



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:08 PM UTC

PDB ID : 1YJN / pdb_00001yjn
Title : Crystal Structure Of Clindamycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-14
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

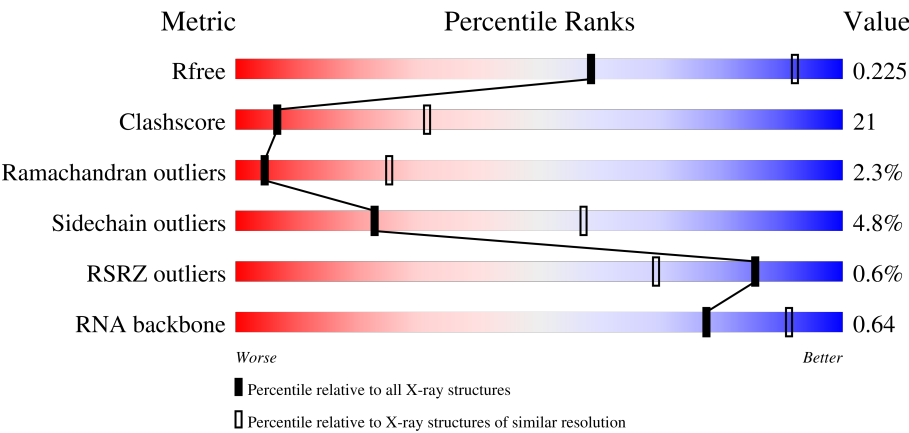
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



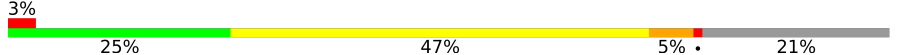
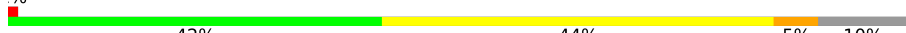
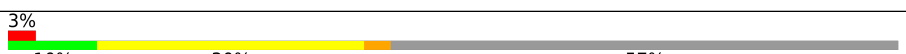
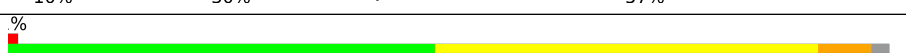
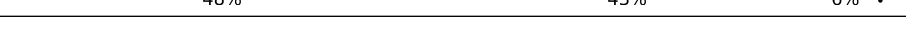
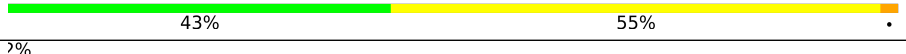
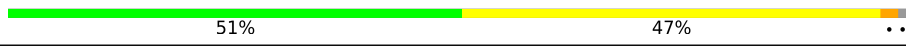
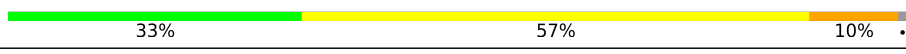
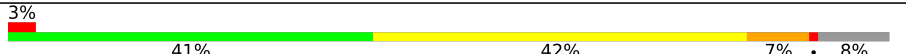
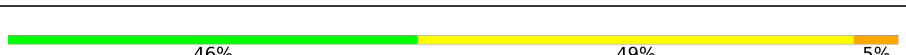
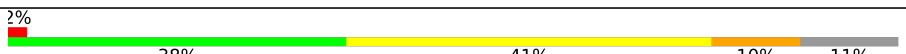
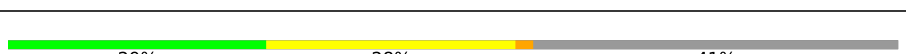
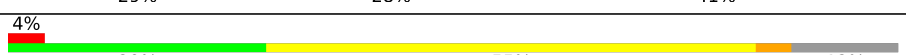
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	52%37%6%6%
2	9	122	2% 39%52%9%
3	A	240	% 50%40%9%
4	B	338	43%49%7%

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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	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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	J	8802	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99060 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
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

- 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
			2599	1160	471	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 L4E.

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

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

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

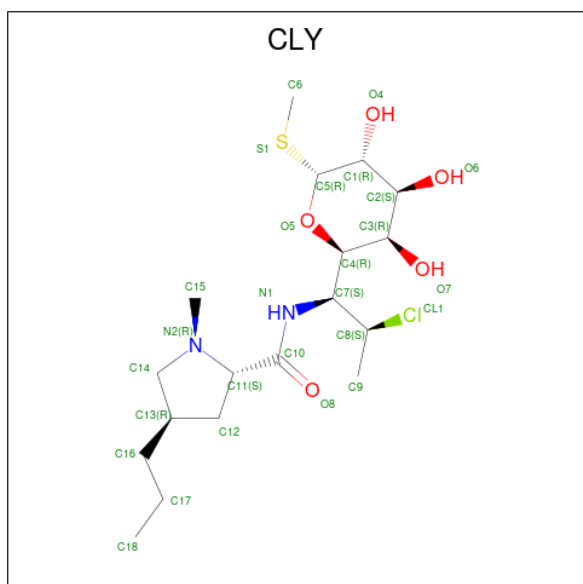
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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

