	W	1196	0	1137	55	0
25	X	654	0	653	22	0
26	Y	1130	0	1133	38	0
27	Z	579	0	540	46	0
28	1	430	0	426	20	0
29	2	396	0	413	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	755	0	729	28	0
31	I	519	0	500	27	0
32	0	12	0	10	0	0
33	0	107	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	4	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	4	0
36	L	1	0	0	0	0
36	M	1	0	0	2	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	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	5893	0	0	184	0
38	1	56	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	40	0	0	3	0
38	3	66	0	0	5	0
38	9	145	0	0	9	0
38	A	118	0	0	10	0
38	B	147	0	0	14	0
38	C	163	0	0	14	0
38	D	48	0	0	8	0
38	E	46	0	0	4	0
38	F	23	0	0	3	0
38	G	19	0	0	0	0
38	H	69	0	0	6	0
38	I	4	0	0	1	0
38	J	58	0	0	4	0
38	K	58	0	0	3	0
38	L	81	0	0	8	0
38	M	115	0	0	5	0
38	N	58	0	0	5	0
38	O	44	0	0	7	0
38	P	61	0	0	1	0
38	Q	55	0	0	4	0
38	R	81	0	0	4	0
38	S	37	0	0	0	0
38	T	39	0	0	3	0
38	U	28	0	0	2	0
38	V	11	0	0	3	0
38	W	70	0	0	5	0
38	X	26	0	0	2	0
38	Y	99	0	0	10	0
38	Z	32	0	0	5	0
All	All	99016	0	59909	2329	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 16.