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

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

- Molecule 32 is CLINDAMYCIN (CCD ID: CLY) (formula: $C_{18}H_{33}ClN_2O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	S	0	0
			27	18	1	2	5	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	9	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
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 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5892	Total 5892	O 5892	0	0
38	9	139	Total 139	O 139	0	0
38	A	120	Total 120	O 120	0	0
38	B	146	Total 146	O 146	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	169	Total 169	O 169	0	0
38	D	49	Total 49	O 49	0	0
38	E	41	Total 41	O 41	0	0
38	F	25	Total 25	O 25	0	0
38	G	19	Total 19	O 19	0	0
38	H	68	Total 68	O 68	0	0
38	I	10	Total 10	O 10	0	0
38	J	56	Total 56	O 56	0	0
38	K	60	Total 60	O 60	0	0
38	L	82	Total 82	O 82	0	0
38	M	128	Total 128	O 128	0	0
38	N	64	Total 64	O 64	0	0
38	O	44	Total 44	O 44	0	0
38	P	64	Total 64	O 64	0	0
38	Q	49	Total 49	O 49	0	0
38	R	79	Total 79	O 79	0	0
38	S	31	Total 31	O 31	0	0
38	T	36	Total 36	O 36	0	0
38	U	27	Total 27	O 27	0	0
38	V	14	Total 14	O 14	0	0
38	W	68	Total 68	O 68	0	0

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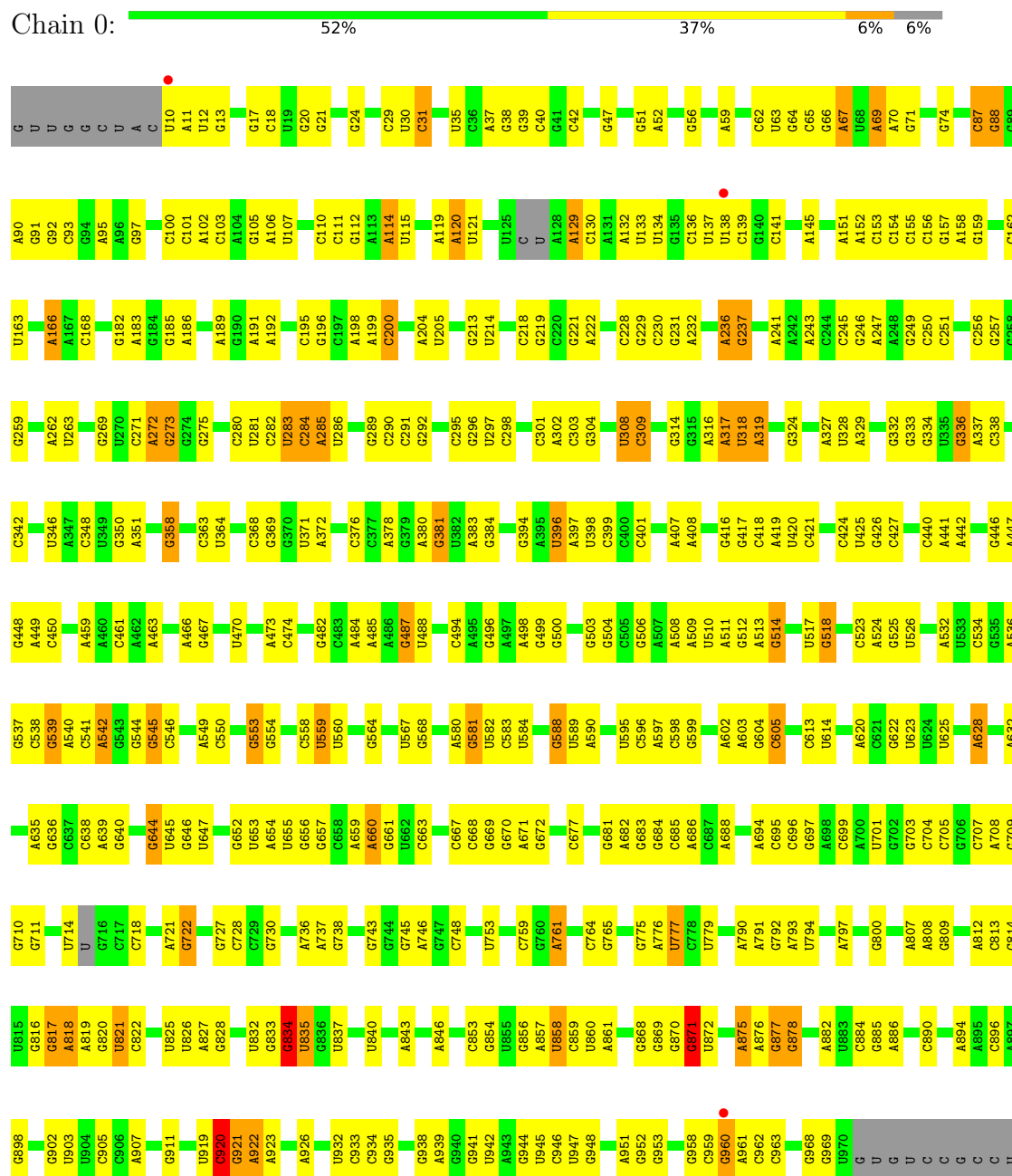
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	24	Total 24	O 24	0	0
38	Y	101	Total 101	O 101	0	0
38	Z	31	Total 31	O 31	0	0
38	1	57	Total 57	O 57	0	0
38	2	39	Total 39	O 39	0	0
38	3	74	Total 74	O 74	0	0

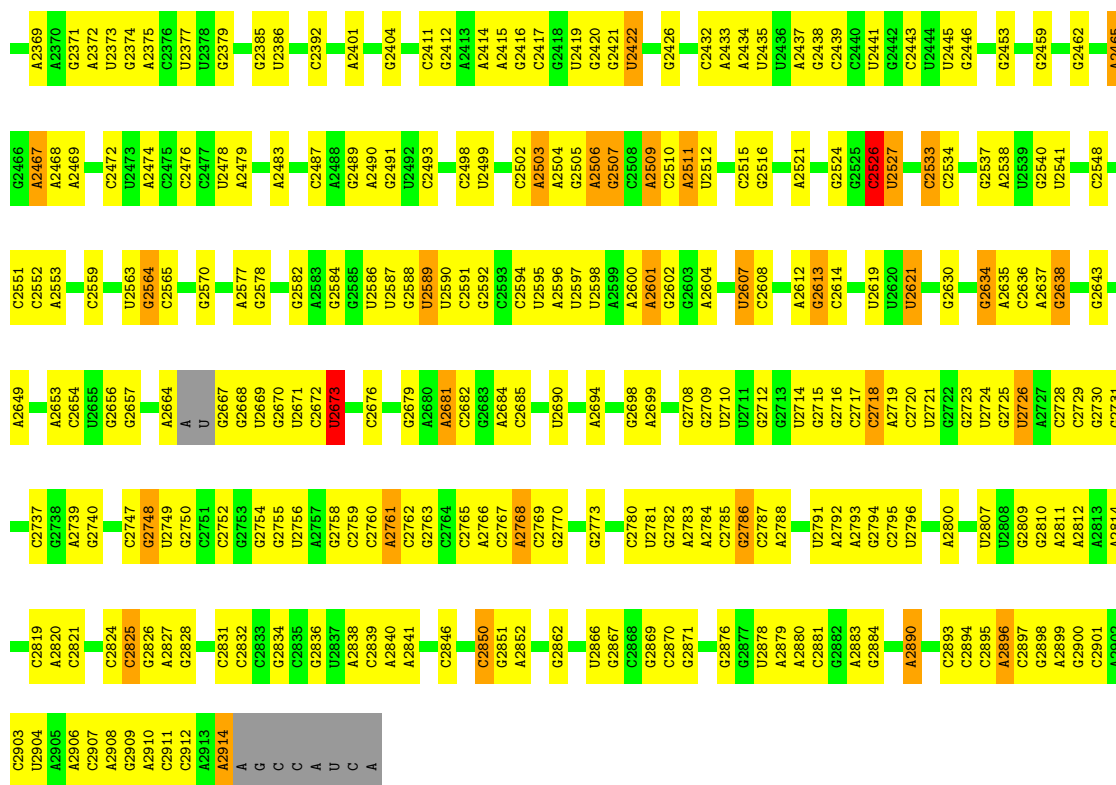
3 Residue-property plots

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.