All (2329) 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)
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.29	1.15
1:0:871:G:H5'	1:0:871:G:H8	1.06	1.12
1:0:656:G:H5'	16:O:3:THR:HG22	1.16	1.12
2:9:3056:A:H2'	2:9:3057:A:H5''	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1559:A:H1'	38:0:5862:HOH:O	1.50	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	1.16	1.09
1:0:871:G:H5'	1:0:871:G:C8	1.86	1.08
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.69	1.07
1:0:1242:A:H5'	11:J:82:THR:HG23	1.35	1.06
1:0:1160:G:C5'	1:0:1161:A:H5'	1.85	1.06
1:0:282:C:H1'	1:0:368:C:N4	1.72	1.02
1:0:156:C:H5''	14:M:171:ARG:HD3	1.40	1.02
1:0:870:G:H2'	1:0:871:G:H5''	1.41	1.01
1:0:1603:A:H5'	1:0:1605:G:O4'	1.61	1.00
1:0:1160:G:H5'	1:0:1161:A:H5'	1.03	1.00
1:0:214:U:H5'	38:0:6131:HOH:O	1.61	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.44	0.99
1:0:1474:C:H6	1:0:1474:C:H5'	1.25	0.99
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.41	0.99
1:0:1160:G:H5'	1:0:1161:A:C5'	1.92	0.99
2:9:3076:G:H3'	2:9:3077:A:H5''	1.44	0.98
1:0:236:A:H4'	1:0:237:G:H5'	1.46	0.98
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.47	0.97
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.46	0.97
1:0:1118:A:C8	1:0:1118:A:H3'	1.99	0.96
1:0:1118:A:H3'	1:0:1118:A:H8	1.26	0.96
1:0:289:G:H22	1:0:363:A:H2	1.05	0.96
27:Z:41:ASN:HB3	27:Z:60:CYS:SG	2.05	0.95
1:0:1835:U:H5	1:0:1840:A:N7	1.62	0.95
1:0:2812:A:H2	1:0:2814:A:H62	1.14	0.94
1:0:2506:A:HO2'	1:0:2507:G:H8	1.00	0.94
1:0:2783:A:H3'	38:0:5224:HOH:O	1.67	0.94
1:0:541:C:H2'	1:0:542:A:H5''	1.48	0.93
1:0:2533:C:H5'	1:0:2533:C:H6	1.32	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.30	0.92
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.50	0.92
1:0:797:A:H4'	27:Z:10:ARG:N	1.85	0.92
17:P:115:SER:H	17:P:118:GLN:HE21	1.03	0.92
1:0:1372:A:H3'	38:0:7168:HOH:O	1.70	0.92
2:9:3006:C:H5''	15:N:37:ARG:HH12	1.30	0.92
1:0:1862:C:H1'	38:0:7198:HOH:O	1.68	0.92
11:J:127:ILE:HG22	36:J:8701:CL:CL	2.07	0.92
12:K:10:GLN:HE21	12:K:10:GLN:H	0.92	0.92
2:9:3054:A:O2'	2:9:3055:U:H5'	1.69	0.91
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:381:G:H5''	38:0:4317:HOH:O	1.71	0.90
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.51	0.90
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.90
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.19	0.90
1:0:1666:C:O2'	1:0:1667:A:H5''	1.72	0.90
1:0:182:G:H5'	38:0:5151:HOH:O	1.71	0.90
1:0:1205:U:H2'	1:0:1206:U:C5'	2.02	0.89
1:0:871:G:H8	1:0:871:G:C5'	1.85	0.89
1:0:1206:U:H5'	1:0:1206:U:H6	1.37	0.89
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.87	0.89
1:0:545:G:H5'	1:0:545:G:H8	1.35	0.89
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.88
1:0:2506:A:O2'	1:0:2507:G:H8	1.57	0.88
1:0:2672:C:H1'	38:B:8833:HOH:O	1.71	0.88
1:0:2850:C:H6	1:0:2850:C:H5'	1.37	0.88
1:0:56:G:H5''	23:V:50:ARG:HH12	1.39	0.87
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.54	0.87
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.16	0.87
2:9:3056:A:C2'	2:9:3057:A:H5''	2.05	0.87
1:0:541:C:C2'	1:0:542:A:H5''	2.05	0.86
1:0:753:U:H3'	38:0:5520:HOH:O	1.75	0.86
1:0:396:U:H1'	38:0:7600:HOH:O	1.75	0.86
1:0:558:C:O2'	1:0:559:U:H5''	1.75	0.86
1:0:2824:C:H5''	1:0:2825:C:H5'	1.56	0.86
1:0:656:G:H5'	16:O:3:THR:CG2	2.01	0.86
1:0:1116:U:HO2'	1:0:1118:A:H2	0.88	0.86
1:0:1450:C:H4'	1:0:1451:C:OP2	1.75	0.86
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.41	0.86
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.39	0.86
12:K:10:GLN:HE21	12:K:10:GLN:N	1.75	0.85
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.85
12:K:10:GLN:H	12:K:10:GLN:NE2	1.74	0.85
1:0:1184:C:H1'	38:0:7436:HOH:O	1.76	0.85
1:0:1189:A:H1'	1:0:1209:C:O4'	1.77	0.84
24:W:149:LEU:HG	24:W:153:MET:HE2	1.57	0.84
1:0:2421:G:H1'	38:0:7002:HOH:O	1.76	0.84
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.58	0.84
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.59	0.84
1:0:1474:C:H5'	1:0:1474:C:C6	2.12	0.84
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.43	0.84
1:0:2570:G:H5''	38:0:4909:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:79:MET:HE3	4:B:144:THR:HG21	1.60	0.83
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.58	0.83
1:0:1120:U:H6	1:0:1120:U:H5'	1.41	0.83
1:0:677:C:O2'	1:0:678:G:H5'	1.78	0.83
4:B:238:ASN:HD22	4:B:240:GLY:H	1.25	0.83
22:U:39:ASN:ND2	22:U:44:ARG:HH11	1.76	0.83
27:Z:42:CYS:SG	27:Z:59:TYR:HD2	2.00	0.83
1:0:877:G:H5'	1:0:878:G:OP1	1.79	0.83
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.60	0.83
36:0:8713:CL:CL	38:0:4680:HOH:O	2.33	0.83
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.61	0.83
1:0:282:C:O2'	1:0:283:U:H5'	1.79	0.82
29:2:41:HIS:H	29:2:45:ASN:HD22	1.28	0.82
1:0:1118:A:H62	1:0:1244:U:H3	1.24	0.82
1:0:2502:C:C2'	1:0:2503:A:H5'	2.10	0.82
1:0:2533:C:H5'	1:0:2533:C:C6	2.13	0.82
14:M:59:GLY:HA3	14:M:141:ILE:HD11	1.62	0.82
1:0:2769:C:O2'	1:0:2770:G:H5'	1.80	0.82
1:0:1119:G:N2	1:0:1246:A:C2	2.48	0.81
36:M:8718:CL:CL	38:M:8819:HOH:O	2.34	0.81
5:C:236:THR:HG22	5:C:239:ALA:N	1.96	0.81
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.61	0.81
1:0:1183:C:N4	1:0:1184:C:H41	1.79	0.81
1:0:21:G:C5'	19:R:2:ILE:HA	2.11	0.81
1:0:21:G:H5'	19:R:2:ILE:HA	1.63	0.81
1:0:1205:U:H2'	1:0:1206:U:H5''	1.60	0.81
1:0:2256:G:C2'	1:0:2257:G:H5'	2.11	0.81
27:Z:46:ARG:HD2	27:Z:59:TYR:HB2	1.60	0.81
1:0:870:G:C2'	1:0:871:G:H5''	2.09	0.80
1:0:2291:A:C8	1:0:2309:C:H5'	2.16	0.80
1:0:2251:G:H2'	1:0:2252:A:C8	2.16	0.80
1:0:2502:C:H2'	1:0:2503:A:H5'	1.62	0.80
1:0:1116:U:O2'	1:0:1118:A:H2	1.65	0.80
19:R:39:THR:HG22	19:R:42:GLU:H	1.46	0.80
23:V:2:VAL:HG21	23:V:45:ARG:NH2	1.96	0.80
2:9:3014:G:H5'	2:9:3014:G:H8	1.46	0.80
1:0:1919:A:H4'	38:0:4847:HOH:O	1.83	0.79
2:9:3049:G:O2'	2:9:3050:G:H5'	1.81	0.79
1:0:1771:U:H1'	27:Z:23:ARG:HH21	1.45	0.79
1:0:1603:A:H5''	1:0:1605:G:H5'	1.63	0.79
1:0:188:C:H5''	14:M:163:LEU:HD21	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:G:N2	1:0:363:A:H2	1.81	0.79
1:0:558:C:C2'	1:0:559:U:H5''	2.12	0.79
1:0:558:C:H2'	1:0:559:U:C5'	2.13	0.79
38:0:5215:HOH:O	12:K:39:GLY:HA2	1.82	0.79
1:0:272:A:H5'	1:0:273:G:OP2	1.83	0.79
1:0:2248:C:H3'	38:0:5439:HOH:O	1.82	0.79
36:0:8717:CL:CL	38:Y:8755:HOH:O	2.37	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
1:0:2890:A:H1'	22:U:56:ARG:NH2	1.98	0.78
24:W:5:VAL:HG11	24:W:153:MET:HE1	1.64	0.78
1:0:199:A:H5''	38:0:3528:HOH:O	1.83	0.78
1:0:2586:U:H3	1:0:2592:G:H22	1.32	0.78
1:0:2256:G:H2'	1:0:2257:G:H5'	1.65	0.78
3:A:36:ASP:HB2	3:A:83:GLY:HA3	1.65	0.78
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.64	0.78
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.64	0.78
1:0:31:C:H4'	38:0:7398:HOH:O	1.84	0.78
1:0:1835:U:C5	1:0:1840:A:N7	2.49	0.78
1:0:1130:U:H5'	38:0:7642:HOH:O	1.84	0.78
1:0:541:C:H2'	1:0:542:A:C5'	2.13	0.78
1:0:2001:G:O2'	1:0:2002:C:H5'	1.84	0.78
1:0:69:A:H5'	1:0:69:A:C8	2.20	0.77
1:0:69:A:H5'	1:0:69:A:H8	1.50	0.77
1:0:2491:G:H1'	38:0:6848:HOH:O	1.84	0.77
2:9:3058:G:H1'	38:D:3839:HOH:O	1.83	0.77
1:0:603:A:H5''	1:0:604:G:OP1	1.84	0.77
1:0:1279:U:O2	1:0:1279:U:H2'	1.85	0.77
26:Y:174:VAL:HG23	26:Y:177:LYS:HD2	1.67	0.77
1:0:2755:G:H1'	38:0:4679:HOH:O	1.84	0.76
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.76
1:0:2851:G:O2'	1:0:2852:A:H5'	1.85	0.76
5:C:139:VAL:HG13	38:C:8642:HOH:O	1.82	0.76
1:0:383:A:H4'	38:0:5323:HOH:O	1.85	0.76
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.68	0.76
23:V:2:VAL:HG21	23:V:45:ARG:HH21	1.46	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.33	0.76
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.68	0.76
1:0:559:U:H6	1:0:559:U:H5'	1.51	0.76
1:0:1537:C:H1'	38:0:6566:HOH:O	1.85	0.76
8:F:38:LYS:HZ1	14:M:3:SER:HA	1.51	0.76
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:338:C:H4'	5:C:174:ILE:CD1	2.16	0.76
1:0:1213:C:O2'	1:0:1214:G:H5'	1.84	0.76
1:0:2489:G:H1'	38:0:7254:HOH:O	1.85	0.76
1:0:1398:G:O2'	1:0:1399:A:H5'	1.86	0.75
1:0:2748:G:H2'	38:0:7511:HOH:O	1.85	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.68	0.75
1:0:1667:A:H5'	1:0:1667:A:C8	2.19	0.75
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.68	0.75
1:0:506:G:H22	1:0:509:A:H5'	1.49	0.75
1:0:2679:G:H2'	1:0:2681:A:OP2	1.86	0.75
1:0:2851:G:C2'	1:0:2852:A:H5'	2.17	0.75
30:3:65:THR:HG22	30:3:67:LEU:HG	1.69	0.75
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.16	0.75
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.69	0.75
24:W:6:GLN:HB2	24:W:26:ILE:CD1	2.17	0.75
1:0:1118:A:C8	1:0:1118:A:C3'	2.65	0.74
1:0:2768:A:H2'	1:0:2769:C:O4'	1.86	0.74
1:0:711:G:H1'	38:0:7076:HOH:O	1.86	0.74
4:B:179:LEU:O	4:B:183:GLU:HG2	1.87	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
1:0:2256:G:O2'	1:0:2257:G:H5'	1.88	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.67	0.74
1:0:1080:C:H4'	1:0:1081:A:OP1	1.87	0.74
1:0:292:G:H2'	1:0:358:G:N2	2.03	0.74
1:0:944:G:H21	24:W:44:MET:HE2	1.52	0.74
1:0:2256:G:H2'	1:0:2257:G:C5'	2.18	0.74
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.68	0.74
6:D:103:ASN:ND2	6:D:134:LEU:H	1.84	0.74
1:0:1657:A:H2'	1:0:1658:A:C8	2.23	0.74
1:0:1205:U:H2'	1:0:1206:U:H5'	1.68	0.74
11:J:19:MET:HE1	11:J:78:ILE:HG22	1.70	0.74
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.70	0.74
1:0:1130:U:H2'	1:0:1131:G:O4'	1.87	0.73
1:0:2414:A:H2'	1:0:2415:A:C8	2.23	0.73
19:R:17:MET:SD	38:R:8745:HOH:O	2.46	0.73
1:0:2426:G:H1'	38:0:6084:HOH:O	1.89	0.73
36:J:8701:CL:CL	38:J:8752:HOH:O	2.44	0.73
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.70	0.73
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.18	0.73
1:0:558:C:H2'	1:0:559:U:H5'	1.71	0.73
1:0:656:G:C5'	16:O:3:THR:HG22	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3055:U:H4'	2:9:3056:A:C8	2.23	0.73
24:W:88:THR:HG22	24:W:89:ASP:H	1.54	0.73
2:9:3039:U:H1'	2:9:3044:A:H61	1.51	0.73
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.89	0.73
1:0:661:G:C5	1:0:686:A:C2	2.76	0.72
1:0:281:U:H3'	38:0:7185:HOH:O	1.88	0.72
2:9:3092:G:H2'	2:9:3093:A:C8	2.25	0.72
1:0:797:A:C4'	27:Z:10:ARG:N	2.52	0.72
3:A:121:ALA:O	3:A:124:VAL:HG22	1.90	0.72
1:0:2252:A:C5	1:0:2253:G:H1'	2.25	0.72
4:B:62:ARG:HA	4:B:65:MET:HE3	1.70	0.72
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.07	0.72
14:M:102:GLU:OE1	14:M:164:THR:HG21	1.89	0.72
1:0:1667:A:H2'	1:0:1668:U:C6	2.25	0.72
1:0:2769:C:C2'	1:0:2770:G:H5'	2.19	0.72
1:0:1168:C:H4'	38:0:5905:HOH:O	1.91	0.71
1:0:284:C:H4'	1:0:285:A:O5'	1.90	0.71
1:0:2840:A:OP1	4:B:211:THR:HG23	1.90	0.71
5:C:145:GLU:HG3	38:C:8573:HOH:O	1.90	0.71
1:0:2635:A:O2'	1:0:2636:C:H5'	1.89	0.71
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.54	0.71
1:0:1878:G:H1'	38:0:6112:HOH:O	1.91	0.71
1:0:1441:G:O2'	1:0:1442:A:H5'	1.90	0.71
1:0:1666:C:H2'	1:0:1667:A:H5'	1.72	0.71
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.72	0.71
15:N:144:GLY:O	15:N:147:ILE:HG22	1.91	0.71
1:0:1205:U:C2'	1:0:1206:U:H5''	2.21	0.70
1:0:2488:A:H61	1:0:2534:C:H42	1.36	0.70
1:0:403:C:H3'	38:0:6290:HOH:O	1.90	0.70
17:P:115:SER:H	17:P:118:GLN:NE2	1.84	0.70
19:R:25:PHE:CE2	19:R:29:LYS:HE2	2.27	0.70
1:0:1342:C:C2'	1:0:1343:C:H5'	2.21	0.70
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.73	0.70
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.26	0.70
38:0:7428:HOH:O	5:C:188:ARG:HD2	1.92	0.70
29:2:35:ARG:HB3	38:2:2691:HOH:O	1.92	0.70
1:0:2524:G:H21	1:0:2526:C:N4	1.89	0.70
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.26	0.70
1:0:1164:U:H3	1:0:1192:A:H2	1.37	0.70
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.56	0.70
1:0:288:A:H61	1:0:364:C:H42	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2320:U:H4'	1:0:2321:A:O4'	1.92	0.69
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.69
1:0:2237:G:H1'	38:0:4851:HOH:O	1.91	0.69
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.52	0.69
1:0:338:C:H4'	5:C:174:ILE:HD11	1.74	0.69
1:0:2827:A:H2'	1:0:2828:G:O4'	1.92	0.69
1:0:2054:A:N3	19:R:128:ARG:NH2	2.40	0.69
21:T:48:VAL:HG11	21:T:96:VAL:HG13	1.74	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.92	0.69
1:0:1701:A:H5'	38:0:6267:HOH:O	1.92	0.69
1:0:1942:A:H3'	38:0:7323:HOH:O	1.91	0.69
1:0:2420:G:O2'	1:0:2421:G:H5'	1.93	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.69
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.58	0.69
17:P:115:SER:N	17:P:118:GLN:HE21	1.86	0.69
17:P:59:ARG:NH2	17:P:66:GLN:HE22	1.90	0.69
1:0:1314:U:H2'	38:0:5871:HOH:O	1.94	0.68
14:M:164:THR:HG22	14:M:167:GLY:H	1.58	0.68
1:0:2716:G:H5''	4:B:206:THR:HG21	1.73	0.68
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.73	0.68
1:0:447:A:OP1	21:T:2:LYS:HG2	1.93	0.68
2:9:3064:C:H2'	2:9:3065:A:H5'	1.76	0.68
38:0:5455:HOH:O	9:G:12:ILE:HA	1.92	0.68
2:9:3014:G:H5'	2:9:3014:G:C8	2.28	0.68
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.09	0.68
1:0:703:G:O2'	1:0:704:C:H5'	1.93	0.68
2:9:3054:A:C2'	2:9:3055:U:H5'	2.24	0.68
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.23	0.68
1:0:380:A:H2'	38:0:7206:HOH:O	1.92	0.68
1:0:1289:C:H3'	38:0:6391:HOH:O	1.93	0.68
38:0:7198:HOH:O	3:A:11:ARG:HA	1.93	0.68
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.42	0.68
1:0:1167:G:H4'	31:I:135:LEU:HD22	1.75	0.68
27:Z:10:ARG:HA	38:Z:8615:HOH:O	1.94	0.68
1:0:702:G:O2'	1:0:703:G:H5'	1.95	0.67
1:0:1189:A:H1'	1:0:1209:C:C1'	2.24	0.67
1:0:2363:G:O2'	18:Q:11:ARG:HG3	1.94	0.67
1:0:156:C:H5''	14:M:171:ARG:CD	2.22	0.67
1:0:1771:U:H1'	27:Z:23:ARG:NH2	2.09	0.67
3:A:51:ARG:HB2	38:A:8801:HOH:O	1.92	0.67
1:0:2505:G:O2'	1:0:2506:A:H5'	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:8712:CL:CL	38:0:5118:HOH:O	2.49	0.67
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.30	0.67
1:0:1189:A:O2'	1:0:1208:C:H2'	1.95	0.67
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.94	0.67
1:0:2779:G:H21	7:E:143:GLN:NE2	1.92	0.67
1:0:2896:A:H5''	38:0:6091:HOH:O	1.94	0.67
1:0:544:G:C2'	1:0:545:G:H5''	2.24	0.67
1:0:871:G:C8	1:0:871:G:C5'	2.66	0.67
1:0:272:A:H3'	38:0:7500:HOH:O	1.94	0.67
1:0:558:C:C2'	1:0:559:U:C5'	2.72	0.67
2:9:3055:U:H4'	2:9:3056:A:H8	1.60	0.67
1:0:2533:C:H6	1:0:2533:C:C5'	2.06	0.67
31:I:131:THR:O	31:I:135:LEU:HG	1.94	0.67
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.77	0.66
1:0:1350:U:H4'	38:0:5116:HOH:O	1.93	0.66
4:B:238:ASN:HD22	4:B:240:GLY:N	1.92	0.66
1:0:285:A:H2'	1:0:286:U:O4'	1.94	0.66
1:0:2559:C:H4'	38:0:7235:HOH:O	1.95	0.66
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.61	0.66
1:0:2269:C:C2'	1:0:2270:G:H5'	2.25	0.66
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.10	0.66
1:0:1524:U:OP1	1:0:1524:U:H4'	1.96	0.66
1:0:1804:A:H2'	1:0:1805:G:C8	2.29	0.66
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.60	0.66
13:L:148:GLU:HA	38:L:8769:HOH:O	1.96	0.66
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.66
1:0:56:G:H5''	23:V:50:ARG:NH1	2.09	0.66
1:0:1058:A:H2'	1:0:1060:C:H5''	1.77	0.66
22:U:20:MET:HE2	22:U:30:HIS:NE2	2.10	0.66
10:H:169:GLY:HA3	38:H:8589:HOH:O	1.95	0.66
1:0:1187:U:O2'	1:0:1189:A:H2	1.79	0.66
2:9:3064:C:C2'	2:9:3065:A:H5'	2.26	0.66
6:D:99:ASP:HB3	6:D:103:ASN:H	1.61	0.65
6:D:103:ASN:HD22	6:D:134:LEU:H	1.44	0.65
1:0:1205:U:C2'	1:0:1206:U:C5'	2.74	0.65
15:N:113:SER:HB2	38:N:8754:HOH:O	1.95	0.65
1:0:447:A:O2'	1:0:448:G:H5'	1.97	0.65
1:0:2587:OMU:O3'	1:0:2587:OMU:HM22	1.96	0.65
4:B:297:VAL:HB	38:B:8804:HOH:O	1.95	0.65
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.78	0.65
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:282:C:H1'	1:0:368:C:H41	1.60	0.65
1:0:1187:U:H2'	38:0:6878:HOH:O	1.97	0.65
1:0:1234:U:N3	4:B:244:PRO:HB3	2.11	0.65
1:0:1730:G:H5'	1:0:1731:C:C5	2.32	0.65
1:0:2004:U:H4'	38:0:5302:HOH:O	1.96	0.65
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.77	0.65
5:C:16:VAL:HG12	5:C:17:ASP:H	1.61	0.65
1:0:2269:C:H2'	1:0:2270:G:H5'	1.77	0.65
4:B:51:VAL:CG1	4:B:53:LEU:HD13	2.26	0.65
15:N:132:ASN:O	15:N:135:VAL:HG12	1.96	0.65
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.78	0.65
1:0:560:C:H42	1:0:597:A:H61	1.43	0.65
3:A:8:ARG:HG2	38:A:8751:HOH:O	1.97	0.65
6:D:65:GLU:HA	38:D:6752:HOH:O	1.97	0.65
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.11	0.65
29:2:39:ARG:HG2	38:2:3143:HOH:O	1.95	0.65
29:2:41:HIS:HD2	29:2:44:ARG:H	1.45	0.65
1:0:644:G:H5'	1:0:644:G:N3	2.11	0.65
1:0:1926:G:H2'	1:0:1927:A:H8	1.61	0.65
1:0:2649:A:H5'	1:0:2649:A:H8	1.62	0.65
27:Z:41:ASN:ND2	27:Z:60:CYS:SG	2.69	0.65
27:Z:27:ALA:HA	38:Z:8615:HOH:O	1.98	0.64
1:0:2248:C:H2'	1:0:2249:G:H8	1.62	0.64
20:S:33:SER:O	20:S:37:VAL:HG23	1.96	0.64
1:0:1528:A:H2'	1:0:1529:G:O4'	1.98	0.64
1:0:2509:A:OP2	1:0:2510:C:H5	1.80	0.64
1:0:450:C:OP1	5:C:184:ARG:NH2	2.30	0.64
1:0:1377:C:H5'	1:0:1377:C:H6	1.63	0.64
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.79	0.64
22:U:47:ARG:HG3	38:U:4381:HOH:O	1.96	0.64
23:V:1:THR:HG23	23:V:2:VAL:H	1.62	0.64
1:0:200:U:H2'	38:0:3441:HOH:O	1.98	0.64
1:0:545:G:H5'	1:0:545:G:C8	2.25	0.64
1:0:960:G:N3	1:0:960:G:H2'	2.12	0.64
1:0:1603:A:C5'	1:0:1605:G:H5'	2.27	0.64
1:0:1625:U:H4'	38:0:4662:HOH:O	1.97	0.64
10:H:166:SER:CB	10:H:167:PRO:HD3	2.27	0.64
13:L:136:ALA:HB3	38:L:8770:HOH:O	1.98	0.64
24:W:88:THR:HB	38:W:6679:HOH:O	1.98	0.64
5:C:132:ASP:HB3	38:C:8561:HOH:O	1.98	0.64
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:151:GLU:O	24:W:154:ARG:HB3	1.98	0.64
1:0:1120:U:H5'	1:0:1120:U:C6	2.31	0.64
1:0:1557:G:O2'	1:0:1558:C:H5'	1.97	0.64
1:0:1636:G:O2'	1:0:1637:A:H5'	1.97	0.64
1:0:2897:C:O2'	1:0:2898:G:H5'	1.98	0.64
1:0:281:U:O2'	1:0:282:C:H5'	1.98	0.63
1:0:856:G:C8	38:0:5424:HOH:O	2.50	0.63
1:0:1462:C:H2'	1:0:1463:A:C8	2.33	0.63
5:C:236:THR:H	5:C:239:ALA:HB3	1.61	0.63
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.27	0.63
1:0:1118:A:H2'	1:0:1120:U:H5''	1.80	0.63
1:0:2717:C:H2'	1:0:2718:C:C5'	2.25	0.63
2:9:3035:C:H5''	38:9:4078:HOH:O	1.98	0.63
2:9:3114:G:O6	15:N:11:ARG:HD3	1.98	0.63
11:J:19:MET:HE2	11:J:79:PHE:HA	1.79	0.63
22:U:52:THR:HG22	22:U:55:ALA:H	1.63	0.63
1:0:2244:A:H1'	38:M:8765:HOH:O	1.97	0.63
1:0:2521:A:OP2	10:H:3:ALA:HB3	1.98	0.63
2:9:3003:A:N6	2:9:3022:G:H1'	2.13	0.63
14:M:164:THR:CG2	14:M:167:GLY:H	2.12	0.63
1:0:814:G:H4'	38:0:3125:HOH:O	1.97	0.63
1:0:2850:C:H5'	1:0:2850:C:C6	2.25	0.63
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.79	0.63
1:0:669:G:O2'	1:0:670:G:H5'	1.99	0.63
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63
2:9:3007:G:H5'	38:9:5071:HOH:O	1.98	0.63
1:0:475:G:OP1	5:C:73:LEU:HD22	1.98	0.63
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.64	0.63
2:9:3069:U:OP1	15:N:4:PRO:HG3	1.99	0.63
27:Z:46:ARG:CD	27:Z:59:TYR:HB2	2.29	0.63
1:0:777:U:O2'	28:1:11:LYS:HG2	1.99	0.63
11:J:41:ALA:HB3	38:J:8768:HOH:O	1.99	0.63
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.64	0.63
1:0:39:G:N2	1:0:444:C:C2	2.67	0.63
1:0:308:U:C4	1:0:342:C:H1'	2.34	0.63
1:0:1185:U:H5'	38:0:7436:HOH:O	1.99	0.63
1:0:1474:C:H6	1:0:1474:C:C5'	2.07	0.63
1:0:1593:C:H5'	17:P:116:SER:O	1.98	0.63
5:C:1:MET:HG2	5:C:2:GLN:H	1.63	0.62
1:0:1342:C:O2'	1:0:1343:C:H5'	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1166:A:H1'	1:0:1192:A:C2	2.34	0.62
1:0:67:A:H5''	1:0:69:A:C8	2.34	0.62
1:0:657:G:OP1	5:C:27:ARG:NH2	2.30	0.62
1:0:1450:C:C4'	1:0:1451:C:OP2	2.48	0.62
1:0:1804:A:H2'	1:0:1805:G:H8	1.64	0.62
1:0:2629:C:H41	3:A:206:ARG:HH21	1.45	0.62
14:M:66:SER:HB3	14:M:128:TRP:CD1	2.33	0.62
1:0:185:G:H4'	1:0:186:A:H4'	1.79	0.62
1:0:396:U:O2'	1:0:418:C:H4'	1.99	0.62
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.64	0.62
1:0:1741:U:O2'	1:0:2723:G:H4'	1.99	0.62
4:B:168:GLY:H	4:B:174:ARG:HD3	1.63	0.62
4:B:280:VAL:HG13	4:B:334:SER:HA	1.80	0.62
1:0:363:A:O2'	1:0:364:C:H5'	1.99	0.62
1:0:814:G:H8	38:0:7188:HOH:O	1.82	0.62
1:0:1422:U:H2'	1:0:1423:C:H6	1.65	0.62
1:0:1603:A:H5'	1:0:1605:G:C4'	2.30	0.62
31:I:118:SER:HB2	31:I:123:ASN:HB2	1.82	0.62
1:0:399:C:H5'	14:M:179:GLY:O	1.99	0.62
1:0:1422:U:H2'	1:0:1423:C:C6	2.35	0.62
8:F:96:ALA:HA	38:F:3111:HOH:O	2.00	0.62
9:G:16:LYS:O	9:G:20:VAL:HG23	2.00	0.62
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.30	0.62
24:W:64:THR:O	24:W:68:THR:HG22	2.00	0.62
1:0:542:A:H5'	1:0:542:A:C8	2.27	0.62
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.82	0.62
10:H:9:ILE:HG23	10:H:126:ARG:CZ	2.29	0.62
14:M:59:GLY:CA	14:M:141:ILE:HD11	2.30	0.62
25:X:25:ARG:HD3	25:X:64:ALA:O	2.00	0.62
1:0:338:C:H5''	38:0:3795:HOH:O	2.00	0.61
1:0:349:U:O2'	1:0:350:C:H5'	2.00	0.61
1:0:2681:A:H4'	1:0:2682:C:H5'	1.80	0.61
2:9:3047:A:C2	2:9:3048:C:C2	2.88	0.61
1:0:303:C:O2'	1:0:304:G:H5'	2.01	0.61
1:0:1507:C:H4'	38:0:3600:HOH:O	2.00	0.61
1:0:1926:G:H2'	1:0:1927:A:C8	2.34	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.14	0.61
2:9:3061:C:H2'	2:9:3062:A:H8	1.64	0.61
3:A:211:LYS:HB2	38:A:8812:HOH:O	2.00	0.61
1:0:1787:C:H4'	1:0:2883:A:O4'	2.00	0.61
10:H:166:SER:HB2	10:H:167:PRO:CD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1159:G:H1	1:0:1208:C:H42	1.48	0.61
2:9:3107:C:H5	38:9:3167:HOH:O	1.84	0.61
4:B:36:PRO:HA	4:B:168:GLY:HA2	1.83	0.61
13:L:134:GLU:HG3	38:L:8754:HOH:O	2.00	0.61
1:0:264:G:H1'	1:0:265:U:H5	1.65	0.61
1:0:2563:U:H2'	1:0:2565:C:O5'	2.01	0.61
2:9:3042:C:H5'	2:9:3043:G:OP2	2.00	0.61
1:0:656:G:OP2	16:O:37:ARG:HD2	2.00	0.61
1:0:1641:A:H2'	1:0:1642:A:H5'	1.83	0.61
38:0:6854:HOH:O	14:M:178:LYS:HB2	2.00	0.61
1:0:1160:G:O2'	1:0:1190:G:H1'	2.01	0.61
1:0:1525:G:H5'	1:0:1526:A:OP2	2.01	0.61
1:0:2729:C:H2'	1:0:2730:G:H8	1.65	0.61
1:0:2880:A:H2'	1:0:2881:C:H5'	1.83	0.61
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.96	0.61
1:0:1342:C:H2'	1:0:1343:C:H5'	1.83	0.61
1:0:2812:A:C2	1:0:2814:A:N6	2.66	0.61
2:9:3049:G:C2'	2:9:3050:G:H5'	2.31	0.61
1:0:371:U:H2'	1:0:372:A:H8	1.66	0.60
1:0:2316:G:H4'	38:0:6084:HOH:O	2.01	0.60
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.83	0.60
1:0:553:G:P	26:Y:204:ARG:HH22	2.25	0.60
1:0:1278:A:H4'	1:0:1279:U:C4	2.36	0.60
1:0:1768:C:C2'	1:0:1769:C:H5'	2.31	0.60
4:B:168:GLY:N	4:B:174:ARG:HD3	2.17	0.60
27:Z:39:CYS:CB	27:Z:57:CYS:SG	2.88	0.60
1:0:2252:A:H2'	1:0:2253:G:H5'	1.84	0.60
1:0:2769:C:H2'	1:0:2770:G:C5'	2.30	0.60
4:B:264:GLU:HG3	4:B:302:PRO:HD3	1.83	0.60
19:R:14:ALA:HB3	19:R:147:LEU:HB2	1.82	0.60
25:X:25:ARG:HD2	38:X:5356:HOH:O	2.00	0.60
1:0:21:G:H4'	19:R:2:ILE:HG22	1.83	0.60
1:0:65:C:O2'	1:0:66:G:H5'	2.01	0.60
1:0:1167:G:H2'	1:0:1168:C:O4'	2.02	0.60
1:0:2526:C:O2'	1:0:2527:U:H5'	2.01	0.60
4:B:137:LEU:HG	38:B:8776:HOH:O	2.01	0.60
1:0:125:U:H3'	38:0:3762:HOH:O	2.00	0.60
1:0:407:A:H5'	38:0:6019:HOH:O	2.00	0.60
1:0:2365:G:H4'	18:Q:45:PRO:O	2.01	0.60
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.60
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:42:GLU:HB2	38:O:2176:HOH:O	2.00	0.60
23:V:44:GLY:O	23:V:48:GLU:HG2	2.01	0.60
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.83	0.60
1:O:638:C:H2'	1:O:639:A:C8	2.37	0.60
1:O:1132:A:N6	1:O:1229:C:H2'	2.17	0.60
4:B:248:ARG:O	4:B:251:VAL:HG13	2.02	0.60
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.84	0.60
1:O:1391:G:H2'	1:O:1392:A:H5'	1.84	0.60
1:O:1945:G:O2'	1:O:1946:C:H5'	2.01	0.60
1:O:354:A:H2'	1:O:355:C:H6	1.66	0.60
38:O:5662:HOH:O	27:Z:17:ARG:HD3	2.02	0.60
23:V:64:GLY:O	23:V:65:ASP:HB2	2.02	0.60
26:Y:189:ASN:C	26:Y:189:ASN:HD22	2.09	0.60
1:O:1299:G:O6	13:L:6:ARG:HD3	2.02	0.59
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.36	0.59
23:V:39:ALA:N	23:V:40:PRO:HD2	2.17	0.59
30:3:70:ARG:HD3	38:3:8767:HOH:O	2.02	0.59
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.36	0.59
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.02	0.59
19:R:9:ASP:O	19:R:13:THR:HB	2.01	0.59
1:O:111:C:O2'	28:1:20:ARG:HG2	2.03	0.59
1:O:283:U:C5	1:O:284:C:N3	2.71	0.59
1:O:1741:U:H5'	1:O:1742:A:OP1	2.03	0.59
1:O:2380:A:N1	30:3:1:MET:HE1	2.16	0.59
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.59
5:C:22:PHE:HA	5:C:116:ALA:HA	1.83	0.59
1:O:136:C:H2'	1:O:137:U:O4'	2.03	0.59
1:O:212:A:O4'	1:O:214:U:C6	2.56	0.59
1:O:962:C:H1'	15:N:5:ARG:NH1	2.18	0.59
1:O:1634:G:H3'	38:O:3886:HOH:O	2.01	0.59
1:O:2694:A:H4'	7:E:91:PHE:HE1	1.67	0.59
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.37	0.59
1:O:1937:U:O2'	1:O:1938:G:H5'	2.03	0.59
2:9:3028:U:H2'	2:9:3029:C:C6	2.38	0.59
18:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.59
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.33	0.59
10:H:58:ARG:HH11	10:H:58:ARG:HG3	1.68	0.59
1:O:283:U:H5	1:O:284:C:H42	1.49	0.59
1:O:2416:G:H2'	1:O:2417:C:C6	2.37	0.59
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.85	0.59
25:X:43:VAL:HG12	25:X:44:ASP:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.42	0.59
29:2:18:ASN:ND2	29:2:40:ARG:H	2.00	0.59
1:0:812:A:H2'	1:0:813:C:C6	2.38	0.59
1:0:1181:A:H5'	31:I:94:GLU:OE2	2.03	0.59
15:N:164:ASP:OD1	15:N:167:ASP:HA	2.03	0.59
1:0:426:G:H2'	1:0:427:C:O4'	2.02	0.59
1:0:2781:U:C2'	1:0:2782:G:H5'	2.33	0.59
6:D:50:VAL:O	6:D:71:ALA:HA	2.03	0.59
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.03	0.59
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.33	0.59
24:W:72:PRO:HG2	24:W:77:ALA:HB3	1.84	0.59
1:0:236:A:C4'	1:0:237:G:H5'	2.26	0.59
1:0:559:U:C5	1:0:560:C:C5	2.91	0.59
1:0:1211:G:O2'	1:0:1212:C:H5'	2.03	0.59
1:0:1625:U:H3'	1:0:1625:U:C6	2.38	0.59
1:0:1790:C:H2'	1:0:1791:U:H6	1.68	0.59
1:0:2000:G:O2'	1:0:2001:G:H5'	2.03	0.59
1:0:2010:A:H2'	38:0:5952:HOH:O	2.01	0.59
1:0:2610:U:H4'	38:B:8726:HOH:O	2.03	0.59
6:D:25:MET:HE3	6:D:41:LEU:HG	1.85	0.59
1:0:944:G:H21	24:W:44:MET:CE	2.15	0.58
1:0:1625:U:H3'	1:0:1625:U:H6	1.68	0.58
1:0:1834:C:H2'	1:0:1840:A:N6	2.18	0.58
9:G:64:ASN:HD22	9:G:64:ASN:N	1.99	0.58
14:M:24:GLN:NE2	14:M:27:ARG:HH11	2.00	0.58
1:0:902:G:N7	13:L:18:HIS:HD2	2.00	0.58
1:0:1773:G:C8	27:Z:16:ALA:HA	2.38	0.58
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.58
1:0:2135:A:O2'	1:0:2136:G:H5'	2.03	0.58
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.85	0.58
1:0:1008:C:H5''	10:H:16:ARG:HH12	1.67	0.58
1:0:2346:C:O2'	6:D:52:THR:HG21	2.03	0.58
11:J:127:ILE:CG2	36:J:8701:CL:CL	2.85	0.58
1:0:1400:C:C2'	1:0:1401:G:H5'	2.33	0.58
2:9:3001:U:O3'	2:9:3003:A:H5'	2.03	0.58
14:M:59:GLY:HA3	14:M:141:ILE:CD1	2.34	0.58
1:0:449:A:N7	5:C:43:LYS:HG2	2.18	0.58
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.86	0.58
1:0:1174:A:C5	1:0:1201:C:H4'	2.38	0.58