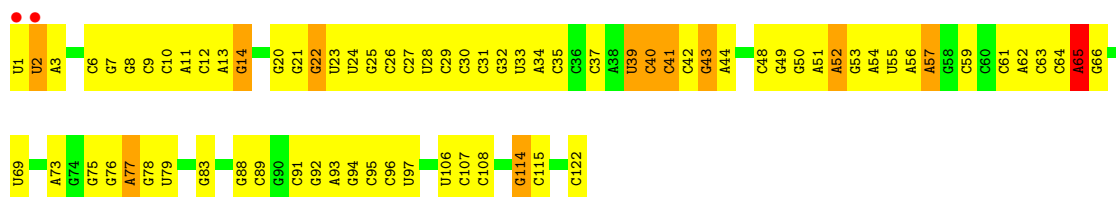
• Molecule 1: 23S Ribosomal RNA



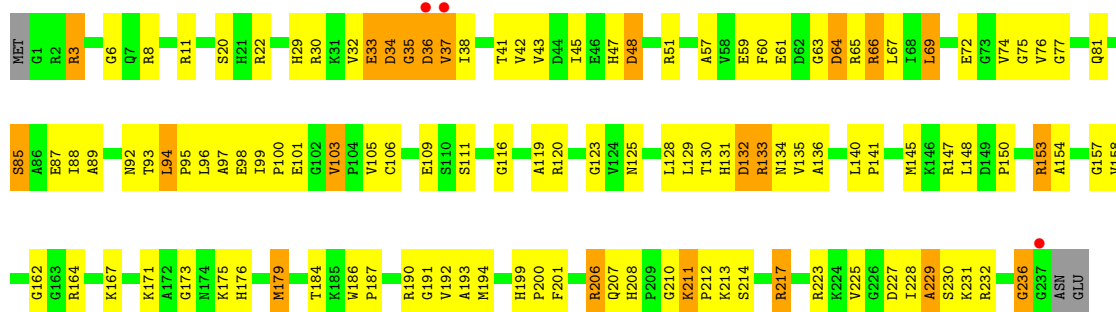




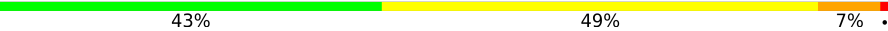
• Molecule 2: 5S Ribosomal RNA

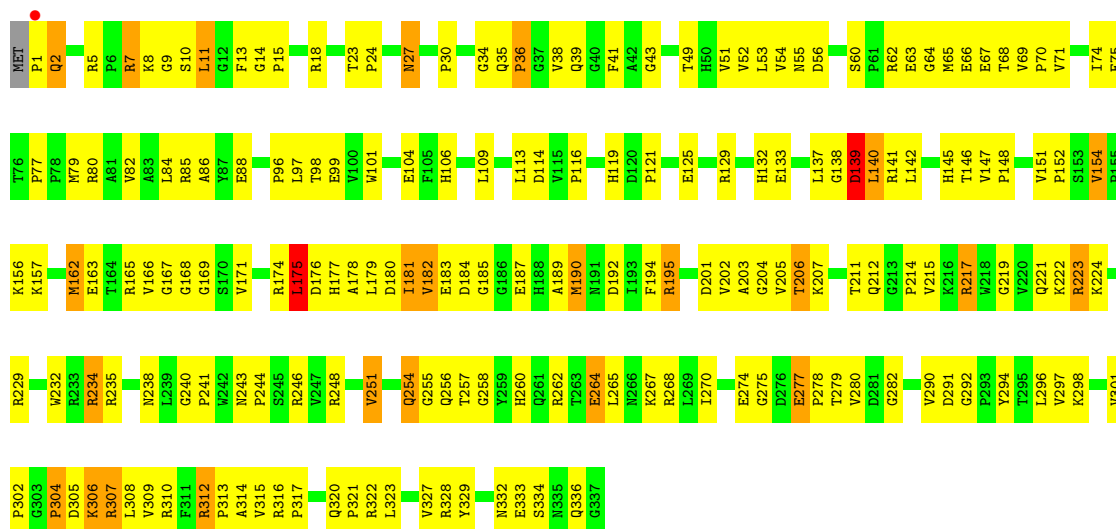


• Molecule 3: 50S ribosomal protein L2P

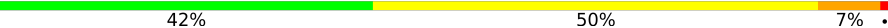


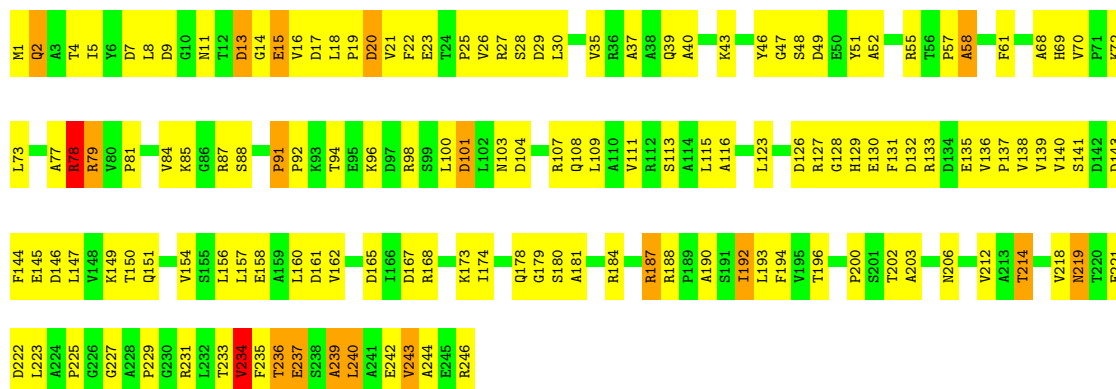
• Molecule 4: 50S ribosomal protein L3P

Chain B:  43% 49% 7%

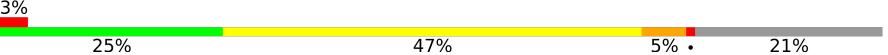


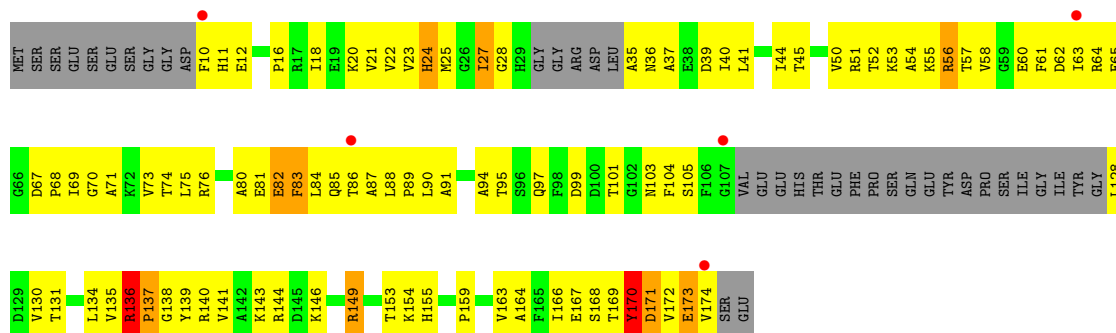
• Molecule 5: 50S ribosomal protein L4E

Chain C:  42% 50% 7%



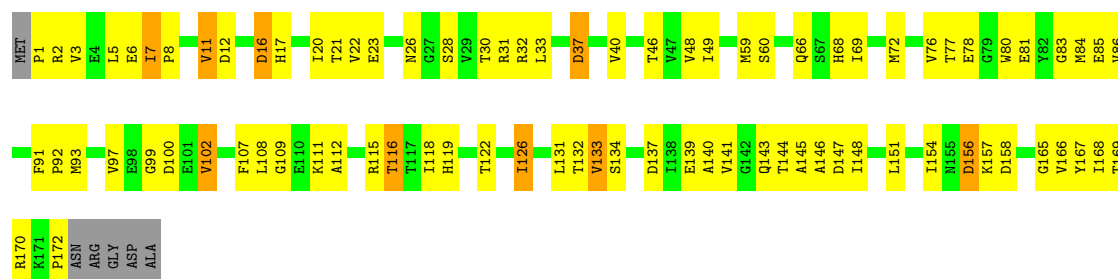
• Molecule 6: 50S ribosomal protein L5P

Chain D:  3% 25% 47% 5% 21%



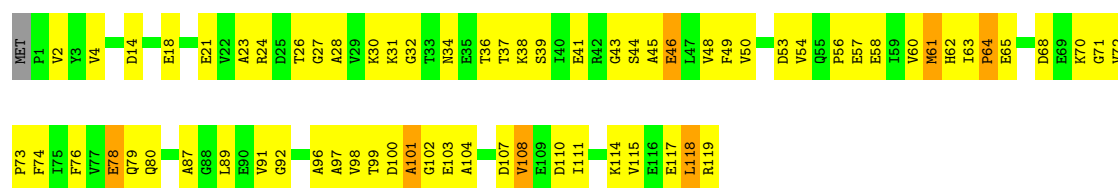
• Molecule 7: 50S ribosomal protein L6P

Chain E:



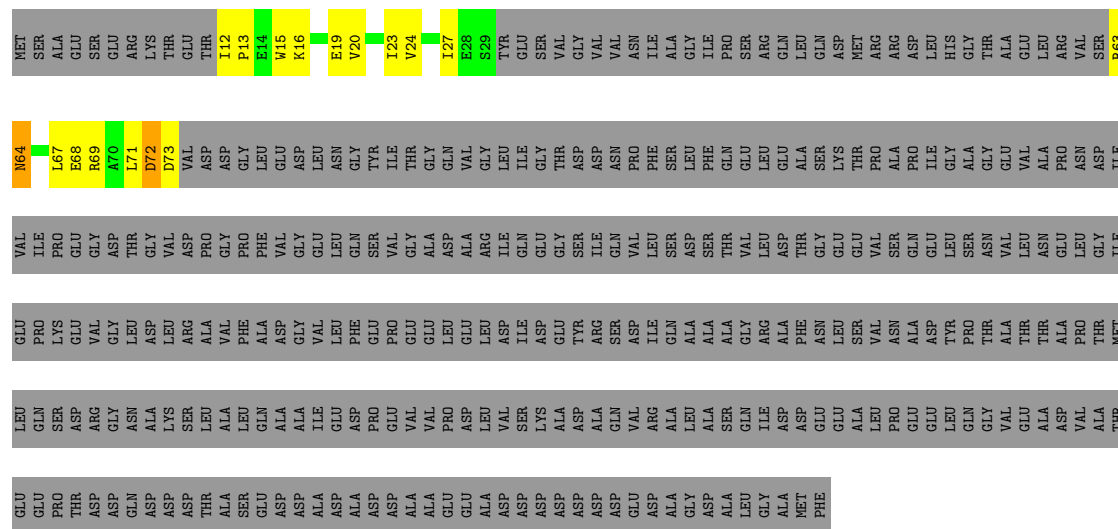
- Molecule 8: 50S ribosomal protein L7AE

Chain F:



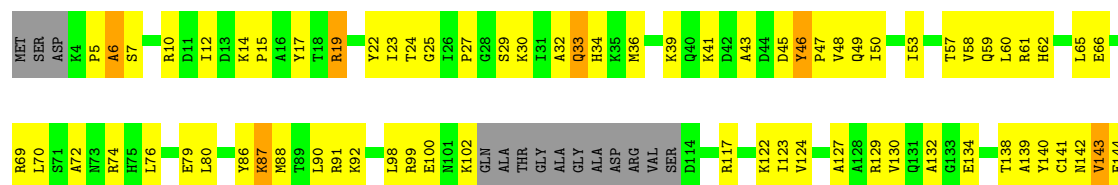
- Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

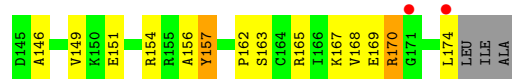
Chain G:



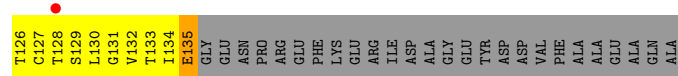
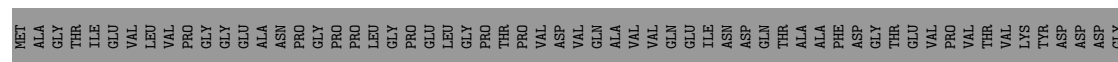
- Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain H:

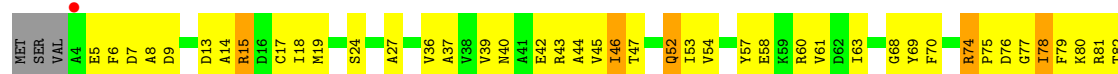




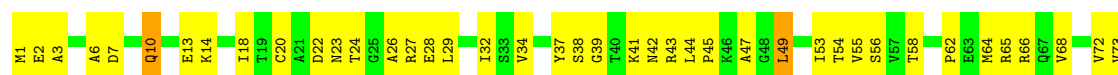
- Molecule 11: 50S RIBOSOMAL PROTEIN L11P