1:0:1477:C:H5'	1:0:1868:G:C5'	2.34	0.58
1:0:1613:C:H2'	1:0:1614:G:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:100:ASP:HB2	38:E:2789:HOH:O	2.04	0.58
1:0:524:A:H5''	19:R:29:LYS:HD3	1.86	0.58
1:0:635:A:H2'	1:0:636:G:H5''	1.86	0.58
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.68	0.58
1:0:1595:G:O2'	1:0:1596:U:H5'	2.04	0.58
21:T:86:GLU:HG3	38:T:6653:HOH:O	2.02	0.58
31:I:113:HIS:NE2	31:I:121:LEU:HD22	2.18	0.58
1:0:821:U:H2'	1:0:822:C:H6	1.68	0.58
1:0:1120:U:H6	1:0:1120:U:C5'	2.16	0.58
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.03	0.58
1:0:1730:G:C5'	1:0:1731:C:C6	2.87	0.58
1:0:1829:A:N6	27:Z:18:TYR:HA	2.19	0.58
1:0:2300:A:H4'	1:0:2301:A:O5'	2.04	0.58
19:R:111:ILE:HG23	19:R:145:LEU:HD11	1.86	0.58
25:X:78:GLU:HG2	25:X:79:GLU:H	1.68	0.58
1:0:1849:G:H1'	1:0:2011:A:N1	2.19	0.58
3:A:48:ASP:HB3	38:A:8801:HOH:O	2.03	0.58
1:0:120:A:H2'	1:0:120:A:N3	2.19	0.57
8:F:101:ALA:HA	38:F:5413:HOH:O	2.04	0.57
10:H:66:ARG:HD3	38:H:8579:HOH:O	2.04	0.57
14:M:64:ARG:HD2	38:M:8778:HOH:O	2.04	0.57
21:T:71:VAL:CG1	21:T:90:PRO:HB3	2.29	0.57
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.85	0.57
1:0:820:G:C6	3:A:171:LYS:HB2	2.39	0.57
1:0:2649:A:H5'	1:0:2649:A:C8	2.39	0.57
1:0:2781:U:H2'	1:0:2782:G:H5'	1.85	0.57
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.57
5:C:2:GLN:HB3	38:C:8536:HOH:O	2.03	0.57
8:F:38:LYS:NZ	14:M:3:SER:HA	2.17	0.57
12:K:23:ASN:HD21	12:K:107:THR:HB	1.68	0.57
19:R:132:ARG:HG2	19:R:133:ALA:N	2.19	0.57
1:0:848:C:H5'	38:0:7251:HOH:O	2.03	0.57
11:J:107:ASN:C	11:J:107:ASN:HD22	2.12	0.57
11:J:131:THR:HG22	11:J:134:GLU:H	1.69	0.57
1:0:297:U:H2'	1:0:298:C:H6	1.69	0.57
1:0:2472:C:O2'	1:0:2634:G:H4'	2.04	0.57
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.20	0.57
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.87	0.57
2:9:3057:A:H8	6:D:141:VAL:HG21	1.70	0.57
6:D:57:THR:HG23	6:D:63:ILE:HA	1.86	0.57
10:H:63:GLU:HA	38:H:8579:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.70	0.57
2:9:3001:U:H5''	2:9:3003:A:OP1	2.05	0.57
4:B:162:MET:CE	4:B:308:LEU:HD21	2.35	0.57
11:J:5:GLU:HA	38:J:8729:HOH:O	2.04	0.57
1:0:475:G:H5'	5:C:73:LEU:HD23	1.86	0.57
1:0:1768:C:H2'	1:0:1769:C:H5'	1.87	0.57
1:0:2667:G:H1'	1:0:2914:A:N3	2.20	0.57
21:T:47:THR:HB	21:T:100:ASP:HB3	1.86	0.57
26:Y:99:ALA:HB2	26:Y:233:TYR:CE2	2.40	0.57
1:0:1666:C:C2'	1:0:1667:A:C5'	2.83	0.57
1:0:1681:G:H5''	1:0:1682:A:H5'	1.86	0.57
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.57
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.86	0.57
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.86	0.57
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.57
1:0:1586:G:O2'	1:0:1587:U:H5'	2.04	0.57
1:0:1916:C:O2'	1:0:1917:G:H5'	2.04	0.57
1:0:128:A:C8	1:0:128:A:H3'	2.40	0.57
4:B:258:GLY:H	4:B:260:HIS:CE1	2.23	0.57
1:0:354:A:H2'	1:0:355:C:C6	2.40	0.56
1:0:775:G:OP1	28:1:16:HIS:HE1	1.88	0.56
1:0:820:G:H5'	1:0:821:U:H5'	1.87	0.56
1:0:1080:C:O5'	1:0:1080:C:H6	1.88	0.56
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.69	0.56
1:0:2909:G:O2'	1:0:2910:A:H5'	2.05	0.56
6:D:16:PRO:HG3	6:D:157:LEU:HD11	1.86	0.56
26:Y:187:VAL:HB	38:Y:8769:HOH:O	2.04	0.56
1:0:1116:U:O2'	1:0:1118:A:C2	2.48	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
2:9:3045:A:H2'	2:9:3046:C:H6	1.70	0.56
17:P:7:LYS:HD3	17:P:21:VAL:CG2	2.35	0.56
1:0:1135:G:H5'	38:0:5924:HOH:O	2.04	0.56
1:0:2768:A:O2'	1:0:2769:C:H5'	2.05	0.56
1:0:2851:G:H2'	1:0:2852:A:H5'	1.86	0.56
38:0:7009:HOH:O	3:A:211:LYS:HG3	2.05	0.56
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.86	0.56
4:B:168:GLY:HA3	4:B:174:ARG:HB3	1.87	0.56
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.86	0.56
6:D:25:MET:CE	6:D:41:LEU:HG	2.35	0.56
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.13	0.56
14:M:164:THR:HG22	14:M:167:GLY:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:49:THR:HB	15:N:58:LEU:HD11	1.85	0.56
21:T:48:VAL:HG11	21:T:96:VAL:CG1	2.35	0.56
1:0:474:C:O2'	5:C:73:LEU:HD21	2.06	0.56
1:0:1181:A:H2'	1:0:1182:C:H5'	1.88	0.56
1:0:1909:A:H2'	1:0:1910:A:C8	2.39	0.56
1:0:1925:G:O2'	1:0:1926:G:H5'	2.06	0.56
1:0:2435:U:H1'	38:0:5427:HOH:O	2.06	0.56
13:L:133:VAL:HA	38:L:8770:HOH:O	2.06	0.56
1:0:832:U:H2'	1:0:833:G:C8	2.41	0.56
1:0:1496:G:H5'	1:0:1572:A:H1'	1.88	0.56
1:0:1768:C:H2'	1:0:1769:C:O4'	2.06	0.56
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.87	0.56
7:E:132:THR:HB	38:E:2227:HOH:O	2.06	0.56
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.21	0.56
18:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.06	0.56
31:I:87:THR:HG22	31:I:88:GLY:H	1.70	0.56
1:0:92:G:H4'	23:V:44:GLY:HA3	1.87	0.56
1:0:1992:U:OP2	12:K:66:ARG:HD2	2.06	0.56
1:0:2324:G:H4'	1:0:2418:G:O2'	2.04	0.56
2:9:3048:C:H4'	15:N:141:ARG:NH2	2.20	0.56
1:0:583:G:H2'	1:0:584:U:C6	2.40	0.56
1:0:2083:A:H3'	38:0:7551:HOH:O	2.05	0.56
1:0:2089:A:O2'	1:0:2090:G:H5'	2.06	0.56
1:0:2717:C:O2'	1:0:2718:C:H5''	2.04	0.56
4:B:88:GLU:HB3	4:B:97:LEU:HG	1.87	0.56
8:F:91:VAL:HG12	8:F:92:GLY:N	2.19	0.56
9:G:20:VAL:O	9:G:24:VAL:HG23	2.06	0.56
20:S:57:THR:HG22	20:S:59:ASP:H	1.70	0.56
21:T:48:VAL:HG22	21:T:98:VAL:HA	1.87	0.56
1:0:538:C:OP2	26:Y:134:HIS:HE1	1.88	0.56
1:0:1701:A:H4'	1:0:1702:U:C5'	2.34	0.56
2:9:3045:A:C5	2:9:3046:C:C5	2.94	0.56
11:J:75:PRO:HB3	11:J:132:LEU:HB3	1.87	0.56
22:U:17:THR:HG22	22:U:18:GLY:N	2.21	0.56
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.88	0.56
1:0:793:A:H5''	17:P:83:LYS:HG2	1.88	0.56
1:0:1730:G:C5'	1:0:1731:C:H6	2.19	0.56
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.56
1:0:1206:U:C5'	1:0:1206:U:H6	2.14	0.56
1:0:1506:U:H6	1:0:1506:U:H5'	1.70	0.56
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:80:GLY:O	14:M:81:ARG:HD3	2.05	0.56
1:0:816:G:H5'	1:0:1598:A:H4'	1.88	0.55
1:0:2064:U:H4'	1:0:2653:A:OP1	2.06	0.55
1:0:2276:U:H2'	1:0:2277:U:C6	2.41	0.55
5:C:233:THR:HG22	5:C:234:VAL:N	2.21	0.55
1:0:1213:C:C2'	1:0:1214:G:H5'	2.37	0.55
3:A:55:VAL:HG12	3:A:67:LEU:HD22	1.88	0.55
12:K:14:LYS:CB	12:K:45:PRO:HG2	2.36	0.55
14:M:60:VAL:C	14:M:61:ILE:HD12	2.32	0.55
1:0:1086:A:C6	24:W:11:VAL:HG11	2.41	0.55
1:0:1555:G:H4'	1:0:1630:A:H2	1.71	0.55
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.55
1:0:2769:C:H2'	1:0:2770:G:H5'	1.88	0.55
5:C:39:GLN:O	5:C:43:LYS:HD3	2.07	0.55
19:R:39:THR:HG23	19:R:107:GLU:O	2.07	0.55
26:Y:144:ARG:CZ	38:Y:8815:HOH:O	2.54	0.55
1:0:2269:C:H2'	1:0:2270:G:C5'	2.36	0.55
1:0:2421:G:H3'	1:0:2422:U:H5''	1.88	0.55
1:0:2748:G:H5'	38:0:7511:HOH:O	2.07	0.55
1:0:2900:G:H2'	1:0:2901:C:O4'	2.07	0.55
2:9:3095:C:O2'	2:9:3096:C:H5'	2.06	0.55
3:A:65:ARG:O	3:A:66:ARG:HG3	2.07	0.55
1:0:263:U:C2	8:F:59:ILE:CD1	2.89	0.55
1:0:2545:U:OP2	4:B:2:GLN:HG3	2.07	0.55
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.88	0.55
22:U:6:CYS:HB2	22:U:32:CYS:HB3	1.87	0.55
29:2:41:HIS:CD2	29:2:43:ARG:H	2.24	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.72	0.55
24:W:125:HIS:HE1	38:W:3071:HOH:O	1.89	0.55
1:0:343:C:O2'	1:0:344:C:H5'	2.06	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:1730:G:H5''	1:0:1731:C:H6	1.71	0.55
38:0:4358:HOH:O	4:B:225:GLY:HA3	2.05	0.55
4:B:51:VAL:HG22	4:B:330:VAL:HG22	1.89	0.55
1:0:731:U:H2'	1:0:732:C:C6	2.42	0.55
1:0:1829:A:H61	27:Z:18:TYR:HD2	1.54	0.55
27:Z:42:CYS:SG	27:Z:42:CYS:O	2.65	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.55
2:9:3044:A:O4'	6:D:76:ARG:NE	2.39	0.55
5:C:79:ARG:O	5:C:87:ARG:HG2	2.07	0.55
1:0:1209:C:C2	1:0:1210:G:C8	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1329:A:N1	36:0:8713:CL:CL	2.77	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.06	0.55
8:F:61:MET:HB3	14:M:19:GLN:OE1	2.07	0.55
1:0:1479:A:H5''	38:0:3736:HOH:O	2.06	0.54
12:K:55:VAL:HG12	12:K:56:SER:N	2.22	0.54
38:0:4058:HOH:O	4:B:27:ASN:HB2	2.07	0.54
38:0:4617:HOH:O	3:A:6:GLY:HA3	2.06	0.54
1:0:262:A:OP2	8:F:91:VAL:HG11	2.08	0.54
1:0:2897:C:H2'	1:0:2898:G:H8	1.70	0.54
2:9:3076:G:C3'	2:9:3077:A:H5''	2.30	0.54
6:D:146:LYS:NZ	15:N:107:ASN:HD21	2.06	0.54
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.89	0.54
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.54
1:0:960:G:N3	1:0:960:G:C2'	2.70	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.07	0.54
1:0:2488:A:H2	38:0:7254:HOH:O	1.89	0.54
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.07	0.54
8:F:14:ASP:O	8:F:18:GLU:HG3	2.07	0.54
10:H:171:ALA:HA	38:H:8568:HOH:O	2.07	0.54
13:L:138:GLY:HA3	38:L:8751:HOH:O	2.07	0.54
20:S:57:THR:HG22	20:S:59:ASP:N	2.23	0.54
30:3:73:GLU:HB3	38:3:8757:HOH:O	2.07	0.54
1:0:1315:G:H1'	26:Y:211:ALA:HB3	1.89	0.54
1:0:1733:A:H4'	4:B:212:GLN:HA	1.89	0.54
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.40	0.54
24:W:4:LEU:O	24:W:32:CYS:HA	2.07	0.54
27:Z:56:GLN:HA	27:Z:62:TYR:O	2.07	0.54
1:0:1400:C:H1'	38:0:4132:HOH:O	2.08	0.54
1:0:1878:G:O2'	1:0:1879:U:H6	1.90	0.54
1:0:2878:U:H2'	1:0:2879:A:O4'	2.07	0.54
20:S:57:THR:C	20:S:59:ASP:H	2.16	0.54
1:0:1174:A:C6	1:0:1201:C:H4'	2.42	0.54
1:0:1343:C:H2'	1:0:1344:G:O5'	2.07	0.54
2:9:3057:A:C8	6:D:141:VAL:HG21	2.43	0.54
11:J:42:GLU:O	11:J:131:THR:HG23	2.08	0.54
21:T:38:ARG:HG3	21:T:38:ARG:HH11	1.73	0.54
24:W:68:THR:HG23	24:W:69:ARG:HG2	1.90	0.54
1:0:960:G:H4'	38:0:7405:HOH:O	2.07	0.54
5:C:236:THR:HA	38:C:8645:HOH:O	2.07	0.54
14:M:65:VAL:HG21	14:M:105:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:816:G:C6	1:0:817:G:N1	2.76	0.54
1:0:1236:A:H2'	1:0:1237:U:O4'	2.08	0.54
1:0:2001:G:C2'	1:0:2002:C:H5'	2.38	0.54
1:0:2467:A:O2'	1:0:2468:A:H2'	2.08	0.54
1:0:2468:A:H61	30:3:48:ASN:HD21	1.55	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.90	0.54
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.53
1:0:157:G:H4'	14:M:95:LYS:HE2	1.90	0.53
1:0:559:U:H2'	1:0:560:C:O4'	2.08	0.53
1:0:709:G:O2'	16:O:25:VAL:HG12	2.08	0.53
1:0:1873:G:H3'	38:0:5204:HOH:O	2.09	0.53
1:0:2251:G:H2'	1:0:2252:A:H8	1.68	0.53
1:0:2419:U:H5''	1:0:2420:G:H5'	1.89	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.40	0.53
4:B:36:PRO:HA	4:B:168:GLY:CA	2.37	0.53
4:B:54:VAL:HB	38:B:8812:HOH:O	2.08	0.53
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.37	0.53
24:W:125:HIS:HD2	24:W:127:GLY:H	1.56	0.53
27:Z:41:ASN:CB	27:Z:60:CYS:SG	2.88	0.53
1:0:1016:U:H1'	38:0:3654:HOH:O	2.08	0.53
1:0:1119:G:H8	11:J:52:GLN:HE22	1.56	0.53
1:0:1168:C:H1'	38:0:7388:HOH:O	2.09	0.53
1:0:1521:C:H2'	1:0:1522:A:H8	1.73	0.53
1:0:1921:A:C6	1:0:1922:A:C2	2.95	0.53
1:0:2768:A:H3'	38:0:4423:HOH:O	2.07	0.53
4:B:27:ASN:HD22	4:B:27:ASN:H	1.57	0.53
28:1:25:LYS:HG3	29:2:49:GLU:H	1.72	0.53
1:0:2507:G:H2'	1:0:2510:C:H42	1.73	0.53
2:9:3031:C:H2'	2:9:3032:G:O4'	2.07	0.53
3:A:199:HIS:HD2	3:A:201:PHE:H	1.55	0.53
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.91	0.53
24:W:65:VAL:HG12	24:W:116:LEU:HD13	1.90	0.53
24:W:139:GLY:O	24:W:141:HIS:HD2	1.91	0.53
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.09	0.53
1:0:155:C:OP2	14:M:188:ARG:HD3	2.08	0.53
1:0:284:C:OP2	1:0:284:C:C6	2.62	0.53
1:0:544:G:H2'	1:0:545:G:C5'	2.38	0.53
1:0:711:G:C2	1:0:718:C:C2	2.97	0.53
1:0:2502:C:H2'	1:0:2503:A:C5'	2.37	0.53
5:C:153:VAL:O	5:C:157:LEU:HG	2.08	0.53
9:G:19:GLU:O	9:G:23:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:88:LYS:HB3	38:O:7061:HOH:O	2.07	0.53
17:P:9:LEU:O	17:P:13:VAL:HG12	2.08	0.53
21:T:101:LEU:HD13	21:T:112:LEU:HD11	1.90	0.53
1:O:407:A:H2'	1:O:408:A:C8	2.43	0.53
1:O:1471:A:H2'	1:O:1472:C:C6	2.43	0.53
1:O:1782:G:O2'	1:O:1783:A:H5'	2.09	0.53
12:K:32:ILE:HD11	12:K:56:SER:HB2	1.91	0.53
16:O:73:ASP:HA	16:O:92:VAL:O	2.08	0.53
19:R:99:ALA:CB	19:R:109:MET:HE1	2.27	0.53
1:O:47:G:N3	1:O:114:A:C2	2.77	0.53
1:O:371:U:H2'	1:O:372:A:C8	2.42	0.53
1:O:1641:A:C2'	1:O:1642:A:H5'	2.39	0.53
1:O:2248:C:H2'	1:O:2249:G:C8	2.42	0.53
17:P:134:VAL:O	17:P:137:LEU:HB3	2.09	0.53
1:O:281:U:H2'	1:O:282:C:O4'	2.08	0.53
1:O:602:A:O2'	1:O:605:C:H4'	2.09	0.53
1:O:1505:U:H6	1:O:1505:U:H5'	1.73	0.53
1:O:1603:A:C5'	1:O:1605:G:O4'	2.48	0.53
19:R:33:ARG:NH2	38:R:8729:HOH:O	2.41	0.53
27:Z:39:CYS:SG	27:Z:40:PRO:N	2.82	0.53
29:2:20:ARG:HD3	38:2:5444:HOH:O	2.08	0.53
1:O:2613:G:O2'	1:O:2614:C:H5'	2.09	0.53
1:O:2712:G:H5'	38:O:5215:HOH:O	2.09	0.53
1:O:810:G:H2'	1:O:811:C:C6	2.44	0.53
1:O:2271:G:H5'	38:O:4749:HOH:O	2.09	0.53
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.91	0.53
8:F:57:GLU:O	8:F:61:MET:HG3	2.09	0.53
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.41	0.53
21:T:48:VAL:CG1	21:T:96:VAL:HG13	2.39	0.53
1:O:353:G:H2'	1:O:354:A:C8	2.44	0.53
1:O:451:C:O2'	1:O:452:G:H5'	2.09	0.53
1:O:512:G:O3'	1:O:513:A:H8	1.92	0.53
1:O:746:A:C6	16:O:65:LEU:HD13	2.44	0.53
1:O:1588:G:C6	1:O:1589:G:N1	2.77	0.53
1:O:1759:A:N3	1:O:1818:C:H2'	2.24	0.53
2:9:3034:A:H2'	2:9:3035:C:O4'	2.09	0.53
3:A:94:LEU:HD23	3:A:94:LEU:N	2.24	0.53
13:L:143:THR:HG22	13:L:144:ASP:N	2.24	0.53
1:O:661:G:C4	1:O:686:A:C2	2.97	0.52
1:O:1118:A:N6	1:O:1244:U:H3	2.01	0.52
1:O:1279:U:O2	1:O:1279:U:C2'	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2045:G:H2'	1:0:2046:G:O4'	2.09	0.52
4:B:305:ASP:O	4:B:306:LYS:HB2	2.10	0.52
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.91	0.52
1:0:1903:U:O2'	1:0:1904:A:C8	2.61	0.52
1:0:2690:U:O2'	7:E:111:LYS:HE3	2.08	0.52
1:0:2720:C:O2	12:K:87:ARG:NH2	2.41	0.52
4:B:16:ARG:NH1	38:B:8816:HOH:O	2.41	0.52
1:0:567:U:H5''	38:W:5817:HOH:O	2.09	0.52
1:0:1544:U:H2'	1:0:1545:C:H6	1.74	0.52
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.39	0.52
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.91	0.52
14:M:49:ALA:C	14:M:54:TYR:HB3	2.33	0.52
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.91	0.52
1:0:138:U:OP2	1:0:139:C:H5	1.93	0.52
1:0:299:U:C2	1:0:300:C:C6	2.98	0.52
1:0:1166:A:H2'	1:0:1166:A:N3	2.25	0.52
1:0:1592:G:O2'	1:0:1593:C:O4'	2.28	0.52
1:0:1702:U:H5'	38:0:3423:HOH:O	2.08	0.52
1:0:1730:G:H5'	1:0:1731:C:H5	1.75	0.52
1:0:1916:C:N4	1:0:1917:G:C6	2.77	0.52
1:0:2254:G:O2'	1:0:2255:A:H5'	2.08	0.52
1:0:2421:G:H3'	1:0:2422:U:C5'	2.39	0.52
1:0:2758:G:H2'	1:0:2759:C:C6	2.45	0.52
6:D:135:VAL:HG22	6:D:136:ARG:H	1.74	0.52
22:U:39:ASN:HD21	22:U:44:ARG:HH11	1.55	0.52
1:0:31:C:H2'	38:0:7659:HOH:O	2.09	0.52
1:0:42:C:H1'	38:0:4672:HOH:O	2.10	0.52
1:0:714:U:H3'	38:0:6924:HOH:O	2.10	0.52
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.44	0.52
1:0:2265:U:H2'	1:0:2266:A:C8	2.45	0.52
2:9:3002:U:OP2	2:9:3003:A:H5'	2.10	0.52
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.91	0.52
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.91	0.52
4:B:17:LYS:O	4:B:260:HIS:HD2	1.91	0.52
15:N:114:LYS:O	15:N:118:ILE:HG13	2.09	0.52
25:X:76:ARG:HG3	25:X:76:ARG:NH1	2.18	0.52
1:0:232:A:H4'	38:0:6075:HOH:O	2.10	0.52
1:0:318:C:H5	38:0:3720:HOH:O	1.92	0.52
1:0:1087:G:H4'	1:0:1088:A:OP1	2.10	0.52
1:0:1200:A:H2'	38:0:5753:HOH:O	2.09	0.52
1:0:1252:A:H2'	1:0:1253:C:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1400:C:H2'	1:0:1401:G:H5'	1.90	0.52
1:0:1625:U:C6	1:0:1625:U:C3'	2.93	0.52
1:0:2360:C:H1'	38:0:3525:HOH:O	2.09	0.52
7:E:11:VAL:HG12	7:E:12:ASP:N	2.25	0.52
27:Z:42:CYS:C	27:Z:44:GLU:H	2.17	0.52
1:0:558:C:H2'	1:0:559:U:H5''	1.79	0.52
1:0:694:A:H2'	1:0:695:C:H5'	1.91	0.52
1:0:1180:U:H2'	1:0:1181:A:O4'	2.09	0.52
1:0:1562:C:H3'	1:0:1563:G:C8	2.44	0.52
1:0:2667:G:N3	1:0:2827:A:H2	2.07	0.52
2:9:3044:A:H1'	6:D:76:ARG:NH2	2.24	0.52
10:H:120:ILE:N	10:H:120:ILE:HD12	2.25	0.52
24:W:81:ASP:OD1	24:W:92:ASP:HB2	2.09	0.52
1:0:332:G:O2'	1:0:333:G:H5'	2.10	0.52
1:0:958:G:O2'	1:0:959:C:H5'	2.10	0.52
1:0:1644:C:C2	1:0:1645:U:C6	2.98	0.52
21:T:61:GLU:HG2	38:T:3851:HOH:O	2.08	0.52
29:2:18:ASN:HD21	29:2:40:ARG:H	1.58	0.52
1:0:11:A:H5'	1:0:12:U:OP2	2.09	0.52
1:0:282:C:O2'	1:0:283:U:C5'	2.53	0.52
1:0:695:C:O2'	1:0:696:C:H5'	2.10	0.52
1:0:1167:G:O2'	1:0:1168:C:H5'	2.09	0.52
1:0:1568:G:O2'	1:0:1569:U:H5'	2.10	0.52
1:0:2064:U:H5'	1:0:2652:U:H4'	1.92	0.52
1:0:2436:U:H5'	30:3:68:LYS:HE2	1.92	0.52
1:0:2699:A:H2'	1:0:2700:G:O4'	2.10	0.52
4:B:320:GLN:HE21	4:B:321:PRO:CD	2.23	0.52
14:M:123:ASP:OD1	14:M:126:GLN:HG2	2.10	0.52
19:R:33:ARG:NH1	38:R:8741:HOH:O	2.39	0.52
1:0:1497:G:H4'	1:0:1627:G:O2'	2.11	0.52
1:0:1666:C:C2'	1:0:1667:A:H5''	2.39	0.52
1:0:1825:U:O2'	1:0:1826:C:H5'	2.10	0.52
1:0:1890:U:H4'	1:0:2010:A:C6	2.45	0.52
1:0:2702:A:H2	38:E:2401:HOH:O	1.92	0.52
38:0:6265:HOH:O	27:Z:49:ARG:HD3	2.10	0.52
3:A:36:ASP:OD2	3:A:85:SER:HB2	2.10	0.52
7:E:8:PRO:HB2	7:E:11:VAL:HG23	1.92	0.52
24:W:88:THR:HG22	24:W:89:ASP:N	2.22	0.52
1:0:87:C:H2'	29:2:28:LYS:O	2.10	0.51
1:0:166:A:N7	13:L:25:GLY:HA2	2.25	0.51
1:0:1242:A:C5'	11:J:82:THR:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1644:C:H2'	1:0:1645:U:H6	1.74	0.51
1:0:1940:C:H1'	38:0:7323:HOH:O	2.11	0.51
1:0:2281:C:C2'	1:0:2282:U:H5'	2.39	0.51
1:0:2588:OMG:H3'	1:0:2589:U:H5''	1.92	0.51
1:0:2781:U:H2'	1:0:2782:G:C5'	2.39	0.51
6:D:101:THR:O	6:D:157:LEU:HB3	2.10	0.51
8:F:56:PRO:HG2	14:M:44:THR:HA	1.92	0.51
20:S:50:GLU:HB3	20:S:67:ARG:HH21	1.74	0.51
1:0:64:G:H2'	1:0:65:C:O4'	2.11	0.51
1:0:681:G:N3	1:0:681:G:H5'	2.25	0.51
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.43	0.51
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.11	0.51
1:0:2134:G:C6	1:0:2258:A:C8	2.97	0.51
1:0:1477:C:H5'	1:0:1868:G:H5''	1.92	0.51
1:0:1878:G:O2'	1:0:1879:U:P	2.69	0.51
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.51
1:0:2252:A:C2'	1:0:2253:G:H5'	2.40	0.51
1:0:2730:G:O2'	1:0:2731:G:H5'	2.11	0.51
1:0:2781:U:O2'	1:0:2782:G:H5'	2.09	0.51
38:0:7333:HOH:O	3:A:177:HIS:HE1	1.92	0.51
3:A:35:GLY:O	3:A:36:ASP:HB3	2.10	0.51
4:B:177:HIS:O	4:B:181:ILE:HG13	2.11	0.51
6:D:154:LYS:H	6:D:154:LYS:HD2	1.76	0.51
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.91	0.51
13:L:125:PHE:CE1	13:L:140:VAL:HG13	2.45	0.51
18:Q:14:LEU:HB3	38:Q:3971:HOH:O	2.09	0.51
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.44	0.51
1:0:195:C:H2'	1:0:196:G:H5'	1.93	0.51
1:0:1496:G:H1	1:0:1509:C:H42	1.57	0.51
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.76	0.51
23:V:42:ASN:HB3	38:V:7247:HOH:O	2.10	0.51
1:0:920:C:H5'	1:0:921:G:C4	2.46	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.51
1:0:1778:A:H2'	1:0:1779:A:H5'	1.92	0.51
1:0:2249:G:C2	1:0:2253:G:C6	2.98	0.51
1:0:2739:A:C4	1:0:2740:G:C8	2.99	0.51
10:H:36:LYS:HA	10:H:84:LYS:NZ	2.25	0.51
1:0:1165:G:O2'	1:0:1174:A:H1'	2.10	0.51
1:0:1819:G:H5'	38:0:4709:HOH:O	2.10	0.51
2:9:3001:U:H4'	2:9:3003:A:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.92	0.51
11:J:45:VAL:HG11	11:J:121:LEU:HD22	1.91	0.51
1:0:1711:A:O2'	1:0:1712:A:H5'	2.10	0.51
1:0:1916:C:C5	1:0:1917:G:N7	2.79	0.51
1:0:1973:A:H5'	1:0:1973:A:H8	1.76	0.51
1:0:2256:G:C2'	1:0:2257:G:C5'	2.83	0.51
1:0:2312:G:H2'	1:0:2313:C:H5'	1.93	0.51
1:0:2404:G:OP1	18:Q:68:GLY:HA3	2.11	0.51
1:0:2598:U:O2	1:0:2600:A:H8	1.94	0.51
2:9:3039:U:C2'	2:9:3040:C:OP1	2.59	0.51
2:9:3043:G:H5'	38:9:1987:HOH:O	2.09	0.51
3:A:36:ASP:HB2	3:A:83:GLY:CA	2.38	0.51
15:N:115:VAL:HG23	38:N:8754:HOH:O	2.11	0.51
15:N:154:LEU:C	15:N:156:GLU:H	2.18	0.51
23:V:1:THR:HG23	23:V:2:VAL:HG23	1.92	0.51
1:0:553:G:H2'	1:0:554:G:H5'	1.92	0.51
1:0:702:G:HO2'	1:0:703:G:H5'	1.76	0.51
1:0:1060:C:H6	1:0:1060:C:H5'	1.76	0.51
1:0:1515:A:O2'	1:0:1516:C:H5'	2.11	0.51
1:0:1523:G:H2'	1:0:1524:U:C6	2.45	0.51
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.11	0.51
1:0:2768:A:H5''	38:0:4423:HOH:O	2.11	0.51
5:C:16:VAL:HG12	5:C:17:ASP:N	2.24	0.51
5:C:49:ASP:HB3	5:C:52:ALA:HB2	1.92	0.51
12:K:24:THR:HB	12:K:64:MET:HE2	1.92	0.51
21:T:28:SER:O	21:T:32:ARG:HG3	2.10	0.51
1:0:319:A:H4'	1:0:338:C:C5	2.46	0.51
1:0:396:U:OP2	30:3:38:ARG:HD2	2.09	0.51
1:0:567:U:C5'	38:W:5817:HOH:O	2.59	0.51
1:0:1517:U:C2	1:0:1670:G:N2	2.79	0.51
1:0:1803:C:H2'	1:0:1804:A:C8	2.46	0.51
1:0:1936:C:H2'	1:0:1937:U:H6	1.75	0.51
1:0:2002:C:H2'	1:0:2003:U:H5'	1.92	0.51
1:0:2010:A:C2'	38:0:5952:HOH:O	2.58	0.51
1:0:2883:A:H2'	1:0:2884:G:O4'	2.11	0.51
2:9:3039:U:HO2'	2:9:3042:C:H5	1.56	0.51
2:9:3074:G:H1	2:9:3107:C:H42	1.57	0.51
3:A:57:ALA:HA	3:A:67:LEU:HD23	1.93	0.51
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.93	0.51
11:J:74:ARG:NH1	11:J:144:THR:HG21	2.26	0.51
13:L:145:LEU:O	13:L:148:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:56:ILE:O	23:V:60:GLN:HG3	2.11	0.51
1:0:417:G:P	38:0:7393:HOH:O	2.68	0.51
1:0:571:C:O5'	1:0:571:C:H6	1.94	0.51
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.11	0.51
1:0:2629:C:N4	3:A:206:ARG:HH21	2.09	0.51
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.92	0.51
22:U:46:ALA:HA	38:U:3805:HOH:O	2.10	0.51
26:Y:216:ARG:HD2	38:Y:8768:HOH:O	2.10	0.51
31:I:125:ALA:O	31:I:129:VAL:HG23	2.11	0.51
1:0:696:C:O2'	1:0:697:G:H5'	2.11	0.50
1:0:1181:A:H2'	1:0:1182:C:C5'	2.41	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.41	0.50
1:0:2054:A:C2	19:R:128:ARG:NH2	2.79	0.50
1:0:2509:A:H2'	1:0:2510:C:O4'	2.11	0.50
1:0:2769:C:H2'	1:0:2770:G:O4'	2.11	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.11	0.50
6:D:18:ILE:HD13	6:D:84:LEU:HD12	1.93	0.50
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.47	0.50
14:M:115:LEU:HD13	14:M:116:ASN:HB2	1.92	0.50
17:P:20:ARG:NH1	17:P:54:LYS:HD3	2.25	0.50
27:Z:60:CYS:SG	27:Z:62:TYR:HB2	2.51	0.50
1:0:2039:A:H4'	1:0:2760:C:O2'	2.12	0.50
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.10	0.50
7:E:69:ILE:HA	7:E:72:MET:HE3	1.93	0.50
23:V:39:ALA:C	23:V:41:GLU:H	2.19	0.50
24:W:130:HIS:O	24:W:136:GLY:HA3	2.11	0.50
1:0:1119:G:H8	11:J:52:GLN:NE2	2.08	0.50
38:0:9690:HOH:O	4:B:254:GLN:HG3	2.10	0.50
2:9:3002:U:OP2	2:9:3002:U:H4'	2.11	0.50
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.92	0.50
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.93	0.50
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.41	0.50
24:W:4:LEU:CD2	24:W:54:PHE:HB3	2.39	0.50
30:3:62:THR:HB	38:3:8747:HOH:O	2.10	0.50
1:0:500:G:H21	19:R:98:ASN:HD21	1.59	0.50
1:0:821:U:H2'	1:0:822:C:C6	2.47	0.50
1:0:1503:U:H2'	1:0:1504:A:O4'	2.11	0.50
1:0:1765:G:H1'	1:0:1780:G:N2	2.27	0.50
1:0:2681:A:H4'	1:0:2682:C:C5'	2.40	0.50
1:0:2786:G:H2'	38:0:7166:HOH:O	2.11	0.50
2:9:3028:U:H3'	2:9:3029:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:132:VAL:HG11	22:U:22:VAL:HG22	1.93	0.50
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.46	0.50
1:0:290:C:O2'	1:0:291:C:H5'	2.12	0.50
1:0:858:U:H2'	1:0:859:C:H6	1.76	0.50
1:0:1209:C:H2'	1:0:1210:G:H8	1.76	0.50
2:9:3012:C:H5'	2:9:3070:U:O4'	2.11	0.50
4:B:43:GLY:HA3	4:B:76:THR:HG22	1.93	0.50
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.80	0.50
14:M:30:GLU:O	14:M:34:GLU:HG3	2.11	0.50
15:N:72:GLU:HB3	15:N:163:PHE:CE1	2.47	0.50
1:0:661:G:C6	1:0:686:A:C2	2.99	0.50
1:0:2065:C:O2'	1:0:2066:C:H5'	2.12	0.50
1:0:2505:G:C2'	1:0:2506:A:H5'	2.42	0.50
19:R:106:GLY:HA2	19:R:109:MET:HE3	1.92	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.93	0.50
2:9:3036:C:C5	2:9:3037:C:C5	3.00	0.50
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.94	0.50
5:C:5:ILE:HG12	38:C:8627:HOH:O	2.11	0.50
5:C:118:THR:O	5:C:136:VAL:HG13	2.11	0.50
9:G:12:ILE:N	9:G:13:PRO:HD3	2.26	0.50
11:J:107:ASN:HD22	11:J:109:TYR:H	1.59	0.50
23:V:4:HIS:HB3	38:V:6622:HOH:O	2.12	0.50
24:W:139:GLY:O	24:W:141:HIS:CD2	2.65	0.50
25:X:43:VAL:HG12	25:X:44:ASP:N	2.26	0.50
1:0:299:U:H2'	1:0:300:C:H6	1.76	0.50
1:0:346:U:H4'	38:0:6822:HOH:O	2.12	0.50
1:0:581:G:O2'	1:0:582:C:H5'	2.12	0.50
1:0:657:G:H2'	1:0:658:C:C6	2.46	0.50
1:0:877:G:C5'	1:0:878:G:OP1	2.56	0.50
1:0:1882:C:O2'	1:0:2012:U:OP2	2.30	0.50
1:0:2452:G:H1'	38:0:5984:HOH:O	2.12	0.50
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.93	0.50
10:H:167:PRO:O	10:H:168:ALA:HB2	2.12	0.50
1:0:1535:G:H2'	1:0:1536:C:C6	2.47	0.50
1:0:1687:C:O2	28:1:9:GLY:HA2	2.12	0.50
1:0:1811:A:C2	1:0:2752:C:H1'	2.47	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.50
1:0:105:G:O2'	1:0:106:A:H5'	2.12	0.49
1:0:1494:A:C4	1:0:1495:C:C5	3.00	0.49
1:0:2264:A:H2'	1:0:2265:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:9072:HOH:O	4:B:214:PRO:HD2	2.11	0.49
10:H:76:GLU:C	10:H:77:LEU:HD23	2.37	0.49
16:O:39:THR:O	16:O:115:ARG:NH2	2.45	0.49
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.93	0.49
28:1:10:LYS:HG3	38:1:2979:HOH:O	2.11	0.49
1:O:35:U:H5'	5:C:47:GLY:O	2.12	0.49
1:O:1185:U:O2'	1:O:1186:C:H5'	2.12	0.49
1:O:1942:A:O2'	1:O:1943:C:H5'	2.12	0.49
1:O:2896:A:N3	1:O:2896:A:H2'	2.28	0.49
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.93	0.49
7:E:101:GLU:HB3	7:E:117:THR:HA	1.94	0.49
26:Y:212:ARG:HD2	38:Y:8803:HOH:O	2.12	0.49
1:O:255:A:H2'	1:O:256:C:O4'	2.11	0.49
1:O:553:G:O4'	1:O:1325:G:H5'	2.12	0.49
1:O:699:C:C2	1:O:744:G:C2	3.00	0.49
1:O:1181:A:C2'	1:O:1182:C:H5'	2.42	0.49
1:O:1201:C:H5''	38:O:6139:HOH:O	2.12	0.49
1:O:1268:C:O2'	1:O:1269:G:H5'	2.12	0.49
1:O:1396:C:H1'	17:P:1:THR:O	2.12	0.49
1:O:1930:A:H2'	1:O:1931:A:C8	2.47	0.49
1:O:2241:C:O2'	1:O:2242:U:H5'	2.13	0.49
1:O:2533:C:C6	1:O:2533:C:C5'	2.90	0.49
2:9:3003:A:OP2	2:9:3025:G:N2	2.44	0.49
12:K:115:ARG:HG3	12:K:116:GLU:N	2.26	0.49
20:S:56:ASN:O	29:2:8:LYS:HE2	2.12	0.49
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.92	0.49
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.95	0.49
1:O:121:U:OP2	29:2:10:ARG:NH2	2.43	0.49
1:O:583:G:H2'	1:O:584:U:H6	1.75	0.49
1:O:1432:U:H5'	38:O:9190:HOH:O	2.12	0.49
1:O:1903:U:O2'	1:O:1904:A:N7	2.45	0.49
1:O:2766:A:O2'	1:O:2767:C:H5'	2.13	0.49
2:9:3045:A:C4	2:9:3046:C:C6	2.99	0.49
5:C:140:VAL:HB	38:C:8645:HOH:O	2.11	0.49
7:E:80:TRP:O	7:E:134:SER:HA	2.12	0.49
14:M:59:GLY:C	14:M:141:ILE:HD11	2.37	0.49
1:O:39:G:C2	1:O:444:C:N3	2.80	0.49
1:O:113:A:OP2	1:O:114:A:H2'	2.12	0.49
1:O:876:A:H2'	1:O:876:A:N3	2.27	0.49
1:O:1183:C:N4	1:O:1184:C:N4	2.56	0.49
1:O:1626:A:H2'	1:O:1627:G:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1664:A:H8	1:0:1664:A:OP1	1.95	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.43	0.49
3:A:68:ILE:HG13	38:A:8782:HOH:O	2.12	0.49
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.94	0.49
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.35	0.49
27:Z:46:ARG:O	27:Z:57:CYS:HA	2.13	0.49
1:0:88:G:H8	1:0:88:G:H5'	1.77	0.49
1:0:1874:U:OP1	3:A:51:ARG:HD2	2.13	0.49
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.28	0.49
7:E:84:MET:HE2	7:E:133:VAL:HG23	1.95	0.49
25:X:10:VAL:HG11	25:X:36:HIS:HE1	1.76	0.49
31:I:123:ASN:HA	31:I:126:LYS:HD2	1.94	0.49
1:0:832:U:H2'	1:0:833:G:H8	1.76	0.49