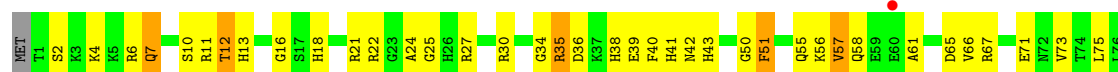
- Molecule 12: 50S ribosomal protein L13P



- Molecule 13: 50S ribosomal protein L14P

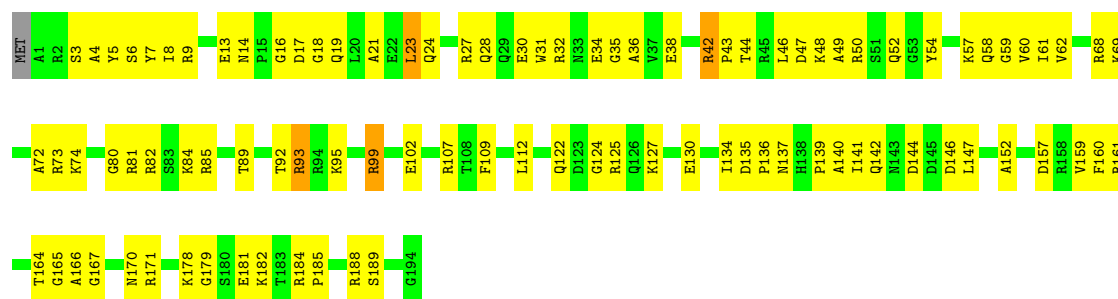


- Molecule 14: 50S ribosomal protein L15P



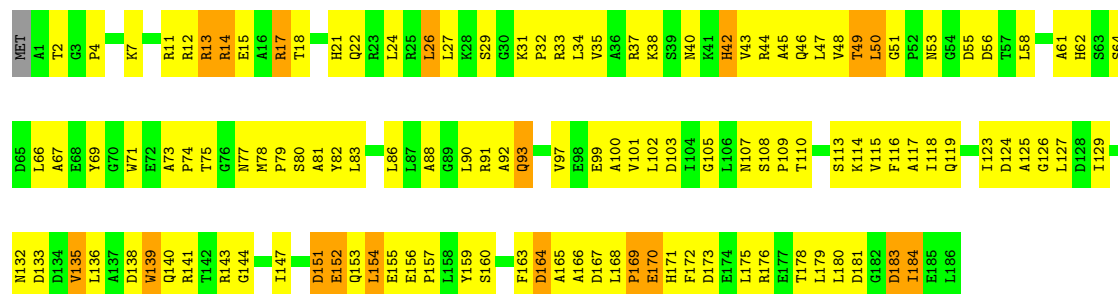
- Molecule 15: 50S Ribosomal Protein L15E

Chain M: 



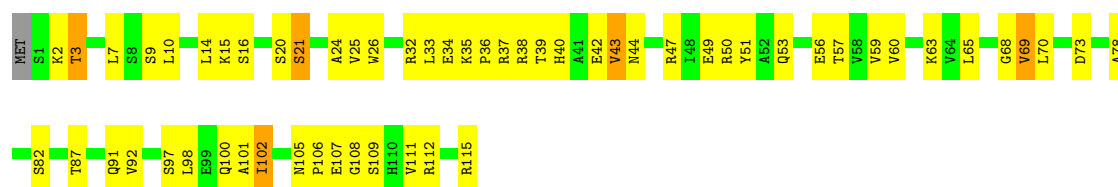
• Molecule 16: 50S ribosomal protein L18P

Chain N: 



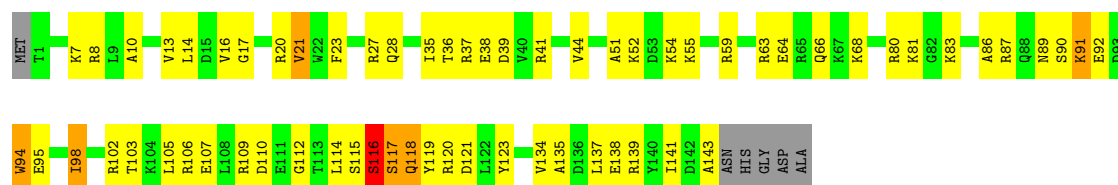
• Molecule 17: 50S ribosomal protein L18e

Chain O: 



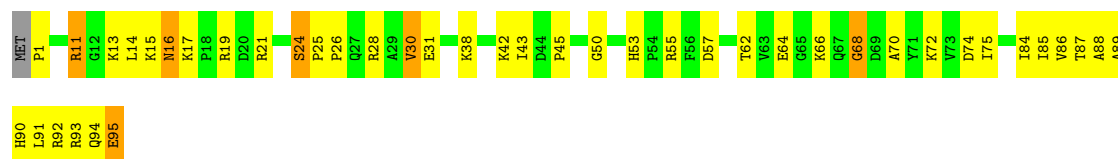
• Molecule 18: 50S ribosomal protein L19E

Chain P: 



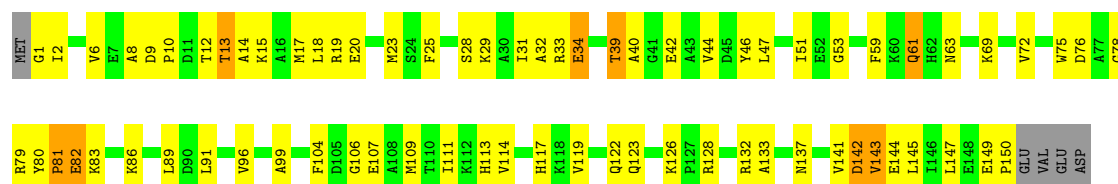
• Molecule 19: 50S ribosomal protein L21e

Chain Q: 



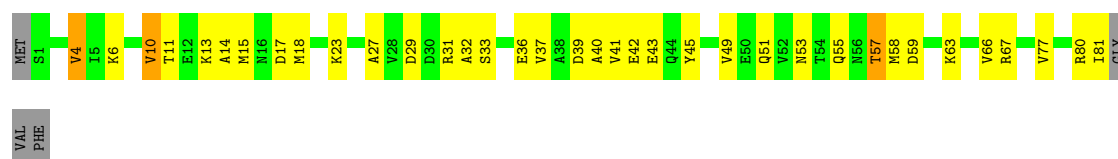
- Molecule 20: 50S ribosomal protein L22P

Chain R: 50% 41% 5% .



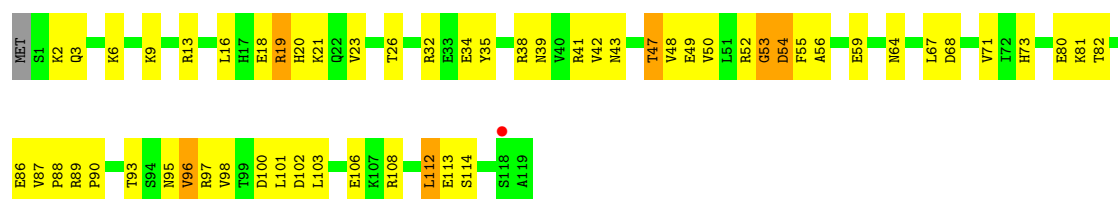
- Molecule 21: 50S ribosomal protein L23P

Chain S: 53% 39% 5% .



- Molecule 22: 50S ribosomal protein L24P

Chain T: 52% 42% 5% .



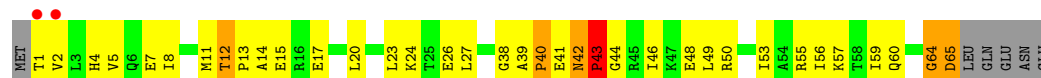
- Molecule 23: 50S ribosomal protein L24E

Chain U: 38% 41% 20% .

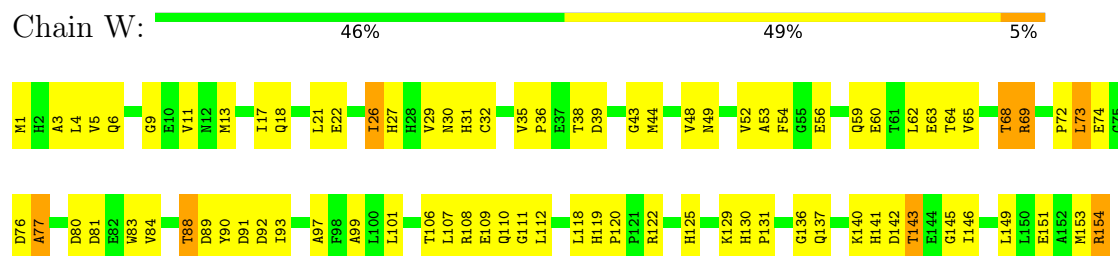


- Molecule 24: 50S ribosomal protein L29P

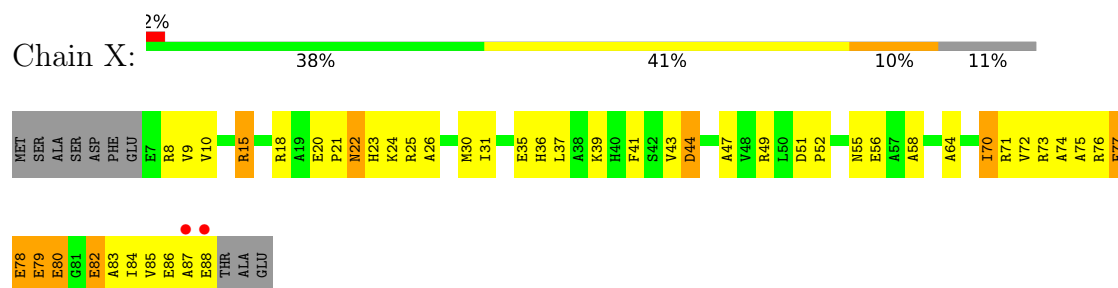
Chain V: 3% 41% 42% 7% 8% .