1:0:1400:C:O2'	1:0:1401:G:H5'	2.12	0.49
1:0:1771:U:O2	27:Z:19:GLY:HA2	2.12	0.49
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.45	0.49
1:0:2436:U:C5'	30:3:68:LYS:HE2	2.42	0.49
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.94	0.49
1:0:275:G:N2	1:0:376:C:C2	2.81	0.49
1:0:275:G:C2	1:0:376:C:N3	2.80	0.49
4:B:125:GLU:O	4:B:129:ARG:HG3	2.13	0.49
11:J:52:GLN:HG3	11:J:53:ILE:N	2.27	0.49
1:0:431:G:O2'	1:0:432:G:H5'	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
1:0:2826:G:C6	1:0:2913:A:N6	2.81	0.49
3:A:192:VAL:HB	38:A:8790:HOH:O	2.12	0.49
4:B:254:GLN:HG2	4:B:255:GLY:N	2.27	0.49
1:0:222:A:H2'	1:0:223:G:O4'	2.12	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.13	0.49
1:0:475:G:H5'	5:C:73:LEU:CD2	2.42	0.49
1:0:506:G:N2	1:0:509:A:H5'	2.24	0.49
1:0:660:A:H4'	1:0:661:G:O5'	2.13	0.49
1:0:1186:C:N4	1:0:1187:U:C4	2.80	0.49
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.95	0.49
1:0:2314:G:C2'	1:0:2315:C:H5'	2.43	0.49
1:0:119:A:H2'	1:0:120:A:H5''	1.95	0.48
1:0:302:A:O2'	1:0:303:C:H5'	2.12	0.48
1:0:834:G:H4'	1:0:835:U:OP2	2.13	0.48
1:0:2346:C:H6	1:0:2346:C:O5'	1.96	0.48
1:0:462:A:C8	29:2:37:HIS:CE1	3.01	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1380:U:H5'	38:0:9209:HOH:O	2.13	0.48
1:0:1925:G:H5'	30:3:29:ARG:HH12	1.78	0.48
1:0:2071:C:H5'	38:0:9520:HOH:O	2.13	0.48
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.48
38:9:3472:HOH:O	15:N:41:LYS:HD3	2.14	0.48
3:A:109:GLU:HG2	3:A:116:GLY:N	2.28	0.48
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.25	0.48
4:B:14:GLY:HA2	4:B:15:PRO:C	2.37	0.48
17:P:115:SER:OG	17:P:118:GLN:HG3	2.13	0.48
1:0:152:A:H2'	1:0:153:C:C6	2.48	0.48
1:0:922:A:N7	1:0:2281:C:H5'	2.28	0.48
1:0:1188:A:C6	1:0:1189:A:C6	3.01	0.48
1:0:1829:A:H5''	38:0:3074:HOH:O	2.13	0.48
1:0:2824:C:C5'	1:0:2825:C:H5'	2.37	0.48
7:E:149:GLU:HG3	7:E:167:TYR:HA	1.94	0.48
8:F:107:ASP:O	8:F:111:ILE:HG13	2.13	0.48
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.42	0.48
15:N:82:TYR:C	15:N:82:TYR:CD2	2.92	0.48
15:N:154:LEU:O	15:N:155:GLU:HB3	2.13	0.48
21:T:25:ALA:CB	21:T:96:VAL:HG12	2.43	0.48
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.95	0.48
1:0:485:A:N3	1:0:487:G:H5''	2.29	0.48
1:0:491:C:O2'	1:0:492:C:H5'	2.13	0.48
1:0:790:A:H1'	1:0:1710:A:H2'	1.95	0.48
1:0:1184:C:O2'	1:0:1185:U:OP2	2.28	0.48
1:0:1753:C:H4'	38:0:5991:HOH:O	2.13	0.48
1:0:1819:G:H2'	1:0:1820:G:C5'	2.43	0.48
1:0:2493:C:O2	1:0:2493:C:H2'	2.12	0.48
3:A:37:VAL:HG22	38:A:8792:HOH:O	2.14	0.48
4:B:85:ARG:NH1	38:B:8833:HOH:O	2.46	0.48
7:E:154:ILE:HD11	7:E:157:LYS:HB2	1.95	0.48
11:J:38:VAL:HB	11:J:103:VAL:HG22	1.95	0.48
24:W:88:THR:HG23	24:W:110:GLN:NE2	2.29	0.48
1:0:522:U:O2'	1:0:1366:C:H5'	2.14	0.48
1:0:1311:G:C2	1:0:1312:G:C8	3.01	0.48
1:0:1477:C:O2'	1:0:1478:U:H5'	2.14	0.48
1:0:1537:C:O2'	1:0:1538:C:H5'	2.13	0.48
1:0:2791:U:H1'	1:0:2792:A:H5''	1.94	0.48
1:0:2880:A:C2'	1:0:2881:C:H5'	2.43	0.48
2:9:3041:C:H4'	6:D:48:MET:HB2	1.96	0.48
2:9:3058:G:H3'	2:9:3059:C:C6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:75:GLU:C	4:B:77:PRO:HD3	2.38	0.48
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.78	0.48
10:H:77:LEU:HD12	10:H:83:TYR:CD2	2.49	0.48
26:Y:99:ALA:HB2	26:Y:233:TYR:CZ	2.48	0.48
30:3:17:HIS:O	30:3:18:GLN:HG3	2.13	0.48
1:0:95:A:H5''	1:0:97:G:O4'	2.13	0.48
1:0:316:A:H5'	21:T:54:ASP:OD2	2.13	0.48
1:0:677:C:C2'	1:0:678:G:H5'	2.44	0.48
1:0:858:U:H2'	1:0:859:C:C6	2.48	0.48
1:0:1936:C:H2'	1:0:1937:U:C6	2.48	0.48
1:0:2504:A:H4'	10:H:71:ARG:NH1	2.28	0.48
1:0:2729:C:H2'	1:0:2730:G:C8	2.47	0.48
3:A:99:ILE:O	3:A:131:HIS:HE1	1.97	0.48
4:B:315:VAL:HG23	4:B:316:ARG:HG2	1.95	0.48
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.94	0.48
24:W:38:THR:HG22	24:W:39:ASP:N	2.28	0.48
27:Z:42:CYS:SG	27:Z:59:TYR:CD2	2.92	0.48
27:Z:49:ARG:HH21	27:Z:52:THR:HA	1.78	0.48
1:0:69:A:H2'	1:0:70:A:OP2	2.13	0.48
1:0:78:G:C6	1:0:79:G:C6	3.02	0.48
1:0:297:U:H2'	1:0:298:C:C6	2.48	0.48
1:0:710:G:O2'	1:0:711:G:H5'	2.13	0.48
1:0:1545:C:H2'	1:0:1546:G:O4'	2.13	0.48
1:0:1574:C:O5'	1:0:1574:C:H6	1.96	0.48
1:0:1878:G:H5''	38:0:5160:HOH:O	2.12	0.48
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.79	0.48
1:0:2825:C:H4'	1:0:2826:G:O5'	2.13	0.48
4:B:148:PRO:HD2	38:B:8777:HOH:O	2.14	0.48
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.96	0.48
25:X:37:LEU:CD1	25:X:85:VAL:HG21	2.34	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:1596:U:H2'	1:0:1598:A:OP2	2.14	0.48
1:0:1682:A:H5''	38:0:9448:HOH:O	2.12	0.48
21:T:41:ARG:HG2	21:T:41:ARG:HH11	1.78	0.48
24:W:38:THR:HG22	24:W:39:ASP:H	1.79	0.48
28:1:28:HIS:HD2	28:1:30:LYS:H	1.61	0.48
1:0:39:G:C2	1:0:444:C:C2	3.02	0.48
1:0:306:A:P	21:T:38:ARG:HH21	2.37	0.48
1:0:319:A:H4'	1:0:338:C:C4	2.49	0.48
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.14	0.48
1:0:1672:G:H8	38:0:3113:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2281:C:H2'	1:0:2282:U:H5'	1.96	0.48
30:3:69:TYR:CZ	30:3:80:ARG:HD2	2.49	0.48
31:I:100:LEU:HD23	31:I:104:GLN:OE1	2.14	0.48
1:0:152:A:O2'	1:0:153:C:H5'	2.14	0.48
1:0:228:C:H2'	1:0:229:G:H5'	1.96	0.48
1:0:317:A:OP1	21:T:52:ARG:O	2.31	0.48
1:0:407:A:H3'	38:0:4457:HOH:O	2.13	0.48
1:0:1189:A:H1'	1:0:1209:C:H1'	1.96	0.48
1:0:1636:G:C2'	1:0:1637:A:H5'	2.43	0.48
1:0:1789:G:H2'	1:0:1790:C:O5'	2.14	0.48
1:0:1886:A:H61	1:0:2016:U:H3	1.60	0.48
38:0:4610:HOH:O	16:O:35:LYS:HD3	2.14	0.48
38:0:7653:HOH:O	14:M:78:LYS:HD3	2.13	0.48
6:D:135:VAL:HG22	6:D:136:ARG:N	2.28	0.48
1:0:128:A:C8	1:0:128:A:C3'	2.96	0.47
1:0:307:G:H3'	1:0:342:C:OP2	2.13	0.47
1:0:441:A:H1'	1:0:442:A:N7	2.29	0.47
1:0:559:U:C2'	1:0:560:C:H5'	2.44	0.47
1:0:853:C:H2'	1:0:854:G:O4'	2.14	0.47
1:0:951:A:O2'	1:0:952:G:H5'	2.14	0.47
1:0:961:A:C6	1:0:1010:C:C5	3.01	0.47
1:0:968:G:O2'	1:0:969:G:H5'	2.14	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:1244:U:H5	38:J:8744:HOH:O	1.96	0.47
1:0:1477:C:C5'	1:0:1868:G:H5''	2.44	0.47
1:0:1669:A:H2	38:0:3699:HOH:O	1.97	0.47
38:0:7398:HOH:O	21:T:9:LYS:HB2	2.14	0.47
8:F:21:GLU:O	8:F:24:ARG:HG2	2.14	0.47
8:F:111:ILE:O	8:F:115:VAL:HG23	2.14	0.47
1:0:283:U:H5	1:0:284:C:N4	2.11	0.47
1:0:392:U:H4'	14:M:193:LYS:HB3	1.95	0.47
1:0:1183:C:H42	1:0:1184:C:H41	1.56	0.47
1:0:1565:C:O4'	1:0:2738:G:H1'	2.14	0.47
1:0:1588:G:C6	1:0:1589:G:C6	3.03	0.47
1:0:1909:A:N1	1:0:2128:G:H1'	2.29	0.47
1:0:2238:A:H3'	38:0:6652:HOH:O	2.14	0.47
1:0:2795:C:O2'	1:0:2796:U:H5'	2.14	0.47
2:9:3028:U:H3'	2:9:3029:C:H6	1.78	0.47
17:P:115:SER:O	17:P:117:SER:N	2.45	0.47
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.47
1:0:569:A:H5''	1:0:587:A:N1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:807:A:H2'	1:0:808:A:O4'	2.15	0.47
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.47
1:0:1850:U:H2'	1:0:1851:G:H8	1.78	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:D:25:MET:HE1	6:D:40:ILE:HG13	1.95	0.47
13:L:73:VAL:HG11	13:L:118:LEU:HD21	1.97	0.47
17:P:94:TRP:CZ2	17:P:98:ILE:HG13	2.49	0.47
23:V:39:ALA:N	23:V:40:PRO:CD	2.77	0.47
28:1:22:CYS:SG	28:1:24:GLU:HB2	2.55	0.47
1:0:307:G:C5	1:0:324:G:C2	3.03	0.47
1:0:734:U:O2'	1:0:737:A:N6	2.47	0.47
1:0:1182:C:H1'	1:0:1192:A:H8	1.80	0.47
1:0:1419:U:H2'	1:0:1685:A:C2	2.48	0.47
1:0:1594:C:O2'	1:0:1607:A:H4'	2.15	0.47
2:9:3053:G:O2'	2:9:3054:A:H5'	2.15	0.47
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.44	0.47
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.44	0.47
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.29	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
8:F:99:THR:HA	38:F:3461:HOH:O	2.15	0.47
19:R:104:PHE:HB3	19:R:109:MET:HE2	1.95	0.47
24:W:119:HIS:HD2	24:W:120:PRO:O	1.97	0.47
1:0:470:U:O2'	28:1:16:HIS:HD2	1.97	0.47
1:0:475:G:C5'	5:C:73:LEU:HD23	2.44	0.47
1:0:1586:G:C5	1:0:1587:U:C5	3.02	0.47
1:0:1593:C:OP1	17:P:117:SER:HB3	2.14	0.47
1:0:2329:C:O2'	1:0:2330:U:H5'	2.14	0.47
38:0:9546:HOH:O	24:W:119:HIS:HE1	1.97	0.47
13:L:129:ALA:O	13:L:133:VAL:HG23	2.15	0.47
30:3:70:ARG:HA	38:3:8767:HOH:O	2.15	0.47
1:0:236:A:H4'	1:0:237:G:OP1	2.14	0.47
1:0:840:U:H2'	19:R:128:ARG:HH12	1.79	0.47
1:0:1032:A:H2'	1:0:1032:A:N3	2.29	0.47
1:0:1577:U:O2'	1:0:1578:C:H5'	2.14	0.47
1:0:1790:C:H2'	1:0:1791:U:C6	2.48	0.47
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.96	0.47
23:V:46:ILE:HA	23:V:49:LEU:HD12	1.96	0.47
26:Y:133:HIS:HD2	38:Y:8782:HOH:O	1.97	0.47
1:0:407:A:C2	1:0:408:A:C4	3.03	0.47
1:0:603:A:H1'	1:0:605:C:C2	2.49	0.47
1:0:883:U:O2	1:0:883:U:C2'	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:894:A:C2	5:C:87:ARG:NH2	2.83	0.47
1:0:1209:C:O2	1:0:1210:G:C8	2.68	0.47
1:0:1512:G:O2'	1:0:1513:C:H5'	2.15	0.47
1:0:1886:A:H4'	38:Z:8606:HOH:O	2.14	0.47
4:B:72:THR:HB	38:B:8804:HOH:O	2.14	0.47
4:B:190:MET:HE2	4:B:194:PHE:CE1	2.49	0.47
5:C:25:PRO:HG2	38:C:8524:HOH:O	2.15	0.47
5:C:236:THR:HG21	38:C:8573:HOH:O	2.15	0.47
6:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.47
19:R:119:VAL:HG21	19:R:142:ASP:CG	2.39	0.47
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.62	0.47
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.63	0.47
28:1:21:ARG:HD2	28:1:39:PHE:HB2	1.96	0.47
28:1:25:LYS:HD2	29:2:49:GLU:H	1.80	0.47
31:I:112:LYS:O	31:I:116:LEU:HG	2.15	0.47
1:0:56:G:N3	1:0:70:A:C2	2.82	0.47
1:0:111:C:O2'	1:0:112:G:H5'	2.15	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.70	0.47
1:0:945:U:H2'	1:0:946:C:C6	2.50	0.47
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.15	0.47
1:0:1352:A:N1	5:C:48:SER:HB3	2.30	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.47
1:0:1925:G:H5''	30:3:29:ARG:HH22	1.80	0.47
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.28	0.47
3:A:164:ARG:NE	38:A:8785:HOH:O	2.47	0.47
5:C:147:LEU:HA	38:C:8613:HOH:O	2.15	0.47
26:Y:141:THR:HG23	38:Y:8790:HOH:O	2.14	0.47
1:0:146:U:H5	38:0:3305:HOH:O	1.97	0.47
1:0:1217:G:C6	1:0:1218:U:C4	3.03	0.47
1:0:1373:G:H1'	38:0:6128:HOH:O	2.14	0.47
38:0:9208:HOH:O	3:A:11:ARG:HD3	2.15	0.47
15:N:22:GLN:HG2	15:N:26:LEU:HD22	1.97	0.47
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.12	0.47
13:L:30:ARG:NH2	38:L:8722:HOH:O	2.45	0.47
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.44	0.47
24:W:137:GLN:NE2	24:W:141:HIS:HE1	2.01	0.47
31:I:87:THR:HG22	31:I:88:GLY:N	2.30	0.47
31:I:92:PRO:C	31:I:94:GLU:H	2.23	0.47
1:0:263:U:C4	8:F:54:VAL:HG13	2.50	0.46
1:0:330:C:H5	5:C:170:ASP:OD2	1.98	0.46
1:0:886:A:OP2	1:0:2113:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1307:A:H2'	1:0:1308:A:C8	2.50	0.46
1:0:1362:U:H5'	38:0:3261:HOH:O	2.14	0.46
1:0:2415:A:H2'	1:0:2416:G:H5'	1.97	0.46
1:0:2885:A:H2'	1:0:2886:C:C6	2.50	0.46
12:K:64:MET:HA	12:K:67:GLN:HE21	1.80	0.46
19:R:132:ARG:CZ	38:R:8780:HOH:O	2.63	0.46
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.97	0.46
1:0:46:U:H4'	1:0:47:G:OP2	2.15	0.46
1:0:106:A:H2'	1:0:107:U:O4'	2.16	0.46
1:0:638:C:H2'	1:0:639:A:H8	1.80	0.46
1:0:1014:A:H2'	1:0:1015:C:H5'	1.96	0.46
1:0:1589:G:N2	1:0:1605:G:H1'	2.31	0.46
1:0:1855:G:H4'	1:0:1856:C:O5'	2.15	0.46
1:0:1877:G:C6	1:0:1878:G:C6	3.03	0.46
1:0:2506:A:N6	1:0:2511:A:O2'	2.48	0.46
1:0:2893:C:O2'	1:0:2894:C:H5'	2.14	0.46
2:9:3054:A:H5''	38:D:3359:HOH:O	2.15	0.46
2:9:3114:G:H2'	2:9:3115:C:C6	2.51	0.46
3:A:170:VAL:HG21	27:Z:26:VAL:HG21	1.97	0.46
5:C:233:THR:HG22	5:C:234:VAL:H	1.80	0.46
15:N:34:LEU:HD22	15:N:129:ILE:HD13	1.97	0.46
15:N:141:ARG:HG3	15:N:146:HIS:ND1	2.30	0.46
30:3:69:TYR:CE1	30:3:80:ARG:HD2	2.50	0.46
31:I:99:ASP:OD1	31:I:138:THR:HB	2.15	0.46
1:0:69:A:H8	1:0:69:A:C5'	2.22	0.46
1:0:138:U:H5''	1:0:139:C:OP2	2.15	0.46
1:0:278:A:H2'	1:0:279:C:O4'	2.15	0.46
1:0:407:A:H8	38:0:4457:HOH:O	1.99	0.46
1:0:812:A:H2'	1:0:813:C:O4'	2.14	0.46
1:0:819:A:H5''	38:Z:8619:HOH:O	2.16	0.46
1:0:1299:G:N7	13:L:6:ARG:NH1	2.64	0.46
1:0:1527:A:H1'	1:0:1528:A:C8	2.50	0.46
1:0:1753:C:O2	4:B:229:ARG:NH2	2.47	0.46
1:0:1883:U:O2'	1:0:1884:G:H5'	2.15	0.46
1:0:1916:C:H2'	1:0:1917:G:O4'	2.16	0.46
2:9:3013:A:O2'	2:9:3014:G:H5''	2.16	0.46
2:9:3091:C:H2'	2:9:3092:G:O4'	2.16	0.46
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.16	0.46
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.48	0.46
4:B:310:ARG:HD2	38:B:8848:HOH:O	2.14	0.46
6:D:54:ALA:HB1	38:D:4069:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:42:HIS:HB3	15:N:62:HIS:HE1	1.80	0.46
17:P:13:VAL:HG11	17:P:40:VAL:CG1	2.46	0.46
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.46
24:W:11:VAL:O	24:W:12:ASN:HB2	2.16	0.46
24:W:125:HIS:CD2	24:W:127:GLY:H	2.34	0.46
1:O:299:U:N3	1:O:300:C:C5	2.83	0.46
1:O:308:U:C4	1:O:342:C:C1'	2.99	0.46
1:O:1218:U:H2'	1:O:1219:U:H6	1.80	0.46
1:O:1850:U:O4'	1:O:1941:A:C2	2.69	0.46
1:O:1916:C:C4	1:O:1917:G:C5	3.03	0.46
3:A:89:ALA:HB3	38:A:8817:HOH:O	2.15	0.46
7:E:68:HIS:O	7:E:72:MET:HG3	2.14	0.46
14:M:159:VAL:HG12	36:M:8718:CL:CL	2.53	0.46
1:O:1130:U:H2'	1:O:1131:G:C4'	2.44	0.46
1:O:1343:C:C2'	1:O:1344:G:O5'	2.63	0.46
1:O:1562:C:N4	38:O:5862:HOH:O	2.48	0.46
1:O:2862:G:H4'	4:B:336:GLN:O	2.16	0.46
11:J:75:PRO:HD3	11:J:136:SER:OG	2.16	0.46
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.98	0.46
13:L:143:THR:HG22	13:L:144:ASP:H	1.81	0.46
14:M:134:ILE:O	14:M:136:PRO:HD3	2.16	0.46
15:N:47:LEU:HD12	15:N:97:VAL:HG11	1.97	0.46
15:N:71:TRP:HE3	15:N:175:LEU:HD22	1.80	0.46
24:W:35:VAL:HG23	24:W:41:TYR:CD2	2.51	0.46
1:O:134:U:C2	1:O:145:A:C2	3.04	0.46
1:O:245:C:H2'	1:O:246:G:H5'	1.97	0.46
1:O:396:U:P	30:3:38:ARG:HH11	2.38	0.46
1:O:1119:G:N2	1:O:1246:A:H2	2.08	0.46
1:O:1414:A:H2'	1:O:1415:G:O4'	2.16	0.46
1:O:1902:G:O2'	1:O:1903:U:H5'	2.15	0.46
1:O:2237:G:O2'	1:O:2238:A:C8	2.68	0.46
1:O:2866:U:C5	22:U:50:GLU:HB2	2.50	0.46
10:H:9:ILE:HD12	10:H:54:THR:HG22	1.98	0.46
27:Z:39:CYS:HB2	27:Z:57:CYS:SG	2.53	0.46
1:O:51:G:O2'	1:O:52:A:H5'	2.16	0.46
1:O:1314:U:H5''	1:O:1316:G:O4'	2.16	0.46
1:O:1834:C:H2'	1:O:1840:A:H62	1.81	0.46
1:O:2081:A:H4'	11:J:69:TYR:CE1	2.50	0.46
1:O:2408:A:H2	38:3:8713:HOH:O	1.98	0.46
1:O:2604:A:H5'	38:O:5788:HOH:O	2.15	0.46
2:9:3078:G:H5'	38:9:4932:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3081:C:C2'	2:9:3082:U:H5'	2.45	0.46
5:C:19:PRO:HD2	5:C:240:LEU:HD22	1.98	0.46
17:P:126:ALA:C	17:P:128:GLY:H	2.23	0.46
18:Q:94:GLN:O	18:Q:95:GLU:HB2	2.16	0.46
1:0:372:A:H2'	1:0:373:G:C8	2.51	0.46
1:0:423:A:C4	1:0:424:C:C6	3.04	0.46
1:0:657:G:H2'	1:0:658:C:H6	1.79	0.46
1:0:944:G:N2	24:W:44:MET:HE2	2.27	0.46
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.50	0.46
5:C:133:ARG:NH2	38:C:8623:HOH:O	2.49	0.46
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.97	0.46
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.46
10:H:2:PRO:HD2	10:H:5:MET:SD	2.56	0.46
17:P:83:LYS:O	17:P:86:ALA:HB3	2.16	0.46
28:1:25:LYS:HD2	29:2:49:GLU:N	2.30	0.46
1:0:80:A:H3'	21:T:43:ASN:OD1	2.15	0.46
1:0:776:A:OP1	28:1:28:HIS:HE1	1.99	0.46
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.46
1:0:1523:G:C6	1:0:1524:U:O4	2.69	0.46
1:0:1634:G:H2'	1:0:1635:U:C6	2.50	0.46
1:0:2246:U:N3	1:0:2256:G:C2	2.84	0.46
1:0:2413:A:N7	15:N:109:PRO:HB3	2.31	0.46
1:0:2478:U:O2'	1:0:2479:A:H5'	2.16	0.46
7:E:84:MET:HE1	7:E:148:ILE:HD13	1.96	0.46
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.15	0.46
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.46
9:G:23:ILE:O	9:G:27:ILE:HG13	2.16	0.46
11:J:107:ASN:ND2	11:J:109:TYR:H	2.14	0.46
15:N:48:VAL:HG12	15:N:49:THR:N	2.30	0.46
17:P:87:ARG:HG2	38:P:181:HOH:O	2.15	0.46
21:T:35:TYR:CG	21:T:112:LEU:HD22	2.51	0.46
21:T:38:ARG:HG3	21:T:38:ARG:NH1	2.31	0.46
21:T:48:VAL:HG13	21:T:97:ARG:O	2.15	0.46
1:0:185:G:H4'	1:0:186:A:OP1	2.15	0.46
1:0:303:C:H2'	1:0:304:G:O4'	2.16	0.46
1:0:786:G:OP1	1:0:1489:G:H4'	2.16	0.46
1:0:820:G:C5	3:A:171:LYS:HB2	2.50	0.46
1:0:1004:C:H1'	38:0:4835:HOH:O	2.15	0.46
1:0:1594:C:O2'	1:0:1595:G:H5'	2.16	0.46
1:0:2320:U:OP2	30:3:1:MET:HA	2.15	0.46
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2361:A:H5''	38:0:9001:HOH:O	2.16	0.46
4:B:119:HIS:O	4:B:121:PRO:HD3	2.15	0.46
8:F:56:PRO:CG	14:M:44:THR:HA	2.46	0.46
8:F:58:GLU:OE1	14:M:27:ARG:NH2	2.46	0.46
1:0:271:C:C2	1:0:273:G:O4'	2.69	0.45
1:0:1197:G:N2	38:0:6222:HOH:O	2.48	0.45
1:0:1484:G:H2'	38:0:9098:HOH:O	2.16	0.45
7:E:15:GLN:HB3	7:E:42:VAL:HG23	1.97	0.45
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.99	0.45
1:0:861:A:H2'	1:0:862:U:C6	2.51	0.45
1:0:1163:G:N2	38:0:4723:HOH:O	2.50	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.45
1:0:2716:G:C5'	4:B:206:THR:HG21	2.44	0.45
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.16	0.45
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.45
25:X:43:VAL:HG11	25:X:82:GLU:HA	1.98	0.45
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.55	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
1:0:858:U:C5	38:0:5424:HOH:O	2.56	0.45
1:0:955:A:C2	1:0:1013:A:C4	3.04	0.45
1:0:1634:G:H2'	1:0:1635:U:H6	1.82	0.45
1:0:1787:C:O2'	1:0:1788:U:H5'	2.16	0.45
10:H:69:ALA:HB2	10:H:153:ALA:HB2	1.99	0.45
16:O:32:ARG:HB2	38:O:4656:HOH:O	2.15	0.45
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.32	0.45
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.45	0.45
1:0:251:C:O2'	1:0:252:C:H5'	2.15	0.45
1:0:259:G:O2'	1:0:260:C:H5'	2.17	0.45
1:0:284:C:C4'	1:0:285:A:O5'	2.62	0.45
1:0:289:G:O2'	1:0:290:C:H5'	2.16	0.45
1:0:612:U:H2'	1:0:613:C:C6	2.52	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.52	0.45
1:0:1391:G:C2'	1:0:1392:A:H5'	2.46	0.45
1:0:1566:C:O2'	1:0:1567:A:H5'	2.15	0.45
1:0:1568:G:C2'	1:0:1569:U:H5'	2.46	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.43	0.45
1:0:1886:A:N6	1:0:2016:U:H3	2.15	0.45
1:0:1896:G:C6	1:0:1897:U:C4	3.04	0.45
1:0:2002:C:H2'	1:0:2003:U:C5'	2.47	0.45
1:0:2252:A:C6	1:0:2253:G:H1'	2.51	0.45
1:0:2255:A:O2'	1:0:2256:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2269:C:O2'	1:0:2270:G:H5'	2.16	0.45
1:0:2638:G:H1'	38:0:4577:HOH:O	2.17	0.45
2:9:3001:U:C4'	2:9:3003:A:OP1	2.64	0.45
10:H:9:ILE:HD12	10:H:54:THR:CG2	2.46	0.45
10:H:9:ILE:HG12	10:H:56:GLN:HG3	1.98	0.45
13:L:10:SER:O	13:L:11:ARG:HB3	2.16	0.45
15:N:110:THR:HB	15:N:113:SER:OG	2.16	0.45
16:O:38:ARG:NH1	38:O:7674:HOH:O	2.46	0.45
24:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.45
26:Y:144:ARG:NH1	38:Y:8776:HOH:O	2.49	0.45
26:Y:184:GLU:OE2	26:Y:204:ARG:HD2	2.17	0.45
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.46	0.45
1:0:215:A:OP1	13:L:52:LYS:NZ	2.45	0.45
1:0:423:A:C5	1:0:424:C:C5	3.04	0.45
1:0:790:A:H1'	1:0:1710:A:O2'	2.16	0.45
1:0:1168:C:H5''	31:I:88:GLY:H	1.82	0.45
1:0:1202:A:H2'	1:0:1203:G:C5'	2.46	0.45
1:0:1299:G:H5'	38:0:4067:HOH:O	2.15	0.45
1:0:1375:A:C2'	1:0:1376:G:H5'	2.46	0.45
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.45
1:0:1842:A:C4	1:0:1979:G:C6	3.04	0.45
1:0:2245:C:H6	1:0:2245:C:O5'	1.99	0.45
1:0:2379:G:H4'	1:0:2380:A:H5''	1.98	0.45
1:0:2656:G:O2'	1:0:2657:G:H5'	2.16	0.45
1:0:2668:G:H2'	1:0:2669:U:C6	2.52	0.45
1:0:2909:G:H2'	1:0:2910:A:C8	2.51	0.45
2:9:3027:C:N3	38:9:3445:HOH:O	2.35	0.45
2:9:3061:C:H2'	2:9:3062:A:C8	2.46	0.45
4:B:16:ARG:HB3	4:B:217:ARG:NH2	2.31	0.45
12:K:113:ILE:HD12	12:K:128:ALA:HB2	1.98	0.45
1:0:187:A:H3'	1:0:188:C:H6	1.82	0.45
1:0:553:G:C2'	1:0:554:G:H5'	2.46	0.45
1:0:1185:U:H2'	1:0:1186:C:H6	1.81	0.45
1:0:1377:C:H6	1:0:1377:C:C5'	2.28	0.45
1:0:1434:A:H2'	1:0:1436:C:C5	2.51	0.45
1:0:1588:G:C5	1:0:1589:G:C6	3.05	0.45
1:0:2630:G:O6	3:A:206:ARG:NH2	2.50	0.45
1:0:2717:C:H5'	4:B:302:PRO:HA	1.98	0.45
1:0:2785:C:H4'	1:0:2786:G:OP2	2.17	0.45
1:0:2872:U:H2'	1:0:2873:C:H6	1.81	0.45
2:9:3034:A:H8	2:9:3034:A:O5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3081:C:O2'	2:9:3082:U:H5'	2.17	0.45
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.99	0.45
10:H:154:TYR:CD1	10:H:154:TYR:C	2.94	0.45
17:P:131:PHE:CD1	17:P:137:LEU:HD13	2.51	0.45
1:0:539:G:H2'	1:0:540:A:C8	2.51	0.45
1:0:875:A:C6	3:A:194:MET:HE2	2.52	0.45
1:0:1406:A:H4'	1:0:1407:A:H5''	1.99	0.45
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.45
1:0:1634:G:C6	1:0:1635:U:C4	3.04	0.45
1:0:1667:A:H2'	1:0:1668:U:H6	1.80	0.45
1:0:2382:A:OP1	30:3:80:ARG:HG2	2.16	0.45
1:0:2444:U:C2	1:0:2445:U:C6	3.04	0.45
38:0:9348:HOH:O	28:1:1:THR:HA	2.17	0.45
4:B:55:ASN:HB3	4:B:64:GLY:H	1.81	0.45
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.86	0.45
21:T:79:LEU:HG	21:T:89:ARG:HB2	1.99	0.45
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.98	0.45
1:0:204:A:C2'	1:0:205:U:H5'	2.47	0.45
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.45
1:0:1236:A:C8	11:J:63:ILE:HD11	2.52	0.45
1:0:1665:G:H2'	1:0:1666:C:H6	1.82	0.45
1:0:1744:G:C2'	1:0:1745:G:H5'	2.47	0.45
1:0:2248:C:C5	1:0:2249:G:N7	2.84	0.45
1:0:2312:G:C2'	1:0:2313:C:H5'	2.47	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.15	0.45
1:0:2820:A:H2'	1:0:2821:C:C6	2.52	0.45
1:0:2885:A:H2'	1:0:2886:C:H6	1.82	0.45
3:A:199:HIS:CD2	3:A:201:PHE:H	2.33	0.45
13:L:67:ARG:O	13:L:71:GLU:HG3	2.17	0.45
30:3:18:GLN:OE1	30:3:73:GLU:HB2	2.17	0.45
1:0:229:G:O2'	1:0:230:C:H5'	2.16	0.45
1:0:1490:G:H4'	1:0:1533:A:OP1	2.16	0.45
1:0:1684:A:C1'	29:2:43:ARG:HH22	2.22	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45
4:B:243:ASN:HA	4:B:244:PRO:C	2.41	0.45
6:D:146:LYS:HG2	15:N:106:LEU:HB2	1.99	0.45
6:D:153:THR:HA	6:D:156:ARG:HG3	1.98	0.45
10:H:169:GLY:C	10:H:170:ASN:HD22	2.25	0.45
14:M:46:LEU:HG	38:M:8812:HOH:O	2.17	0.45
1:0:69:A:C2'	1:0:70:A:OP2	2.65	0.45
1:0:185:G:C4'	1:0:186:A:H4'	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:559:U:C5'	1:0:559:U:H6	2.27	0.45
1:0:820:G:OP2	3:A:171:LYS:NZ	2.43	0.45
1:0:2506:A:O2'	1:0:2507:G:C8	2.43	0.45
1:0:2898:G:H4'	4:B:288:GLY:HA2	1.99	0.45
2:9:3001:U:O3'	2:9:3003:A:C5'	2.65	0.45
2:9:3107:C:C5	38:9:3167:HOH:O	2.56	0.45
3:A:105:VAL:HG13	3:A:155:THR:O	2.17	0.45
4:B:145:HIS:HD2	4:B:146:THR:O	2.00	0.45
1:0:249:G:H2'	1:0:250:C:C6	2.53	0.44
1:0:941:G:C5	1:0:942:U:C4	3.05	0.44
1:0:1118:A:H8	1:0:1119:G:H5''	1.81	0.44
1:0:1619:G:H2'	1:0:1620:C:O4'	2.16	0.44
1:0:1679:C:H5'	38:0:9314:HOH:O	2.16	0.44
1:0:1733:A:C6	1:0:1734:C:C2	3.05	0.44
1:0:2002:C:C2'	1:0:2003:U:H5'	2.47	0.44
1:0:2856:A:OP1	25:X:15:ARG:NH2	2.50	0.44
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.84	0.44
7:E:81:GLU:O	7:E:172:PRO:HD3	2.17	0.44
14:M:139:PRO:HA	14:M:142:GLN:HB2	1.98	0.44
15:N:23:ARG:O	15:N:27:LEU:HG	2.17	0.44
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.47	0.44
21:T:24:ARG:HH21	21:T:39:ASN:ND2	2.15	0.44
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.15	0.44
1:0:154:C:H2'	1:0:155:C:H6	1.82	0.44
1:0:697:G:H4'	1:0:730:G:O3'	2.17	0.44
1:0:794:U:H2'	1:0:795:G:H5'	1.99	0.44
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.44
1:0:1789:G:C2'	1:0:1790:C:O5'	2.65	0.44
1:0:1882:C:H2'	1:0:1883:U:H6	1.81	0.44
1:0:1902:G:N2	1:0:1936:C:C2	2.85	0.44
1:0:2248:C:C2	1:0:2254:G:C2	3.05	0.44
1:0:2378:U:H3'	30:3:8:ASN:O	2.17	0.44
1:0:2664:A:H8	1:0:2664:A:OP1	2.00	0.44
1:0:2834:G:OP1	25:X:39:LYS:HE2	2.17	0.44
1:0:2890:A:C1'	22:U:56:ARG:NH2	2.76	0.44
4:B:81:ALA:HB1	4:B:142:LEU:HD13	1.98	0.44
5:C:228:ALA:HA	5:C:229:PRO:HD3	1.87	0.44
7:E:6:GLU:HA	7:E:46:THR:HG22	1.99	0.44
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.99	0.44
8:F:52:GLU:HG3	8:F:77:VAL:O	2.18	0.44
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:306:A:H2'	1:0:341:C:O2'	2.17	0.44
1:0:1202:A:H2'	1:0:1203:G:H5'	1.99	0.44
1:0:1798:C:H1'	17:P:66:GLN:OE1	2.17	0.44
1:0:1851:G:O2'	1:0:1852:A:H5'	2.17	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.52	0.44
1:0:2375:G:H2'	1:0:2376:C:C6	2.53	0.44
1:0:2598:U:O2	1:0:2600:A:C8	2.70	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.57	0.44
2:9:3018:U:OP2	6:D:154:LYS:HE2	2.17	0.44
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.44
8:F:27:GLY:HA3	8:F:101:ALA:O	2.17	0.44
10:H:138:CYS:HB2	38:H:8543:HOH:O	2.17	0.44
11:J:19:MET:CE	11:J:132:LEU:HD11	2.41	0.44
16:O:44:ASN:OD1	16:O:65:LEU:HB2	2.16	0.44
24:W:69:ARG:HD2	24:W:117:ARG:O	2.17	0.44
1:0:138:U:C5	1:0:140:G:O6	2.71	0.44
1:0:883:U:O2	1:0:883:U:H2'	2.16	0.44
1:0:1925:G:H5'	30:3:29:ARG:NH1	2.32	0.44
1:0:2255:A:C2'	1:0:2256:G:H5'	2.48	0.44
1:0:2314:G:H2'	1:0:2315:C:H5'	2.00	0.44
1:0:2355:G:H5''	1:0:2356:A:OP2	2.18	0.44
38:0:4225:HOH:O	29:2:38:LYS:HE3	2.17	0.44
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.47	0.44
26:Y:107:PRO:HB3	26:Y:182:PHE:CE2	2.53	0.44
29:2:35:ARG:HH11	29:2:37:HIS:CD2	2.36	0.44
1:0:255:A:H2'	1:0:256:C:C6	2.52	0.44
1:0:382:U:C5	1:0:406:G:N2	2.85	0.44
1:0:818:A:O2'	27:Z:13:ARG:HD3	2.18	0.44
1:0:907:A:H4'	1:0:1328:A:C2	2.53	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.17	0.44
1:0:1165:G:O2'	1:0:1174:A:C1'	2.65	0.44
1:0:1520:G:C6	1:0:1521:C:C4	3.05	0.44
1:0:1537:C:C2	1:0:1649:G:C2	3.06	0.44
1:0:1557:G:C2'	1:0:1558:C:H5'	2.47	0.44
1:0:1768:C:H2'	1:0:1769:C:C5'	2.47	0.44
1:0:2004:U:H2'	1:0:2005:G:OP1	2.18	0.44
1:0:2073:G:C6	1:0:2489:G:H4'	2.52	0.44
1:0:2506:A:H1'	38:0:3742:HOH:O	2.16	0.44
1:0:2853:U:C4	1:0:2906:A:N6	2.86	0.44
38:0:3012:HOH:O	28:1:46:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:3230:HOH:O	31:I:92:PRO:HD3	2.17	0.44
38:O:3980:HOH:O	21:T:82:THR:HA	2.17	0.44
6:D:86:THR:C	6:D:89:PRO:HD2	2.43	0.44
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.99	0.44
8:F:34:ASN:HA	14:M:4:ALA:HB2	2.00	0.44
15:N:119:GLN:O	15:N:123:ILE:HG13	2.18	0.44
17:P:59:ARG:HH22	17:P:66:GLN:NE2	2.14	0.44
1:O:216:A:O2'	1:O:217:C:H5'	2.18	0.44
1:O:1894:C:C2	1:O:1939:U:C4	3.05	0.44
1:O:2112:A:H2'	1:O:2113:G:C8	2.52	0.44
1:O:2401:A:H5'	38:O:9485:HOH:O	2.18	0.44
5:C:131:PHE:CD2	5:C:131:PHE:N	2.85	0.44
15:N:179:LEU:HD23	15:N:184:ILE:CD1	2.48	0.44
1:O:21:G:H5''	19:R:2:ILE:HA	1.95	0.44
1:O:151:A:C2	1:O:442:A:C8	3.06	0.44
1:O:731:U:H2'	1:O:732:C:H6	1.82	0.44
1:O:1131:G:C6	1:O:1230:A:C4	3.06	0.44
1:O:1383:U:H5''	38:X:6177:HOH:O	2.18	0.44
1:O:1453:G:H2'	1:O:1454:U:O4'	2.18	0.44
1:O:1805:G:O2'	1:O:1806:G:H5'	2.18	0.44
1:O:2337:G:O3'	6:D:97:GLN:HA	2.17	0.44
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.29	0.44
6:D:10:PHE:CG	6:D:11:HIS:N	2.86	0.44
10:H:23:ILE:HA	10:H:120:ILE:HG21	1.99	0.44
10:H:162:ARG:HD3	38:H:8582:HOH:O	2.16	0.44
15:N:58:LEU:N	15:N:58:LEU:HD12	2.33	0.44
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.47	0.44
21:T:9:LYS:HE3	21:T:13:ARG:HH11	1.80	0.44
26:Y:144:ARG:HH11	26:Y:144:ARG:CG	2.31	0.44
1:O:241:A:N1	1:O:378:A:H4'	2.33	0.44
1:O:282:C:O2'	1:O:283:U:C4'	2.66	0.44
1:O:678:G:H3'	38:O:4438:HOH:O	2.18	0.44
1:O:1181:A:N1	1:O:1192:A:O2'	2.50	0.44
1:O:1185:U:OP1	31:I:126:LYS:HD3	2.17	0.44
1:O:1446:U:H2'	20:S:55:GLN:NE2	2.33	0.44
1:O:1520:G:N1	1:O:1667:A:C6	2.86	0.44
1:O:1538:C:O2'	1:O:1539:U:H5'	2.18	0.44
1:O:1644:C:N3	1:O:1645:U:C5	2.86	0.44
1:O:1787:C:C4'	1:O:2883:A:O4'	2.65	0.44
1:O:1850:U:H2'	1:O:1851:G:C8	2.52	0.44
1:O:1928:C:C2'	1:O:1929:G:H5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2092:G:H2'	1:0:2613:G:OP1	2.18	0.44
38:0:5074:HOH:O	4:B:216:LYS:HA	2.17	0.44
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.16	0.44
10:H:46:GLN:NE2	10:H:137:TYR:HE2	2.15	0.44
11:J:45:VAL:HG11	11:J:121:LEU:CD2	2.48	0.44
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.99	0.44
14:M:164:THR:HG23	14:M:165:GLY:N	2.32	0.44
15:N:43:VAL:CG1	15:N:118:ILE:HD11	2.48	0.44
1:0:243:A:H61	1:0:269:G:H1'	1.83	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.44
1:0:1167:G:H4'	31:I:135:LEU:CD2	2.45	0.44
1:0:1209:C:H2'	1:0:1210:G:C8	2.53	0.44
1:0:1659:A:H2'	1:0:1660:G:O4'	2.18	0.44
1:0:2524:G:H21	1:0:2526:C:H41	1.61	0.44
2:9:3045:A:C8	2:9:3046:C:C5	3.06	0.44
3:A:113:GLY:HA2	3:A:153:ARG:NH2	2.33	0.44
5:C:34:ALA:HB3	5:C:220:THR:HG21	2.00	0.44
6:D:167:GLU:C	6:D:169:THR:H	2.26	0.44
6:D:172:VAL:HG12	6:D:173:GLU:N	2.32	0.44
11:J:93:ARG:HB3	11:J:93:ARG:HH11	1.83	0.44
15:N:37:ARG:NH2	38:N:8731:HOH:O	2.51	0.44
17:P:103:THR:HA	17:P:106:ARG:NH1	2.33	0.44
21:T:48:VAL:CG1	21:T:49:GLU:N	2.81	0.44
1:0:226:A:H1'	1:0:393:G:C5	2.53	0.43
1:0:288:A:H2'	1:0:289:G:C8	2.52	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.43
1:0:629:A:C2	1:0:2074:A:C2	3.06	0.43
1:0:700:A:C2	13:L:71:GLU:HG2	2.52	0.43
1:0:968:G:C2	1:0:1001:U:O2	2.71	0.43
1:0:1183:C:H42	1:0:1184:C:N4	2.15	0.43
1:0:1215:A:O3'	1:0:1216:G:C4'	2.66	0.43
1:0:1279:U:H5''	1:0:1280:A:OP2	2.17	0.43
1:0:1450:C:O2'	1:0:1493:A:H2'	2.17	0.43
1:0:1780:G:O2'	1:0:1781:G:H5'	2.17	0.43
1:0:2403:C:H2'	1:0:2404:G:O5'	2.18	0.43
1:0:2672:C:O2'	1:0:2673:U:H5'	2.18	0.43
5:C:214:THR:HG23	38:C:8633:HOH:O	2.17	0.43
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.47	0.43
14:M:37:VAL:HG21	14:M:108:THR:OG1	2.17	0.43
31:I:113:HIS:N	31:I:114:PRO:HD2	2.33	0.43
1:0:145:A:H4'	14:M:137:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:276:C:H6	1:0:276:C:O5'	2.00	0.43
1:0:764:C:H2'	1:0:765:G:O4'	2.18	0.43
1:0:814:G:N2	1:0:815:U:H1'	2.33	0.43
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.43
1:0:1662:C:H2'	1:0:1663:G:O4'	2.17	0.43
1:0:1973:A:H2'	1:0:1974:G:O4'	2.18	0.43
1:0:2249:G:N1	1:0:2253:G:C6	2.86	0.43
1:0:2667:G:N3	1:0:2827:A:C2	2.85	0.43
1:0:2729:C:H1'	1:0:2864:U:O2'	2.18	0.43
3:A:88:ILE:O	3:A:88:ILE:HG22	2.18	0.43
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.47	0.43
5:C:154:VAL:O	5:C:158:GLU:HG3	2.18	0.43
7:E:40:VAL:HA	7:E:48:VAL:O	2.18	0.43
7:E:101:GLU:HB2	7:E:116:THR:O	2.18	0.43
14:M:28:GLN:O	14:M:32:ARG:HG3	2.18	0.43
19:R:119:VAL:HG12	19:R:119:VAL:O	2.18	0.43
24:W:21:LEU:HD22	24:W:26:ILE:HD13	1.98	0.43
1:0:289:G:N2	1:0:363:A:C2	2.66	0.43
1:0:454:U:C2	38:0:9027:HOH:O	2.56	0.43
1:0:947:U:O2'	1:0:948:G:H5'	2.18	0.43
1:0:1167:G:H3'	38:0:7466:HOH:O	2.18	0.43
1:0:1644:C:O2'	1:0:1645:U:H5'	2.18	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.36	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2444:U:C4	1:0:2445:U:C5	3.06	0.43
38:0:3751:HOH:O	21:T:9:LYS:HD3	2.17	0.43
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.83	0.43
12:K:18:ILE:HG22	12:K:93:ASN:HB2	1.98	0.43
14:M:67:VAL:HB	14:M:97:ILE:HG23	1.99	0.43
20:S:37:VAL:O	20:S:41:VAL:HG23	2.17	0.43
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.54	0.43
1:0:37:A:C2	1:0:446:G:C2	3.07	0.43
1:0:394:G:H1	14:M:181:GLU:CD	2.27	0.43
1:0:488:U:O2'	21:T:82:THR:HG21	2.19	0.43
1:0:1592:G:C5	1:0:1593:C:C4	3.07	0.43
1:0:1785:G:H1'	1:0:1812:G:N3	2.33	0.43
1:0:2443:C:H5'	13:L:57:VAL:HG21	1.99	0.43
1:0:2511:A:H2'	1:0:2512:U:O4'	2.19	0.43
1:0:2624:A:O2'	1:0:2625:C:H5'	2.18	0.43
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.82	0.43
16:O:88:LYS:HD3	38:O:7061:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:30:VAL:HG12	18:Q:30:VAL:O	2.18	0.43
23:V:1:THR:HG23	23:V:2:VAL:N	2.32	0.43
1:0:34:C:C4	1:0:35:U:C4	3.07	0.43
1:0:160:A:C4	1:0:177:A:C2	3.06	0.43
1:0:559:U:H2'	1:0:560:C:C5'	2.49	0.43
1:0:1055:G:OP2	10:H:96:ARG:NH1	2.52	0.43
1:0:1520:G:C6	1:0:1521:C:N4	2.87	0.43
1:0:1556:G:O2'	1:0:1557:G:H5'	2.19	0.43
1:0:2028:U:H2'	1:0:2029:C:C6	2.53	0.43
1:0:2105:C:H2'	1:0:2106:C:C6	2.54	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.17	0.43
1:0:2607:U:H4'	38:0:9432:HOH:O	2.17	0.43
1:0:2834:G:C4	1:0:2847:G:N2	2.86	0.43
12:K:125:ALA:C	12:K:127:ALA:H	2.25	0.43
18:Q:43:ILE:HG13	18:Q:52:PHE:CZ	2.54	0.43
24:W:65:VAL:CG1	24:W:116:LEU:HD13	2.47	0.43
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.43
1:0:510:U:H6	38:0:7411:HOH:O	1.99	0.43
1:0:559:U:O2'	1:0:560:C:H5'	2.18	0.43
1:0:1400:C:H2'	1:0:1401:G:C5'	2.48	0.43
1:0:1513:C:O2'	1:0:1514:C:H5'	2.18	0.43
1:0:1581:A:C5	1:0:1582:C:C5	3.07	0.43
1:0:1644:C:C4	1:0:1645:U:C5	3.06	0.43
1:0:1878:G:C1'	38:0:6112:HOH:O	2.56	0.43
1:0:2761:A:C4	1:0:2763:G:C8	3.06	0.43
1:0:2911:C:O2'	1:0:2912:C:H5'	2.19	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.54	0.43
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.43
28:1:25:LYS:HD2	29:2:48:ASP:HA	1.99	0.43
1:0:195:C:H5''	38:M:8796:HOH:O	2.17	0.43
1:0:372:A:H2'	1:0:373:G:H8	1.83	0.43
1:0:1204:C:H1'	38:0:4743:HOH:O	2.18	0.43
1:0:1215:A:O3'	1:0:1216:G:H4'	2.18	0.43
1:0:1649:G:O2'	1:0:1650:C:H5'	2.19	0.43
1:0:1669:A:H2'	1:0:1670:G:C8	2.54	0.43
1:0:1829:A:H61	27:Z:18:TYR:HA	1.82	0.43
1:0:2072:G:N2	38:0:6848:HOH:O	2.41	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
1:0:2897:C:H2'	1:0:2898:G:C8	2.53	0.43
1:0:2912:C:H2'	1:0:2913:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:O2'	2:9:3042:C:H5	2.00	0.43
2:9:3065:A:C2'	2:9:3066:G:OP2	2.66	0.43
11:J:90:LYS:HB2	36:J:8702:CL:CL	2.55	0.43
16:O:47:ARG:HH11	16:O:47:ARG:HG3	1.84	0.43
24:W:108:ARG:HG3	24:W:114:PRO:HG3	2.00	0.43
30:3:48:ASN:ND2	30:3:50:GLY:H	2.16	0.43
1:0:69:A:C8	1:0:69:A:C5'	2.97	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.43
1:0:301:G:O2'	1:0:302:A:H5'	2.19	0.43
1:0:432:G:H2'	1:0:433:C:H6	1.84	0.43
1:0:1052:G:N3	1:0:1052:G:H2'	2.34	0.43
1:0:1462:C:H2'	1:0:1463:A:H8	1.79	0.43
1:0:1592:G:H2'	1:0:1593:C:C6	2.54	0.43
1:0:2252:A:H2'	1:0:2253:G:C5'	2.48	0.43
1:0:2338:G:H1'	6:D:105:SER:OG	2.19	0.43
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.52	0.43
3:A:65:ARG:C	3:A:66:ARG:HG3	2.43	0.43
4:B:307:ARG:HG2	4:B:308:LEU:N	2.33	0.43
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.77	0.43
15:N:22:GLN:HA	15:N:25:ARG:CZ	2.49	0.43
24:W:126:ASP:HB3	24:W:135:GLY:O	2.19	0.43
30:3:22:VAL:HG12	30:3:67:LEU:HD22	2.01	0.43
1:0:20:G:H21	19:R:117:HIS:HD2	1.66	0.43
1:0:527:U:H2'	1:0:528:G:C8	2.54	0.43
1:0:1298:U:H2'	1:0:1299:G:C8	2.54	0.43
1:0:1463:A:H8	1:0:1463:A:O5'	2.01	0.43
1:0:1500:U:P	17:P:41:ARG:HH22	2.42	0.43
1:0:1573:A:H2'	1:0:1574:C:H5'	2.00	0.43
38:0:7425:HOH:O	4:B:211:THR:HG21	2.18	0.43
6:D:86:THR:O	6:D:90:LEU:HG	2.19	0.43
1:0:17:G:H2'	1:0:18:C:C6	2.54	0.43
1:0:298:C:N3	1:0:299:U:C5	2.87	0.43
1:0:311:C:H2'	1:0:312:U:C6	2.54	0.43
1:0:321:A:H1'	38:0:7016:HOH:O	2.19	0.43
1:0:595:U:O2'	1:0:596:C:H5'	2.19	0.43
1:0:932:U:H2'	1:0:933:C:C6	2.54	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.54	0.43
1:0:1285:U:H4'	24:W:74:GLU:OE1	2.19	0.43
1:0:1717:A:H5''	17:P:54:LYS:HB2	2.01	0.43
1:0:1730:G:H5''	1:0:1731:C:C6	2.52	0.43
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2119:C:O2'	1:0:2120:U:H5'	2.19	0.43
1:0:2487:C:H5	38:0:4883:HOH:O	2.01	0.43
2:9:3096:C:O2'	2:9:3097:U:H5'	2.19	0.43
3:A:69:LEU:HB3	38:A:8775:HOH:O	2.18	0.43
3:A:167:LYS:CE	27:Z:26:VAL:HG22	2.49	0.43
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.49	0.43
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.99	0.43
15:N:154:LEU:HD11	38:N:8723:HOH:O	2.19	0.43
21:T:41:ARG:NH1	21:T:42:VAL:O	2.52	0.43
27:Z:24:ARG:HG2	27:Z:28:GLU:OE2	2.19	0.43
1:0:797:A:N6	1:0:816:G:H1'	2.34	0.42
1:0:825:U:H5''	1:0:826:U:OP1	2.19	0.42
1:0:876:A:N3	1:0:876:A:C2'	2.82	0.42
1:0:1175:G:H1'	1:0:1193:A:C2'	2.46	0.42
1:0:1421:C:O2'	1:0:1422:U:H5'	2.19	0.42
1:0:1568:G:C5	1:0:1569:U:C5	3.07	0.42
1:0:1713:G:H1'	38:0:5065:HOH:O	2.19	0.42
1:0:2132:C:H1'	14:M:124:GLY:HA3	2.01	0.42
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.30	0.42
5:C:33:LYS:HE2	38:C:8558:HOH:O	2.19	0.42
10:H:166:SER:CB	10:H:167:PRO:CD	2.92	0.42
25:X:76:ARG:HH11	25:X:76:ARG:CG	2.21	0.42
1:0:36:C:C2	1:0:447:A:C2	3.07	0.42
1:0:40:C:H4'	38:0:6982:HOH:O	2.18	0.42
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.42
1:0:432:G:O2'	1:0:433:C:H5'	2.19	0.42
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.42
1:0:666:A:H2'	1:0:667:C:H5'	1.99	0.42
1:0:789:C:H1'	1:0:827:A:C2	2.53	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.42
1:0:2531:U:O2'	1:0:2532:A:H5'	2.19	0.42
38:0:6279:HOH:O	6:D:99:ASP:HA	2.19	0.42
38:0:7398:HOH:O	21:T:9:LYS:HD2	2.18	0.42
4:B:82:VAL:O	4:B:82:VAL:HG12	2.18	0.42
5:C:95:GLU:H	5:C:95:GLU:CD	2.28	0.42
10:H:47:ILE:HD12	10:H:146:VAL:HG11	2.00	0.42
15:N:73:ALA:HB1	15:N:74:PRO:HD2	2.00	0.42
16:O:63:LYS:NZ	38:O:2363:HOH:O	2.49	0.42
27:Z:49:ARG:HB2	27:Z:55:TRP:CZ3	2.54	0.42
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.19	0.42
1:0:152:A:H1'	1:0:440:C:O2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:364:C:H2'	1:0:365:G:C8	2.54	0.42
1:0:450:C:H4'	5:C:46:TYR:CE1	2.54	0.42
1:0:670:G:H2'	1:0:671:A:O4'	2.19	0.42
1:0:800:G:H2'	1:0:801:U:C6	2.54	0.42
1:0:1159:G:H1	1:0:1208:C:N4	2.15	0.42
1:0:1164:U:OP1	31:I:74:PRO:HA	2.19	0.42
1:0:1202:A:C2'	1:0:1203:G:H5'	2.49	0.42
1:0:1246:A:H5'	1:0:1246:A:H8	1.85	0.42
1:0:1822:A:O2'	1:0:1823:G:H5'	2.19	0.42
1:0:2467:A:H2'	38:0:5453:HOH:O	2.19	0.42
1:0:2577:A:H5'	38:0:7721:HOH:O	2.18	0.42
38:0:5628:HOH:O	17:P:58:SER:HB3	2.19	0.42
38:0:6782:HOH:O	4:B:282:GLY:HA2	2.19	0.42
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.50	0.42
14:M:42:ARG:HA	14:M:43:PRO:HD3	1.85	0.42
15:N:175:LEU:HA	15:N:175:LEU:HD12	1.79	0.42
25:X:76:ARG:NH1	25:X:76:ARG:CG	2.81	0.42
1:0:285:A:C2	1:0:368:C:H4'	2.54	0.42
1:0:461:C:H6	38:0:5831:HOH:O	2.03	0.42
1:0:645:U:OP2	13:L:4:LYS:HE2	2.19	0.42
1:0:856:G:H2'	38:0:5424:HOH:O	2.19	0.42
1:0:1501:A:C6	1:0:1502:A:C6	3.07	0.42
1:0:2044:G:OP1	25:X:23:HIS:HE1	2.01	0.42
1:0:2504:A:H2'	1:0:2505:G:O4'	2.19	0.42
1:0:2509:A:OP2	1:0:2510:C:C5	2.68	0.42
1:0:2635:A:C2'	1:0:2636:C:H5'	2.48	0.42
2:9:3003:A:O5'	2:9:3003:A:C8	2.72	0.42
11:J:131:THR:HB	11:J:134:GLU:HG3	2.00	0.42
13:L:41:HIS:CD2	13:L:41:HIS:H	2.38	0.42
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.42
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.42
1:0:1205:U:O2'	1:0:1206:U:H5''	2.19	0.42
1:0:1661:A:O2'	1:0:1662:C:H5'	2.20	0.42
1:0:2377:U:H6	1:0:2377:U:O5'	2.02	0.42
1:0:2863:G:C2	1:0:2894:C:O2	2.72	0.42
2:9:3001:U:C5'	2:9:3003:A:OP1	2.66	0.42
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.86	0.42
5:C:218:VAL:HG12	38:C:8621:HOH:O	2.19	0.42
6:D:146:LYS:HZ1	15:N:107:ASN:HD21	1.68	0.42
13:L:114:VAL:HG11	38:L:8770:HOH:O	2.19	0.42
20:S:33:SER:OG	20:S:36:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:58:MET:SD	29:2:8:LYS:HE3	2.59	0.42
21:T:53:GLY:HA3	38:T:6384:HOH:O	2.18	0.42
26:Y:219:GLU:HG3	26:Y:220:GLU:N	2.34	0.42
31:I:93:GLN:HA	31:I:96:PHE:CE2	2.55	0.42
1:0:240:C:O2	1:0:240:C:H2'	2.20	0.42
1:0:750:A:O3'	5:C:101:ASP:HB2	2.20	0.42
1:0:1176:C:H1'	38:0:3922:HOH:O	2.19	0.42
1:0:1189:A:H3'	38:0:7650:HOH:O	2.18	0.42
3:A:217:ARG:CG	3:A:217:ARG:NH1	2.83	0.42
15:N:69:TYR:CD2	15:N:184:ILE:HD11	2.54	0.42
23:V:12:THR:HG23	23:V:14:ALA:H	1.85	0.42
27:Z:39:CYS:SG	27:Z:41:ASN:N	2.93	0.42
27:Z:39:CYS:SG	27:Z:57:CYS:HB2	2.60	0.42
1:0:298:C:C2	1:0:299:U:C6	3.07	0.42
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.42
1:0:794:U:C2'	1:0:795:G:H5'	2.49	0.42
1:0:1407:A:O2'	1:0:1408:U:H3'	2.19	0.42
1:0:1553:C:H2'	1:0:1554:U:H6	1.85	0.42
1:0:1626:A:H2'	1:0:1627:G:C5'	2.49	0.42
1:0:1773:G:H2'	1:0:1774:G:H5'	2.02	0.42
1:0:2064:U:H2'	1:0:2065:C:C6	2.55	0.42
38:0:7388:HOH:O	31:I:90:GLY:HA2	2.19	0.42
38:0:9656:HOH:O	16:O:112:ARG:HD2	2.19	0.42
2:9:3094:G:O2'	2:9:3095:C:H5'	2.20	0.42
10:H:154:TYR:C	10:H:154:TYR:HD1	2.28	0.42
14:M:109:PHE:HB3	14:M:112:LEU:HG	2.02	0.42
15:N:143:ARG:HA	15:N:172:PHE:CD2	2.55	0.42
24:W:73:LEU:HD12	24:W:73:LEU:HA	1.75	0.42
1:0:24:G:N2	1:0:518:G:H1'	2.34	0.42
1:0:275:G:C2	1:0:376:C:C2	3.07	0.42
1:0:506:G:H22	1:0:509:A:H5''	1.82	0.42
1:0:1156:C:O2'	1:0:1157:C:H5'	2.20	0.42
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.48	0.42
1:0:1947:G:O2'	1:0:1948:G:H5'	2.19	0.42
1:0:1972:U:C2'	1:0:1973:A:H5''	2.49	0.42
1:0:2488:A:N6	1:0:2534:C:H42	2.10	0.42
3:A:35:GLY:O	3:A:36:ASP:CB	2.68	0.42
4:B:149:ASP:HA	38:B:8861:HOH:O	2.19	0.42
8:F:91:VAL:CG1	8:F:92:GLY:N	2.81	0.42
12:K:34:VAL:HG22	12:K:47:ALA:HB2	2.01	0.42
12:K:98:VAL:HG13	12:K:102:GLU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:47:ASP:CG	14:M:48:LYS:N	2.78	0.42
26:Y:189:ASN:HD22	26:Y:192:ASP:H	1.67	0.42
1:0:53:C:H2'	1:0:54:G:O4'	2.20	0.42
1:0:283:U:C6	1:0:284:C:N3	2.88	0.42
1:0:807:A:H2'	1:0:808:A:C8	2.54	0.42
1:0:1183:C:N3	1:0:1184:C:C5	2.87	0.42
1:0:1597:A:O4'	17:P:95:GLU:HG2	2.20	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.34	0.42
1:0:2871:G:H2'	1:0:2872:U:C6	2.55	0.42
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.02	0.42
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.42
12:K:72:VAL:HG11	12:K:121:PHE:CD1	2.54	0.42
15:N:108:SER:HA	15:N:109:PRO:HD3	1.78	0.42
16:O:96:VAL:CG1	16:O:100:GLN:HB2	2.49	0.42
18:Q:40:HIS:CE1	18:Q:94:GLN:HG3	2.55	0.42
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.42
1:0:2073:G:OP2	1:0:2490:A:H5'	2.20	0.42
1:0:2283:G:C6	10:H:113:MET:HB3	2.55	0.42
1:0:2444:U:N3	1:0:2445:U:C5	2.88	0.42
1:0:2769:C:C2'	1:0:2770:G:C5'	2.87	0.42
1:0:2815:G:N7	11:J:80:LYS:NZ	2.63	0.42
1:0:2836:G:H1'	38:0:6818:HOH:O	2.19	0.42
1:0:2853:U:C5	1:0:2906:A:N6	2.88	0.42
38:0:6235:HOH:O	22:U:56:ARG:HD3	2.20	0.42
5:C:194:PHE:CE2	5:C:234:VAL:HG11	2.55	0.42
10:H:143:ALA:O	10:H:147:LYS:HG3	2.20	0.42
15:N:37:ARG:HD3	36:N:8707:CL:CL	2.57	0.42
15:N:42:HIS:CB	15:N:62:HIS:HE1	2.33	0.42
21:T:48:VAL:HG12	21:T:49:GLU:N	2.35	0.42
30:3:11:CYS:HB2	30:3:20:HIS:HE1	1.85	0.42
1:0:61:G:C2	1:0:62:C:C2	3.08	0.41
1:0:484:A:C6	1:0:486:A:C6	3.08	0.41
1:0:634:G:O2'	1:0:1358:A:OP1	2.34	0.41
1:0:635:A:H2	38:0:9207:HOH:O	2.02	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.08	0.41
1:0:1543:G:N1	1:0:1641:A:OP2	2.38	0.41
1:0:1836:A:H1'	28:1:1:THR:O	2.20	0.41
1:0:2272:G:OP1	3:A:223:ARG:HD2	2.20	0.41
1:0:2414:A:H1'	38:0:4703:HOH:O	2.19	0.41
17:P:109:ARG:NH1	17:P:119:TYR:CE2	2.88	0.41
1:0:138:U:OP2	1:0:139:C:C5	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:154:C:H2'	1:0:155:C:C6	2.55	0.41
1:0:392:U:C5'	14:M:193:LYS:HB3	2.50	0.41
1:0:843:A:C2	1:0:846:A:C8	3.08	0.41
1:0:1188:A:C5	1:0:1189:A:N1	2.88	0.41
1:0:1352:A:H5''	1:0:1353:C:OP2	2.19	0.41
1:0:1444:G:O2'	1:0:1445:G:H5'	2.19	0.41
1:0:1494:A:H1'	1:0:1495:C:C6	2.55	0.41
8:F:99:THR:HG23	8:F:99:THR:O	2.20	0.41
15:N:87:LEU:HG	15:N:91:ARG:NH1	2.34	0.41
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.41
19:R:113:HIS:HE1	19:R:144:GLU:CD	2.28	0.41
1:0:216:A:N6	1:0:225:G:C2	2.88	0.41
1:0:353:G:C6	1:0:354:A:C6	3.08	0.41
1:0:581:G:H4'	1:0:1254:C:O2'	2.19	0.41
1:0:622:G:P	26:Y:148:GLY:HA3	2.60	0.41
1:0:812:A:H2'	1:0:813:C:H6	1.85	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.55	0.41
1:0:1262:C:H1'	24:W:120:PRO:HG3	2.02	0.41
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.41
1:0:1425:G:O2'	1:0:1426:C:H5'	2.19	0.41
1:0:1433:G:O2'	1:0:1434:A:H5'	2.20	0.41
1:0:1915:U:O2'	1:0:1916:C:H5'	2.20	0.41
1:0:1928:C:H2'	1:0:1929:G:H5'	2.02	0.41
1:0:2250:G:C6	1:0:2251:G:C2	3.08	0.41
1:0:2255:A:N1	1:0:2256:G:C4	2.88	0.41
1:0:2374:A:H2'	1:0:2375:G:C8	2.55	0.41
2:9:3039:U:H2'	2:9:3040:C:OP1	2.21	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.91	0.41
21:T:18:GLU:O	21:T:21:LYS:HE2	2.20	0.41
26:Y:122:ARG:NH2	38:Y:8735:HOH:O	2.53	0.41
1:0:89:G:H4'	38:0:4762:HOH:O	2.20	0.41
1:0:99:A:C8	1:0:100:C:C5	3.09	0.41
1:0:331:A:C6	1:0:332:G:C4	3.08	0.41
1:0:813:C:H3'	38:0:7188:HOH:O	2.20	0.41
1:0:821:U:H4'	38:Z:8631:HOH:O	2.20	0.41
1:0:2335:C:C2	1:0:2350:G:C2	3.09	0.41
1:0:2345:A:N6	38:0:9272:HOH:O	2.53	0.41
1:0:2582:G:H4'	38:K:4440:HOH:O	2.20	0.41
4:B:43:GLY:O	4:B:308:LEU:HD12	2.20	0.41
5:C:19:PRO:CD	5:C:240:LEU:HD22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:35:ALA:N	38:D:5576:HOH:O	2.53	0.41
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.34	0.41
26:Y:151:SER:HB3	26:Y:154:ARG:HB3	2.03	0.41
1:0:184:G:O2'	1:0:185:G:H5'	2.20	0.41
1:0:254:C:N4	1:0:255:A:C6	2.89	0.41
1:0:451:C:C2'	1:0:452:G:H5'	2.51	0.41
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.41
1:0:912:A:C4	1:0:1294:A:C2	3.08	0.41
1:0:1102:C:H5	38:0:3488:HOH:O	2.04	0.41
1:0:1117:A:C2	1:0:1244:U:C2	3.09	0.41
1:0:1180:U:H2'	1:0:1181:A:C8	2.56	0.41
1:0:1427:A:H61	1:0:1440:U:C1'	2.33	0.41
1:0:1447:U:H3'	1:0:1506:U:O2	2.20	0.41
1:0:1773:G:C2'	1:0:1774:G:H5'	2.51	0.41
1:0:2368:A:H8	38:N:8730:HOH:O	2.04	0.41
1:0:2407:G:O2'	1:0:2408:A:H5'	2.19	0.41
1:0:2473:U:O3'	1:0:2474:A:H3'	2.20	0.41
1:0:2768:A:C2'	1:0:2769:C:O4'	2.63	0.41
17:P:114:LEU:HA	17:P:118:GLN:NE2	2.35	0.41
26:Y:144:ARG:HH11	26:Y:144:ARG:HG3	1.85	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
1:0:834:G:H3'	1:0:835:U:H4'	2.02	0.41
1:0:1055:G:O4'	10:H:113:MET:HE1	2.21	0.41
1:0:1196:C:H2'	1:0:1197:G:H5'	2.02	0.41
1:0:1882:C:H2'	1:0:1883:U:C6	2.55	0.41
2:9:3054:A:C5'	38:D:3359:HOH:O	2.69	0.41
3:A:179:MET:HG2	3:A:186:TRP:CG	2.55	0.41
4:B:260:HIS:HE1	38:B:8783:HOH:O	2.02	0.41
4:B:329:TYR:HE2	22:U:15:PRO:HG2	1.81	0.41
14:M:48:LYS:HE3	14:M:52:GLN:NE2	2.36	0.41
26:Y:189:ASN:C	26:Y:189:ASN:ND2	2.78	0.41
1:0:111:C:H2'	1:0:112:G:C5'	2.51	0.41
1:0:189:A:OP1	14:M:171:ARG:NH2	2.53	0.41
1:0:365:G:C5	1:0:366:U:C5	3.09	0.41
1:0:731:U:C2	1:0:732:C:C5	3.09	0.41
1:0:1191:A:H2'	1:0:1193:A:H5'	2.03	0.41
1:0:1241:G:N3	11:J:86:MET:HE2	2.35	0.41
1:0:1747:A:C8	12:K:44:LEU:HD13	2.56	0.41
1:0:1964:U:O2	1:0:1964:U:H2'	2.20	0.41
3:A:135:VAL:HG22	3:A:136:ALA:N	2.36	0.41
4:B:60:SER:HA	4:B:61:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:80:ARG:HA	4:B:186:GLY:O	2.21	0.41
14:M:75:ARG:HE	14:M:75:ARG:HB3	1.76	0.41
16:O:7:LEU:O	16:O:11:ILE:HG13	2.21	0.41
17:P:20:ARG:HH12	17:P:54:LYS:HD3	1.84	0.41
19:R:149:GLU:HA	19:R:150:PRO:HD3	1.86	0.41
20:S:52:VAL:HG22	20:S:66:VAL:HG13	2.02	0.41
22:U:14:GLU:HA	22:U:15:PRO:HD2	1.94	0.41
23:V:31:ARG:NE	38:V:2682:HOH:O	2.53	0.41
24:W:3:ALA:O	24:W:54:PHE:HA	2.19	0.41
26:Y:115:ARG:NE	38:Y:8755:HOH:O	2.53	0.41
1:O:77:G:O2'	1:O:78:G:H5'	2.21	0.41
1:O:263:U:O4'	8:F:59:ILE:HD13	2.21	0.41
1:O:333:G:O2'	1:O:334:G:H5'	2.21	0.41
1:O:1162:G:C6	1:O:1163:G:C6	3.09	0.41
1:O:1195:G:C2	1:O:1205:U:C2	3.08	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.20	0.41
1:O:2102:G:C2	1:O:2104:C:C4	3.09	0.41
1:O:2110:G:H5''	38:O:6390:HOH:O	2.20	0.41
1:O:2524:G:N2	1:O:2526:C:H41	2.18	0.41
1:O:2599:A:C6	1:O:2600:A:N1	2.89	0.41
1:O:2615:U:C5	1:O:2616:G:C6	3.09	0.41
2:9:3076:G:H3'	2:9:3077:A:C5'	2.33	0.41
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.20	0.41
4:B:198:GLU:HA	38:B:8858:HOH:O	2.21	0.41
16:O:49:GLU:HG2	38:O:5191:HOH:O	2.21	0.41
16:O:53:GLN:HG2	16:O:56:GLU:OE1	2.20	0.41
19:R:17:MET:HE1	19:R:19:ARG:NH2	2.35	0.41
1:O:466:A:H2'	1:O:467:G:O4'	2.21	0.41
1:O:665:A:C6	1:O:666:A:C6	3.09	0.41
1:O:731:U:O2'	1:O:732:C:H5'	2.21	0.41
1:O:960:G:C2'	1:O:961:A:OP2	2.69	0.41
1:O:1236:A:C8	11:J:63:ILE:CD1	3.04	0.41
1:O:1746:A:O4'	1:O:1747:A:C2	2.73	0.41
1:O:1945:G:C2'	1:O:1946:C:H5'	2.51	0.41
1:O:1976:G:O2'	1:O:1977:U:H5'	2.21	0.41
1:O:2241:C:H2'	1:O:2242:U:C6	2.55	0.41
1:O:2247:C:O2'	1:O:2248:C:H5'	2.20	0.41
1:O:2296:C:H2'	1:O:2297:U:C6	2.56	0.41
1:O:2437:A:H2'	1:O:2438:G:C8	2.55	0.41
1:O:2503:A:H2	1:O:2517:A:N7	2.18	0.41
1:O:2504:A:H4'	10:H:71:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2526:C:H5''	38:0:7578:HOH:O	2.20	0.41
2:9:3041:C:O4'	6:D:50:VAL:HG22	2.21	0.41
2:9:3065:A:O2'	2:9:3066:G:P	2.79	0.41
3:A:48:ASP:HA	3:A:49:PRO:HD3	1.88	0.41
3:A:126:ALA:HB1	3:A:138:VAL:HG12	2.03	0.41
13:L:143:THR:HG21	38:L:8738:HOH:O	2.21	0.41
15:N:42:HIS:HB3	15:N:62:HIS:CE1	2.56	0.41
19:R:59:PHE:O	19:R:63:ASN:HB3	2.20	0.41
19:R:84:ALA:O	19:R:88:PHE:HD1	2.04	0.41
25:X:30:MET:CE	25:X:58:ALA:HB3	2.46	0.41
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	2.03	0.41
27:Z:47:VAL:HA	27:Z:56:GLN:O	2.21	0.41
31:I:133:THR:N	38:I:5371:HOH:O	2.54	0.41
1:0:66:G:H4'	1:0:69:A:O4'	2.20	0.41
1:0:154:C:C2	1:0:155:C:C5	3.09	0.41
1:0:803:C:O2'	1:0:804:C:H5'	2.21	0.41
1:0:962:C:C1'	15:N:5:ARG:NH1	2.84	0.41
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.54	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
2:9:3037:C:O2'	2:9:3038:A:H5'	2.21	0.41
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.36	0.41
6:D:55:LYS:O	6:D:56:ARG:HB2	2.21	0.41
12:K:98:VAL:HG11	12:K:102:GLU:HA	2.03	0.41
17:P:59:ARG:NH2	17:P:66:GLN:NE2	2.62	0.41
25:X:43:VAL:HG22	25:X:76:ARG:NH1	2.36	0.41
30:3:3:MET:O	30:3:90:PHE:HA	2.21	0.41
1:0:307:G:C2	1:0:309:C:C4	3.09	0.40
1:0:696:C:C2'	1:0:697:G:H5'	2.51	0.40
1:0:724:G:O2'	1:0:725:C:H5'	2.21	0.40
1:0:1024:G:C6	1:0:1025:C:N3	2.90	0.40
1:0:1081:A:H5''	38:0:3145:HOH:O	2.20	0.40
1:0:1586:G:H2'	1:0:1587:U:H6	1.86	0.40
1:0:1857:A:H5''	38:0:6684:HOH:O	2.21	0.40
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.21	0.40
1:0:2686:C:H1'	38:0:7593:HOH:O	2.22	0.40
38:0:6510:HOH:O	18:Q:3:SER:HB3	2.20	0.40
3:A:144:GLU:HG2	3:A:145:MET:N	2.36	0.40
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.50	0.40
4:B:146:THR:C	4:B:148:PRO:HD3	2.46	0.40
6:D:67:ASP:HA	6:D:68:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:132:LEU:HD23	11:J:132:LEU:HA	1.88	0.40
17:P:13:VAL:HG11	17:P:40:VAL:HG11	2.03	0.40
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.57	0.40
1:0:503:G:H2'	1:0:504:G:H8	1.86	0.40
1:0:626:U:C4	1:0:627:G:C6	3.09	0.40
1:0:800:G:H4'	38:0:7041:HOH:O	2.21	0.40
1:0:1587:U:O2'	1:0:1588:G:H5'	2.21	0.40
1:0:1735:C:OP2	4:B:234:ARG:HG3	2.20	0.40
1:0:2582:G:H5''	4:B:3:PRO:HB3	2.02	0.40
1:0:2659:U:H4'	19:R:76:ASP:HB3	2.03	0.40
1:0:2716:G:H5'	4:B:262:ARG:HG3	2.02	0.40
1:0:2780:C:H2'	1:0:2781:U:C6	2.57	0.40
1:0:2842:G:H5'	19:R:68:HIS:O	2.21	0.40
2:9:3042:C:C5'	2:9:3043:G:OP2	2.68	0.40
2:9:3065:A:C5	2:9:3113:C:C5	3.09	0.40
3:A:167:LYS:HE3	27:Z:26:VAL:HA	2.03	0.40
5:C:193:LEU:HD13	5:C:222:ASP:HB2	2.04	0.40
7:E:108:LEU:HD12	7:E:108:LEU:HA	1.94	0.40
11:J:74:ARG:NH1	11:J:105:LEU:HD11	2.35	0.40
31:I:101:SER:O	31:I:105:VAL:HG23	2.21	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.22	0.40
1:0:461:C:H2'	38:0:5831:HOH:O	2.21	0.40
1:0:682:A:H2'	1:0:683:G:O4'	2.21	0.40
1:0:805:G:N2	1:0:807:A:H3'	2.36	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.56	0.40
1:0:1207:A:C8	1:0:1208:C:C5	3.10	0.40
1:0:1393:A:H2'	1:0:1394:C:C6	2.56	0.40
1:0:1416:G:C2'	1:0:1417:G:H5'	2.51	0.40
1:0:2599:A:C6	1:0:2600:A:C6	3.09	0.40
38:0:4065:HOH:O	14:M:97:ILE:HB	2.20	0.40
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.22	0.40
12:K:59:LYS:HA	38:K:5358:HOH:O	2.20	0.40
17:P:103:THR:HA	17:P:106:ARG:CZ	2.52	0.40
25:X:21:PRO:HG2	25:X:24:LYS:HD3	2.02	0.40
1:0:68:U:O2'	1:0:69:A:H5''	2.21	0.40
1:0:541:C:C2'	1:0:542:A:C5'	2.83	0.40
1:0:588:G:O6	24:W:154:ARG:NH1	2.54	0.40
1:0:599:G:H2'	1:0:600:G:H8	1.87	0.40
1:0:820:G:H5'	1:0:821:U:C5'	2.50	0.40
1:0:1684:A:H1'	29:2:43:ARG:NH2	2.22	0.40
1:0:1976:G:H1'	1:0:2005:G:N2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.56	0.40
1:0:2589:U:H2'	1:0:2590:U:C6	2.57	0.40
2:9:3057:A:N6	38:9:3535:HOH:O	2.46	0.40
3:A:76:VAL:HG23	27:Z:63:LYS:HB3	2.04	0.40
4:B:26:PHE:HE1	38:B:8848:HOH:O	2.04	0.40
4:B:41:PHE:HB3	4:B:190:MET:CE	2.51	0.40
7:E:69:ILE:HA	7:E:72:MET:CE	2.51	0.40
15:N:163:PHE:O	15:N:164:ASP:O	2.40	0.40
21:T:89:ARG:O	21:T:89:ARG:HG3	2.22	0.40
27:Z:42:CYS:O	27:Z:44:GLU:N	2.53	0.40
1:0:366:U:H2'	1:0:367:G:O4'	2.21	0.40
1:0:484:A:N6	1:0:486:A:C6	2.89	0.40
1:0:921:G:H4'	1:0:924:G:N1	2.36	0.40
1:0:1139:U:H2'	1:0:1140:C:C6	2.57	0.40
1:0:1195:G:N2	1:0:1205:U:C2	2.89	0.40
1:0:1460:G:OP1	3:A:17:ARG:NH1	2.54	0.40
1:0:1592:G:O2'	1:0:1593:C:O5'	2.37	0.40
1:0:1634:G:C5	1:0:1635:U:C5	3.09	0.40
1:0:1795:G:H2'	1:0:1796:A:O4'	2.21	0.40
1:0:1889:C:O2	1:0:2010:A:H2	2.05	0.40
1:0:1972:U:C2'	1:0:1973:A:C5'	3.00	0.40
1:0:2415:A:N3	15:N:26:LEU:HD13	2.37	0.40
2:9:3056:A:C3'	2:9:3057:A:H5''	2.50	0.40
8:F:57:GLU:HB2	14:M:23:LEU:HD11	2.04	0.40
11:J:6:PHE:HB3	11:J:109:TYR:OH	2.21	0.40
12:K:78:LYS:HA	12:K:79:PRO:HD3	1.95	0.40
12:K:130:MET:SD	22:U:25:ASP:O	2.80	0.40
15:N:169:PRO:O	15:N:172:PHE:HB3	2.21	0.40
27:Z:33:MET:HG3	27:Z:69:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/239 (98%)	209 (89%)	23 (10%)	3 (1%)	9	25
4	B	335/337 (99%)	305 (91%)	24 (7%)	6 (2%)	6	18
5	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	30	54
6	D	134/177 (76%)	107 (80%)	23 (17%)	4 (3%)	3	8
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	14	35
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	143 (92%)	9 (6%)	4 (3%)	4	11
11	J	140/145 (97%)	128 (91%)	11 (8%)	1 (1%)	18	41
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	24	48
15	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	7	20
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	9	23
18	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	29
19	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	18	41
20	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	9	25
21	T	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
22	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
23	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	7	20
24	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	9	25
25	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	4	11
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	58 (82%)	9 (13%)	4 (6%)	1	2
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
31	I	68/162 (42%)	65 (96%)	3 (4%)	0	100	100
All	All	3705/4418 (84%)	3435 (93%)	232 (6%)	38 (1%)	12	32

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	137	PRO
6	D	173	GLU
8	F	101	ALA
10	H	166	SER
10	H	168	ALA
15	N	154	LEU
15	N	164	ASP
24	W	77	ALA
25	X	87	ALA
27	Z	81	ARG
3	A	34	ASP
3	A	36	ASP
6	D	27	ILE
10	H	16	ARG
10	H	140	VAL
11	J	5	GLU
15	N	139	TRP
17	P	117	SER
4	B	185	GLY
17	P	116	SER
3	A	27	LEU
4	B	138	GLY
4	B	169	GLY
4	B	206	THR
5	C	201	SER
24	W	76	ASP
27	Z	42	CYS
4	B	2	GLN
4	B	34	GLY
20	S	58	MET
27	Z	36	ASP
27	Z	43	GLY
14	M	88	VAL
18	Q	18	PRO
6	D	28	GLY
19	R	81	PRO
23	V	43	PRO
25	X	70	ILE

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	168 (94%)	11 (6%)	17	40
4	B	282/282 (100%)	263 (93%)	19 (7%)	15	36
5	C	193/193 (100%)	173 (90%)	20 (10%)	7	17
6	D	117/148 (79%)	112 (96%)	5 (4%)	26	54
7	E	152/156 (97%)	147 (97%)	5 (3%)	33	63
8	F	93/94 (99%)	90 (97%)	3 (3%)	34	64
9	G	27/283 (10%)	26 (96%)	1 (4%)	30	59
10	H	132/138 (96%)	126 (96%)	6 (4%)	24	52
11	J	118/121 (98%)	110 (93%)	8 (7%)	14	35
12	K	106/106 (100%)	104 (98%)	2 (2%)	50	77
13	L	113/127 (89%)	109 (96%)	4 (4%)	32	61
14	M	158/158 (100%)	151 (96%)	7 (4%)	25	53
15	N	149/150 (99%)	142 (95%)	7 (5%)	23	51
16	O	93/94 (99%)	89 (96%)	4 (4%)	26	54
17	P	113/117 (97%)	109 (96%)	4 (4%)	32	61
18	Q	79/80 (99%)	78 (99%)	1 (1%)	61	83
19	R	117/122 (96%)	112 (96%)	5 (4%)	26	54
20	S	71/74 (96%)	68 (96%)	3 (4%)	26	55
21	T	105/106 (99%)	101 (96%)	4 (4%)	29	58
22	U	44/52 (85%)	42 (96%)	2 (4%)	24	52
23	V	51/57 (90%)	50 (98%)	1 (2%)	48	76
24	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
25	X	66/74 (89%)	62 (94%)	4 (6%)	17	40
26	Y	120/196 (61%)	115 (96%)	5 (4%)	26	55
27	Z	60/60 (100%)	58 (97%)	2 (3%)	33	63
28	1	46/47 (98%)	45 (98%)	1 (2%)	45	74
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	72
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	71
31	I	58/130 (45%)	56 (97%)	2 (3%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3093/3601 (86%)	2947 (95%)	146 (5%)	23 51

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	64	ASP
3	A	69	LEU
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	49	THR
4	B	51	VAL
4	B	53	LEU
4	B	56	ASP
4	B	97	LEU
4	B	98	THR
4	B	171	VAL
4	B	175	LEU
4	B	190	MET
4	B	195	ARG
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	257	THR
4	B	280	VAL
5	C	2	GLN
5	C	27	ARG
5	C	73	LEU
5	C	76	ARG
5	C	78	ARG
5	C	115	LEU
5	C	131	PHE

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Mol	Chain	Res	Type
5	C	135	GLU
5	C	136	VAL
5	C	151	GLN
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	237	GLU
5	C	240	LEU
5	C	243	VAL
6	D	24	HIS
6	D	50	VAL
6	D	69	ILE
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	16	ASP
7	E	36	PRO
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	60	VAL
8	F	65	GLU
9	G	64	ASN
10	H	1	LYS
10	H	30	GLN
10	H	62	LEU
10	H	84	LYS
10	H	88	ARG
10	H	154	TYR
11	J	7	ASP
11	J	32	ASP
11	J	39	VAL
11	J	45	VAL
11	J	46	ILE
11	J	52	GLN
11	J	127	ILE
11	J	131	THR
12	K	10	GLN

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Mol	Chain	Res	Type
12	K	98	VAL
13	L	99	GLU
13	L	101	ASP
13	L	104	ASP
13	L	114	VAL
14	M	23	LEU
14	M	46	LEU
14	M	81	ARG
14	M	93	ARG
14	M	99	ARG
14	M	120	VAL
14	M	164	THR
15	N	26	LEU
15	N	47	LEU
15	N	49	THR
15	N	50	LEU
15	N	53	ASN
15	N	127	LEU
15	N	135	VAL
16	O	3	THR
16	O	43	VAL
16	O	67	SER
16	O	98	LEU
17	P	16	VAL
17	P	21	VAL
17	P	98	ILE
17	P	110	ASP
18	Q	16	ASN
19	R	13	THR
19	R	39	THR
19	R	55	GLN
19	R	82	GLU
19	R	143	VAL
20	S	10	VAL
20	S	12	GLU
20	S	71	ASP
21	T	26	THR
21	T	39	ASN
21	T	96	VAL
21	T	112	LEU
22	U	52	THR
22	U	54	THR

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Mol	Chain	Res	Type
23	V	12	THR
24	W	13	MET
24	W	26	ILE
24	W	52	VAL
24	W	73	LEU
24	W	142	ASP
24	W	146	ILE
24	W	154	ARG
25	X	49	ARG
25	X	66	THR
25	X	72	VAL
25	X	82	GLU
26	Y	154	ARG
26	Y	163	THR
26	Y	189	ASN
26	Y	203	VAL
26	Y	235	GLU
27	Z	36	ASP
27	Z	60	CYS
28	1	25	LYS
29	2	31	ARG
30	3	3	MET
30	3	14	CYS
31	I	113	HIS
31	I	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	176	HIS
3	A	188	ASN
3	A	199	HIS
3	A	218	ASN
4	B	27	ASN
4	B	55	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	243	ASN
4	B	256	GLN
4	B	260	HIS

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Mol	Chain	Res	Type
4	B	320	GLN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	47	GLN
6	D	103	ASN
6	D	133	ASN
7	E	55	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
8	F	55	GLN
9	G	64	ASN
10	H	31	HIS
10	H	46	GLN
10	H	56	GLN
10	H	72	HIS
10	H	128	GLN
10	H	170	ASN
11	J	29	GLN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	67	GLN
13	L	18	HIS
13	L	41	HIS
13	L	42	ASN
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	22	GLN
15	N	53	ASN
15	N	93	GLN
15	N	107	ASN
15	N	132	ASN
16	O	100	GLN
17	P	50	GLN
17	P	66	GLN
17	P	118	GLN
18	Q	40	HIS
19	R	22	GLN

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Mol	Chain	Res	Type
19	R	94	ASN
19	R	98	ASN
19	R	113	HIS
19	R	117	HIS
19	R	122	GLN
20	S	9	HIS
20	S	25	GLN
20	S	53	ASN
20	S	55	GLN
21	T	39	ASN
21	T	73	HIS
22	U	39	ASN
23	V	4	HIS
23	V	60	GLN
24	W	14	HIS
24	W	25	ASN
24	W	27	HIS
24	W	28	HIS
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	36	HIS
25	X	40	HIS
26	Y	119	GLN
26	Y	133	HIS
26	Y	134	HIS
26	Y	149	GLN
26	Y	153	GLN
26	Y	189	ASN
27	Z	37	HIS
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	37	HIS
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	20	HIS
30	3	30	GLN
30	3	39	GLN

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Mol	Chain	Res	Type
30	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	242 (8%)	35 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	260 (9%)	36 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U

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Mol	Chain	Res	Type
1	0	309	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	630	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	699	C
1	0	701	U
1	0	705	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	870	G
1	0	871	G
1	0	872	U

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Mol	Chain	Res	Type
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G

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Mol	Chain	Res	Type
1	0	1246	A
1	0	1247	A
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1419	U
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1507	C
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1562	C
1	0	1592	G
1	0	1605	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A

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Mol	Chain	Res	Type
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2346	C
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U

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Mol	Chain	Res	Type
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A

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Mol	Chain	Res	Type
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3034	A
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	169	A
1	0	284	C
1	0	603	A
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1120	U
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A

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Mol	Chain	Res	Type
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1667	A
1	0	1685	A
1	0	1730	G
1	0	1856	C
1	0	1878	G
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2850	C
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	1MA	0	628	35,1	21,25,26	0.72	1 (4%)	30,37,40	0.71	1 (3%)
1	OMU	0	2587	1	19,22,23	0.32	0	25,31,34	0.43	0
1	PSU	0	2621	1	18,21,22	1.56	2 (11%)	21,30,33	1.40	3 (14%)
1	OMG	0	2588	1	23,26,27	0.29	0	32,38,41	0.37	0
1	UR3	0	2619	1	19,22,23	0.45	0	26,32,35	0.71	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	0	628	35,1	-	2/7/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.33	1.43	1.36
1	0	628	1MA	C6-N6	2.45	1.33	1.28
1	0	2621	PSU	C6-C5	2.26	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.77	120.72	118.17
1	0	2621	PSU	C6-N1-C2	-3.03	119.88	122.69
1	0	2621	PSU	O2-C2-N1	3.00	125.88	122.79
1	0	628	1MA	N1-C2-N3	2.82	129.34	126.00
1	0	2619	UR3	C4-N3-C2	2.79	126.82	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 230 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	GIR	0	9000	-	8,12,12	1.26	0	8,16,16	2.26	2 (25%)

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
32	GIR	0	9000	-	-	0/8/10/10	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	GIR	C6-C8-N9	-4.24	107.00	111.46
32	0	9000	GIR	C8-C6-N7	3.82	110.56	105.61

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, 95th 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 ²)	Q<0.9
1	0	2749/2922 (94%)	-0.31	53 (1%) 66 63	24, 49, 93, 153	0
2	9	122/122 (100%)	0.18	5 (4%) 41 37	38, 64, 91, 149	0
3	A	237/239 (99%)	0.31	9 (3%) 44 40	30, 58, 99, 119	0
4	B	337/337 (100%)	0.19	2 (0%) 85 85	28, 56, 84, 95	0
5	C	246/246 (100%)	0.14	3 (1%) 76 75	25, 49, 74, 80	0
6	D	140/177 (79%)	1.54	43 (30%) 1 1	61, 105, 127, 136	0
7	E	172/178 (96%)	0.52	10 (5%) 29 25	46, 68, 87, 93	0
8	F	119/120 (99%)	0.81	7 (5%) 28 25	53, 78, 99, 117	0
9	G	29/348 (8%)	1.44	8 (27%) 1 1	77, 94, 105, 107	0
10	H	160/171 (93%)	0.26	7 (4%) 39 35	40, 58, 92, 100	0
11	J	142/145 (97%)	0.14	4 (2%) 55 51	35, 50, 74, 90	0
12	K	132/132 (100%)	0.25	1 (0%) 82 81	36, 54, 77, 87	0
13	L	145/165 (87%)	0.72	17 (11%) 9 7	29, 71, 118, 130	0
14	M	194/194 (100%)	-0.01	3 (1%) 72 70	35, 47, 63, 73	0
15	N	186/187 (99%)	0.79	22 (11%) 9 7	41, 68, 115, 120	0
16	O	115/116 (99%)	0.39	2 (1%) 69 67	41, 57, 75, 80	0
17	P	143/149 (95%)	0.34	3 (2%) 63 61	43, 59, 78, 83	0
18	Q	95/96 (98%)	-0.07	0 100 100	37, 48, 62, 78	0
19	R	150/155 (96%)	-0.13	0 100 100	33, 47, 66, 74	0
20	S	81/85 (95%)	0.28	2 (2%) 58 55	47, 67, 87, 94	0
21	T	119/120 (99%)	0.34	2 (1%) 69 67	41, 61, 88, 108	0
22	U	53/66 (80%)	0.36	1 (1%) 66 63	44, 61, 77, 83	0
23	V	65/71 (91%)	1.12	8 (12%) 8 7	60, 84, 118, 121	0
24	W	154/154 (100%)	-0.01	0 100 100	34, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.46	6 (7%) 21 18	45, 61, 87, 102	0
26	Y	142/241 (58%)	0.01	4 (2%) 55 51	28, 47, 71, 92	0
27	Z	73/73 (100%)	2.20	40 (54%) 0 0	61, 98, 111, 115	0
28	1	56/57 (98%)	-0.44	0 100 100	29, 37, 43, 50	0
29	2	46/50 (92%)	0.72	6 (13%) 7 6	39, 68, 101, 114	0
30	3	92/92 (100%)	0.29	1 (1%) 78 76	40, 62, 75, 83	0
31	I	70/162 (43%)	2.24	36 (51%) 0 0	105, 124, 141, 141	0
All	All	6646/7462 (89%)	0.11	305 (4%) 37 34	24, 55, 105, 153	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	I	133	THR	7.5
27	Z	26	VAL	7.3
23	V	1	THR	7.2
6	D	10	PHE	6.0
14	M	194	ALA	5.4
6	D	63	ILE	5.3
27	Z	14	PHE	5.2
2	9	3002	U	5.2
27	Z	34	ASN	5.2
3	A	37	VAL	5.2
6	D	174	VAL	5.1
27	Z	29	ILE	4.9
27	Z	16	ALA	4.7
27	Z	21	VAL	4.7
27	Z	12	GLY	4.7
13	L	82	ALA	4.6
1	0	1171	A	4.5
1	0	1175	G	4.4
15	N	168	LEU	4.4
7	E	10	ASP	4.3
31	I	76	ALA	4.2
6	D	101	THR	4.2
15	N	154	LEU	4.2
1	0	138	U	4.2
27	Z	22	SER	4.1
23	V	2	VAL	4.1
15	N	169	PRO	4.1
27	Z	11	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	0	1173	A	4.0
2	9	3001	U	4.0
31	I	102	VAL	4.0
27	Z	18	TYR	4.0
27	Z	20	ARG	3.9
9	G	27	ILE	3.9
31	I	96	PHE	3.9
31	I	88	GLY	3.9
1	0	10	U	3.8
23	V	40	PRO	3.8
31	I	93	GLN	3.8
31	I	117	LEU	3.7
23	V	39	ALA	3.7
1	0	1161	A	3.7
31	I	90	GLY	3.7
13	L	148	GLU	3.6
13	L	81	VAL	3.6
3	A	36	ASP	3.6
15	N	148	ALA	3.6
27	Z	23	ARG	3.5
27	Z	27	ALA	3.5
9	G	63	ARG	3.5
31	I	78	LEU	3.5
10	H	169	GLY	3.4
27	Z	10	ARG	3.4
27	Z	30	GLU	3.4
2	9	3023	U	3.4
9	G	12	ILE	3.4
21	T	119	ALA	3.4
1	0	2344	G	3.4
4	B	1	PRO	3.4
31	I	139	ILE	3.3
31	I	137	VAL	3.3
1	0	1176	C	3.3
27	Z	13	ARG	3.3
25	X	85	VAL	3.3
27	Z	40	PRO	3.2
31	I	135	LEU	3.2
1	0	1192	A	3.2
6	D	35	ALA	3.2
31	I	109	ALA	3.2
23	V	43	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
10	H	168	ALA	3.2
31	I	119	TYR	3.2
31	I	138	THR	3.2
1	0	1204	C	3.1
25	X	87	ALA	3.1
10	H	111	ASP	3.1
1	0	2345	A	3.1
27	Z	19	GLY	3.1
2	9	3024	U	3.1
6	D	11	HIS	3.1
15	N	167	ASP	3.1
31	I	113	HIS	3.1
6	D	66	GLY	3.1
6	D	44	ILE	3.1
13	L	150	GLN	3.0
27	Z	43	GLY	3.0
31	I	87	THR	3.0
27	Z	17	ARG	3.0
15	N	165	ALA	3.0
1	0	1193	A	3.0
15	N	1	ALA	3.0
25	X	83	ALA	3.0
1	0	1172	G	3.0
27	Z	44	GLU	2.9
10	H	170	ASN	2.9
15	N	147	ILE	2.9
15	N	161	GLY	2.9
13	L	99	GLU	2.9
1	0	1177	A	2.9
27	Z	41	ASN	2.9
15	N	159	TYR	2.9
31	I	79	ILE	2.9
6	D	107	GLY	2.9
13	L	83	GLU	2.9
29	2	42	TRP	2.9
1	0	1166	A	2.9
1	0	960	G	2.9
9	G	73	ASP	2.9
27	Z	39	CYS	2.9
1	0	735	C	2.9
8	F	99	THR	2.9
1	0	1951	G	2.9

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Mol	Chain	Res	Type	RSRZ
13	L	89	PHE	2.9
8	F	90	GLU	2.8
21	T	1	SER	2.8
31	I	118	SER	2.8
6	D	40	ILE	2.8
9	G	71	LEU	2.8
1	0	1202	A	2.8
25	X	88	GLU	2.8
1	0	1167	G	2.8
6	D	59	GLY	2.8
1	0	1199	A	2.8
31	I	106	LYS	2.8
15	N	145	ALA	2.8
15	N	160	SER	2.8
11	J	76	ASP	2.8
13	L	78	ALA	2.8
6	D	172	VAL	2.7
6	D	75	LEU	2.7
13	L	145	LEU	2.7
6	D	26	GLY	2.7
17	P	143	ALA	2.7
1	0	2637	A	2.7
3	A	211	LYS	2.7
27	Z	59	TYR	2.7
27	Z	15	GLY	2.7
10	H	40	ALA	2.7
15	N	166	ALA	2.7
1	0	970	U	2.7
31	I	82	GLU	2.7
8	F	101	ALA	2.7
31	I	95	ASP	2.7
31	I	100	LEU	2.6
31	I	132	CYS	2.6
29	2	49	GLU	2.6
17	P	116	SER	2.6
15	N	157	PRO	2.6
1	0	1561	U	2.6
2	9	3025	G	2.6
11	J	4	ALA	2.6
31	I	72	VAL	2.6
1	0	999	C	2.6
1	0	1130	U	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1160	G	2.6
1	0	2249	G	2.6
8	F	91	VAL	2.6
27	Z	82	SER	2.6
9	G	26	MET	2.6
6	D	90	LEU	2.6
11	J	62	ASP	2.5
27	Z	61	ASP	2.5
7	E	154	ILE	2.5
3	A	237	GLY	2.5
7	E	13	ALA	2.5
11	J	70	PHE	2.5
27	Z	33	MET	2.5
27	Z	31	SER	2.5
6	D	69	ILE	2.5
15	N	150	TYR	2.5
3	A	32	VAL	2.5
13	L	91	VAL	2.5
31	I	105	VAL	2.5
8	F	28	ALA	2.5
31	I	125	ALA	2.5
29	2	38	LYS	2.5
6	D	100	ASP	2.5
1	0	1524	U	2.5
6	D	12	GLU	2.5
29	2	47	THR	2.4
23	V	45	ARG	2.4
5	C	166	ILE	2.4
1	0	2251	G	2.4
22	U	37	GLU	2.4
1	0	1169	U	2.4
6	D	56	ARG	2.4
6	D	18	ILE	2.4
6	D	128	LEU	2.4
15	N	158	LEU	2.4
1	0	1279	U	2.4
23	V	36	ALA	2.4
30	3	8	ASN	2.4
31	I	129	VAL	2.4
7	E	87	PHE	2.4
1	0	1198	U	2.4
7	E	126	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
7	E	53	GLU	2.4
27	Z	32	GLU	2.4
6	D	13	MET	2.4
3	A	31	LYS	2.4
20	S	44	GLN	2.4
8	F	47	LEU	2.3
6	D	27	ILE	2.3
1	0	1170	U	2.3
15	N	149	GLU	2.3
1	0	368	C	2.3
10	H	167	PRO	2.3
14	M	125	ARG	2.3
15	N	186	LEU	2.3
1	0	1174	A	2.3
1	0	1181	A	2.3
31	I	77	GLU	2.3
1	0	2250	G	2.3
13	L	97	VAL	2.3
31	I	124	ALA	2.3
8	F	26	THR	2.3
13	L	102	ASP	2.3
6	D	17	ARG	2.3
6	D	58	VAL	2.3
25	X	84	ILE	2.3
6	D	57	THR	2.3
26	Y	235	GLU	2.3
7	E	170	ARG	2.3
16	O	23	GLY	2.3
7	E	11	VAL	2.3
4	B	57	GLU	2.2
27	Z	28	GLU	2.2
27	Z	35	GLU	2.2
27	Z	62	TYR	2.2
26	Y	216	ARG	2.2
5	C	16	VAL	2.2
3	A	38	ILE	2.2
27	Z	37	HIS	2.2
31	I	140	GLU	2.2
15	N	164	ASP	2.2
1	0	2254	G	2.2
26	Y	187	VAL	2.2
26	Y	236	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
5	C	135	GLU	2.2
9	G	65	THR	2.2
31	I	92	PRO	2.2
6	D	53	LYS	2.2
6	D	62	ASP	2.2
15	N	162	ASP	2.2
31	I	134	SER	2.2
27	Z	47	VAL	2.2
25	X	77	PHE	2.2
29	2	35	ARG	2.2
1	0	1559	A	2.2
6	D	158	ASN	2.2
12	K	119	GLN	2.2
6	D	138	GLY	2.2
7	E	128	GLY	2.2
6	D	171	ASP	2.2
6	D	96	SER	2.2
27	Z	58	SER	2.2
10	H	171	ALA	2.1
1	0	1165	G	2.1
1	0	1190	G	2.1
1	0	1203	G	2.1
6	D	159	PRO	2.1
9	G	13	PRO	2.1
6	D	154	LYS	2.1
13	L	149	ARG	2.1
1	0	1168	C	2.1
6	D	134	LEU	2.1
23	V	44	GLY	2.1
7	E	156	ASP	2.1
6	D	61	PHE	2.1
6	D	165	PHE	2.1
1	0	734	U	2.1
17	P	77	ALA	2.1
1	0	2769	C	2.1
6	D	166	ILE	2.1
3	A	60	PHE	2.1
13	L	80	ASP	2.1
20	S	1	SER	2.1
14	M	22	GLU	2.1
29	2	44	ARG	2.1
1	0	1162	G	2.1

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Mol	Chain	Res	Type	RSRZ
15	N	139	TRP	2.1
1	0	1964	U	2.1
1	0	2252	A	2.1
1	0	2664	A	2.1
6	D	95	THR	2.1
31	I	114	PRO	2.1
3	A	88	ILE	2.1
13	L	105	TYR	2.1
6	D	21	VAL	2.1
27	Z	45	ASP	2.0
16	O	24	ALA	2.0
6	D	25	MET	2.0
1	0	128	A	2.0
1	0	285	A	2.0
31	I	71	GLY	2.0
27	Z	46	ARG	2.0
27	Z	81	ARG	2.0
13	L	104	ASP	2.0
31	I	94	GLU	2.0
1	0	87	C	2.0
13	L	118	LEU	2.0
15	N	184	ILE	2.0
6	D	76	ARG	2.0
27	Z	24	ARG	2.0
6	D	170	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UR3	0	2619	21/22	0.97	0.06	36,39,42,48	0
1	OMU	0	2587	21/22	0.98	0.06	34,36,37,39	0
1	OMG	0	2588	24/25	0.98	0.06	33,36,38,39	0
1	1MA	0	628	23/24	0.98	0.06	28,32,33,35	0
1	PSU	0	2621	20/21	0.98	0.05	28,30,33,34	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8049	1/1	0.67	0.24	92,92,92,92	0
35	NA	0	8566	1/1	0.67	0.26	66,66,66,66	0
35	NA	0	8568	1/1	0.68	0.24	71,71,71,71	0
33	MG	9	8095	1/1	0.71	0.15	76,76,76,76	0
35	NA	9	8551	1/1	0.73	0.25	50,50,50,50	0
35	NA	0	8524	1/1	0.76	0.31	62,62,62,62	0
35	NA	0	8529	1/1	0.78	0.17	77,77,77,77	0
35	NA	R	8586	1/1	0.80	0.63	95,95,95,95	0
35	NA	0	8577	1/1	0.81	0.27	71,71,71,71	0
35	NA	0	8540	1/1	0.82	0.13	58,58,58,58	0
33	MG	0	8087	1/1	0.83	0.13	66,66,66,66	0
35	NA	0	8582	1/1	0.83	0.23	79,79,79,79	0
35	NA	0	8584	1/1	0.84	0.12	62,62,62,62	0
33	MG	0	8090	1/1	0.84	0.26	69,69,69,69	0
35	NA	9	8583	1/1	0.84	0.18	65,65,65,65	0
35	NA	0	8526	1/1	0.84	0.14	58,58,58,58	0
35	NA	0	8571	1/1	0.86	0.34	65,65,65,65	0
35	NA	0	8508	1/1	0.86	0.16	56,56,56,56	0
35	NA	0	8585	1/1	0.86	0.28	51,51,51,51	0
33	MG	0	8114	1/1	0.87	0.17	67,67,67,67	0
35	NA	0	8563	1/1	0.87	0.18	57,57,57,57	0
33	MG	0	8094	1/1	0.88	0.17	77,77,77,77	0
35	NA	0	8533	1/1	0.88	0.15	39,39,39,39	0
35	NA	0	8503	1/1	0.89	0.17	47,47,47,47	0
35	NA	0	8564	1/1	0.89	0.13	53,53,53,53	0
35	NA	0	8570	1/1	0.90	0.38	69,69,69,69	0
32	GIR	0	9000	12/12	0.90	0.15	23,40,50,53	0
35	NA	0	8557	1/1	0.90	0.16	61,61,61,61	0
35	NA	0	8579	1/1	0.90	0.17	64,64,64,64	0
35	NA	0	8534	1/1	0.90	0.17	45,45,45,45	0
35	NA	S	8512	1/1	0.90	0.07	43,43,43,43	0
35	NA	0	8552	1/1	0.91	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8556	1/1	0.91	0.15	49,49,49,49	0
35	NA	0	8505	1/1	0.91	0.11	33,33,33,33	0
33	MG	0	8044	1/1	0.91	0.08	46,46,46,46	0
35	NA	0	8521	1/1	0.91	0.18	61,61,61,61	0
35	NA	0	8541	1/1	0.91	0.10	50,50,50,50	0
35	NA	0	8560	1/1	0.92	0.20	51,51,51,51	0
35	NA	0	8562	1/1	0.92	0.16	60,60,60,60	0
33	MG	0	8043	1/1	0.92	0.09	48,48,48,48	0
33	MG	0	8101	1/1	0.92	0.12	69,69,69,69	0
33	MG	0	8103	1/1	0.92	0.14	82,82,82,82	0
35	NA	0	8567	1/1	0.92	0.17	59,59,59,59	0
33	MG	0	8070	1/1	0.92	0.12	50,50,50,50	0
35	NA	R	8537	1/1	0.92	0.09	48,48,48,48	0
35	NA	0	8532	1/1	0.92	0.15	49,49,49,49	0
35	NA	0	8510	1/1	0.92	0.08	36,36,36,36	0
36	CL	3	8704	1/1	0.92	0.12	71,71,71,71	0
33	MG	0	8046	1/1	0.93	0.10	53,53,53,53	0
35	NA	0	8572	1/1	0.93	0.15	54,54,54,54	0
35	NA	0	8574	1/1	0.93	0.16	66,66,66,66	0
35	NA	C	8504	1/1	0.93	0.06	49,49,49,49	0
33	MG	T	8073	1/1	0.93	0.07	71,71,71,71	0
33	MG	0	8041	1/1	0.93	0.13	56,56,56,56	0
33	MG	0	8096	1/1	0.93	0.06	52,52,52,52	0
36	CL	0	8722	1/1	0.93	0.27	81,81,81,81	0
36	CL	A	8709	1/1	0.93	0.15	77,77,77,77	0
35	NA	0	8555	1/1	0.93	0.16	57,57,57,57	0
35	NA	0	8535	1/1	0.94	0.14	56,56,56,56	0
33	MG	0	8100	1/1	0.94	0.14	66,66,66,66	0
33	MG	0	8092	1/1	0.94	0.12	89,89,89,89	0
35	NA	0	8565	1/1	0.94	0.21	40,40,40,40	0
35	NA	0	8542	1/1	0.94	0.12	47,47,47,47	0
33	MG	0	8102	1/1	0.94	0.10	73,73,73,73	0
33	MG	0	8023	1/1	0.94	0.12	41,41,41,41	0
35	NA	M	8547	1/1	0.94	0.11	34,34,34,34	0
35	NA	0	8569	1/1	0.94	0.15	74,74,74,74	0
35	NA	R	8538	1/1	0.94	0.05	60,60,60,60	0
33	MG	0	8082	1/1	0.94	0.11	63,63,63,63	0
33	MG	0	8116	1/1	0.94	0.06	58,58,58,58	0
36	CL	0	8705	1/1	0.94	0.12	67,67,67,67	0
36	CL	0	8715	1/1	0.94	0.15	86,86,86,86	0
35	NA	0	8559	1/1	0.94	0.22	49,49,49,49	0
35	NA	0	8511	1/1	0.94	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	J	8701	1/1	0.94	0.13	66,66,66,66	0
35	NA	0	8561	1/1	0.94	0.08	56,56,56,56	0
35	NA	0	8502	1/1	0.95	0.08	51,51,51,51	0
33	MG	0	8053	1/1	0.95	0.06	45,45,45,45	0
33	MG	0	8063	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	8506	1/1	0.95	0.16	48,48,48,48	0
33	MG	0	8047	1/1	0.95	0.15	74,74,74,74	0
35	NA	0	8539	1/1	0.95	0.04	30,30,30,30	0
35	NA	A	8545	1/1	0.95	0.08	62,62,62,62	0
33	MG	0	8039	1/1	0.95	0.09	52,52,52,52	0
35	NA	H	8509	1/1	0.95	0.08	39,39,39,39	0
35	NA	J	8546	1/1	0.95	0.06	53,53,53,53	0
33	MG	0	8085	1/1	0.95	0.06	54,54,54,54	0
35	NA	0	8513	1/1	0.95	0.05	62,62,62,62	0
35	NA	0	8550	1/1	0.95	0.09	45,45,45,45	0
33	MG	A	8066	1/1	0.95	0.07	72,72,72,72	0
35	NA	0	8523	1/1	0.95	0.13	43,43,43,43	0
33	MG	B	8055	1/1	0.95	0.05	48,48,48,48	0
36	CL	0	8713	1/1	0.95	0.09	65,65,65,65	0
35	NA	0	8573	1/1	0.95	0.07	69,69,69,69	0
33	MG	0	8050	1/1	0.95	0.05	59,59,59,59	0
35	NA	0	8575	1/1	0.95	0.23	61,61,61,61	0
35	NA	0	8527	1/1	0.95	0.07	44,44,44,44	0
36	CL	J	8702	1/1	0.95	0.07	57,57,57,57	0
35	NA	0	8578	1/1	0.95	0.23	51,51,51,51	0
33	MG	0	8113	1/1	0.96	0.05	53,53,53,53	0
35	NA	0	8530	1/1	0.96	0.07	50,50,50,50	0
34	K	0	8401	1/1	0.96	0.18	85,85,85,85	0
35	NA	0	8558	1/1	0.96	0.23	82,82,82,82	0
33	MG	0	8088	1/1	0.96	0.04	38,38,38,38	0
35	NA	0	8514	1/1	0.96	0.14	38,38,38,38	0
35	NA	0	8516	1/1	0.96	0.09	54,54,54,54	0
35	NA	0	8536	1/1	0.96	0.06	55,55,55,55	0
35	NA	0	8520	1/1	0.96	0.04	34,34,34,34	0
35	NA	0	8581	1/1	0.96	0.06	48,48,48,48	0
33	MG	0	8057	1/1	0.96	0.07	45,45,45,45	0
36	CL	0	8717	1/1	0.96	0.06	65,65,65,65	0
33	MG	0	8051	1/1	0.96	0.09	59,59,59,59	0
33	MG	0	8104	1/1	0.96	0.07	65,65,65,65	0
35	NA	0	8507	1/1	0.96	0.11	59,59,59,59	0
33	MG	0	8112	1/1	0.96	0.09	42,42,42,42	0
36	CL	L	8710	1/1	0.96	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	N	8707	1/1	0.96	0.06	66,66,66,66	0
36	CL	O	8708	1/1	0.96	0.12	73,73,73,73	0
35	NA	0	8553	1/1	0.96	0.06	30,30,30,30	0
33	MG	0	8097	1/1	0.97	0.06	34,34,34,34	0
35	NA	0	8543	1/1	0.97	0.08	39,39,39,39	0
35	NA	0	8544	1/1	0.97	0.04	28,28,28,28	0
35	NA	0	8549	1/1	0.97	0.10	51,51,51,51	0
33	MG	0	8042	1/1	0.97	0.07	38,38,38,38	0
35	NA	0	8531	1/1	0.97	0.07	50,50,50,50	0
36	CL	0	8714	1/1	0.97	0.06	54,54,54,54	0
35	NA	0	8518	1/1	0.97	0.10	42,42,42,42	0
36	CL	0	8716	1/1	0.97	0.14	56,56,56,56	0
33	MG	0	8072	1/1	0.97	0.05	63,63,63,63	0
33	MG	0	8075	1/1	0.97	0.04	44,44,44,44	0
33	MG	0	8076	1/1	0.97	0.05	55,55,55,55	0
33	MG	0	8093	1/1	0.97	0.05	56,56,56,56	0
35	NA	0	8525	1/1	0.97	0.06	56,56,56,56	0
35	NA	H	8522	1/1	0.97	0.26	67,67,67,67	0
33	MG	0	8045	1/1	0.97	0.09	53,53,53,53	0
33	MG	0	8064	1/1	0.97	0.09	30,30,30,30	0
36	CL	Y	8720	1/1	0.97	0.06	46,46,46,46	0
35	NA	Q	8548	1/1	0.97	0.04	42,42,42,42	0
37	CD	O	8605	1/1	0.97	0.06	93,93,93,93	0
35	NA	0	8515	1/1	0.98	0.08	42,42,42,42	0
35	NA	L	8580	1/1	0.98	0.09	57,57,57,57	0
33	MG	0	8117	1/1	0.98	0.03	32,32,32,32	0
35	NA	0	8517	1/1	0.98	0.06	51,51,51,51	0
33	MG	0	8062	1/1	0.98	0.05	54,54,54,54	0
33	MG	0	8098	1/1	0.98	0.08	40,40,40,40	0
33	MG	0	8048	1/1	0.98	0.06	54,54,54,54	0
33	MG	0	8052	1/1	0.98	0.04	54,54,54,54	0
36	CL	0	8703	1/1	0.98	0.07	58,58,58,58	0
33	MG	Y	8109	1/1	0.98	0.06	37,37,37,37	0
36	CL	0	8712	1/1	0.98	0.06	49,49,49,49	0
33	MG	0	8067	1/1	0.98	0.06	52,52,52,52	0
35	NA	0	8576	1/1	0.98	0.09	46,46,46,46	0
35	NA	0	8554	1/1	0.98	0.14	40,40,40,40	0
35	NA	0	8501	1/1	0.98	0.11	32,32,32,32	0
33	MG	0	8089	1/1	0.98	0.06	74,74,74,74	0
35	NA	0	8528	1/1	0.98	0.14	42,42,42,42	0
33	MG	0	8014	1/1	0.98	0.04	32,32,32,32	0
36	CL	B	8719	1/1	0.98	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8106	1/1	0.98	0.03	65,65,65,65	0
33	MG	0	8108	1/1	0.98	0.11	70,70,70,70	0
36	CL	J	8721	1/1	0.98	0.05	58,58,58,58	0
33	MG	0	8110	1/1	0.98	0.04	27,27,27,27	0
33	MG	0	8024	1/1	0.98	0.04	21,21,21,21	0
33	MG	0	8059	1/1	0.98	0.05	43,43,43,43	0
33	MG	0	8061	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8115	1/1	0.98	0.04	52,52,52,52	0
33	MG	0	8081	1/1	0.98	0.05	49,49,49,49	0
33	MG	0	8022	1/1	0.99	0.03	38,38,38,38	0
33	MG	0	8071	1/1	0.99	0.03	69,69,69,69	0
33	MG	0	8011	1/1	0.99	0.07	27,27,27,27	0
33	MG	0	8074	1/1	0.99	0.02	36,36,36,36	0
33	MG	0	8012	1/1	0.99	0.04	39,39,39,39	0
33	MG	0	8025	1/1	0.99	0.02	37,37,37,37	0
33	MG	0	8111	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	8079	1/1	0.99	0.03	37,37,37,37	0
33	MG	0	8080	1/1	0.99	0.06	45,45,45,45	0
33	MG	0	8027	1/1	0.99	0.03	44,44,44,44	0
33	MG	0	8029	1/1	0.99	0.03	35,35,35,35	0
33	MG	0	8084	1/1	0.99	0.04	47,47,47,47	0
33	MG	0	8031	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8086	1/1	0.99	0.04	52,52,52,52	0
33	MG	0	8033	1/1	0.99	0.02	31,31,31,31	0
33	MG	0	8035	1/1	0.99	0.03	46,46,46,46	0
33	MG	B	8056	1/1	0.99	0.03	55,55,55,55	0
33	MG	K	8069	1/1	0.99	0.03	58,58,58,58	0
33	MG	0	8037	1/1	0.99	0.02	43,43,43,43	0
33	MG	0	8058	1/1	0.99	0.04	39,39,39,39	0
33	MG	3	8078	1/1	0.99	0.04	43,43,43,43	0
33	MG	0	8091	1/1	0.99	0.04	51,51,51,51	0
34	K	0	8402	1/1	0.99	0.18	57,57,57,57	0
33	MG	0	8006	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	8060	1/1	0.99	0.07	40,40,40,40	0
33	MG	0	8040	1/1	0.99	0.03	60,60,60,60	0
33	MG	0	8015	1/1	0.99	0.03	35,35,35,35	0
36	CL	M	8718	1/1	0.99	0.05	47,47,47,47	0
33	MG	0	8016	1/1	0.99	0.04	40,40,40,40	0
33	MG	0	8018	1/1	0.99	0.06	50,50,50,50	0
36	CL	Q	8711	1/1	0.99	0.07	55,55,55,55	0
36	CL	R	8706	1/1	0.99	0.04	46,46,46,46	0
33	MG	0	8099	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8021	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8068	1/1	0.99	0.04	61,61,61,61	0
37	CD	Z	8603	1/1	0.99	0.03	98,98,98,98	0
37	CD	1	8602	1/1	0.99	0.05	63,63,63,63	0
37	CD	3	8604	1/1	0.99	0.02	68,68,68,68	0
33	MG	0	8007	1/1	1.00	0.02	22,22,22,22	0
33	MG	0	8038	1/1	1.00	0.02	34,34,34,34	0
33	MG	0	8019	1/1	1.00	0.04	35,35,35,35	0
33	MG	0	8020	1/1	1.00	0.02	33,33,33,33	0
33	MG	A	8065	1/1	1.00	0.03	41,41,41,41	0
33	MG	0	8008	1/1	1.00	0.03	37,37,37,37	0
33	MG	0	8009	1/1	1.00	0.01	35,35,35,35	0
33	MG	0	8010	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8002	1/1	1.00	0.04	34,34,34,34	0
33	MG	0	8003	1/1	1.00	0.03	35,35,35,35	0
33	MG	0	8026	1/1	1.00	0.03	26,26,26,26	0
33	MG	0	8013	1/1	1.00	0.02	38,38,38,38	0
33	MG	0	8028	1/1	1.00	0.02	38,38,38,38	0
33	MG	0	8004	1/1	1.00	0.04	29,29,29,29	0
33	MG	0	8077	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8030	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8005	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8032	1/1	1.00	0.07	28,28,28,28	0
33	MG	0	8107	1/1	1.00	0.02	36,36,36,36	0
33	MG	0	8001	1/1	1.00	0.01	36,36,36,36	0
33	MG	0	8083	1/1	1.00	0.01	43,43,43,43	0
33	MG	0	8054	1/1	1.00	0.02	37,37,37,37	0
37	CD	U	8601	1/1	1.00	0.02	62,62,62,62	0
33	MG	0	8034	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8017	1/1	1.00	0.01	26,26,26,26	0
33	MG	0	8036	1/1	1.00	0.03	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.