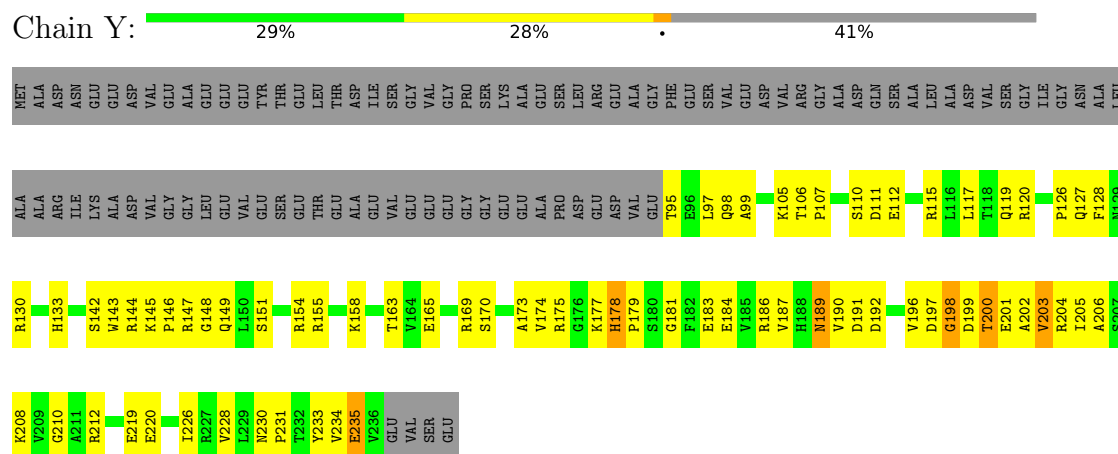
- Molecule 25: 50S ribosomal protein L30P



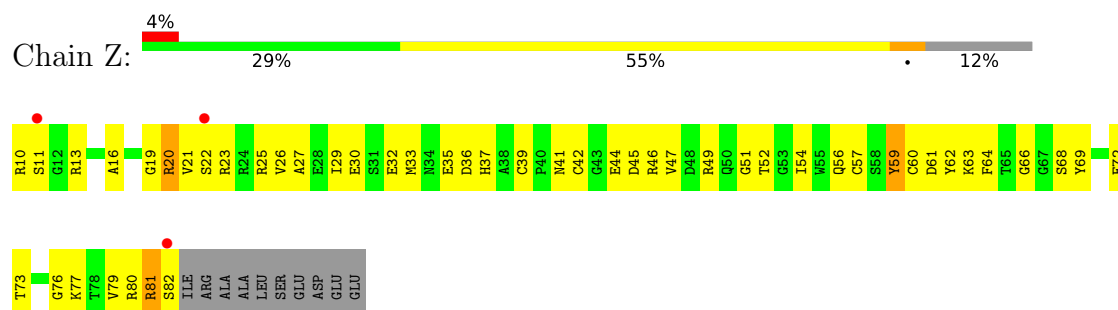
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e

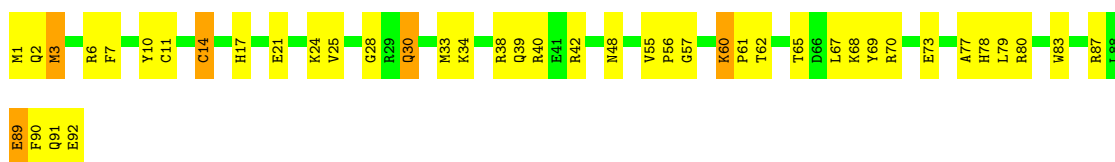




- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.51Å 300.12Å 573.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.00 29.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (29.97-3.00) 92.0 (29.97-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.170 , 0.228 0.169 , 0.225	Depositor DCC
R_{free} test set	3275 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.3	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	99060	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: CD, 1MA, OMG, MG, K, UR3, NA, CL, PSU, OMU, CLY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.38	0/65957	0.61	20/102867 (0.0%)
2	9	0.38	0/2904	0.61	3/4526 (0.1%)
3	A	0.43	0/1786	1.00	7/2408 (0.3%)
4	B	0.45	0/2690	1.01	13/3652 (0.4%)
5	C	0.50	0/1884	1.01	7/2551 (0.3%)
6	D	0.37	0/1111	0.95	4/1498 (0.3%)
7	E	0.41	0/1382	0.96	5/1880 (0.3%)
8	F	0.38	0/901	0.91	2/1224 (0.2%)
9	G	0.41	0/241	0.77	0/324
10	H	0.43	0/1302	0.99	6/1743 (0.3%)
11	I	0.38	0/526	0.91	3/716 (0.4%)
12	J	0.48	0/1136	0.95	6/1530 (0.4%)
13	K	0.45	0/1001	0.99	3/1347 (0.2%)
14	L	0.39	0/1130	0.98	4/1509 (0.3%)
15	M	0.45	0/1582	0.96	6/2117 (0.3%)
16	N	0.40	0/1474	1.07	12/1999 (0.6%)
17	O	0.46	0/874	0.91	3/1181 (0.3%)
18	P	0.44	0/1147	0.90	1/1528 (0.1%)
19	Q	0.46	0/749	1.08	6/1005 (0.6%)
20	R	0.50	0/1172	0.96	6/1578 (0.4%)
21	S	0.41	0/648	0.89	4/875 (0.5%)
22	T	0.41	0/958	0.99	3/1289 (0.2%)
23	U	0.41	0/417	0.96	1/562 (0.2%)
24	V	0.40	0/502	1.05	4/675 (0.6%)
25	W	0.51	0/1219	1.03	3/1655 (0.2%)
26	X	0.47	0/664	1.00	2/895 (0.2%)
27	Y	0.47	0/1146	0.96	4/1536 (0.3%)
28	Z	0.38	0/589	0.89	0/787
29	1	0.47	0/438	0.89	0/578
30	2	0.41	0/401	0.77	0/529
31	3	0.37	0/771	0.86	2/1024 (0.2%)
All	All	0.40	0/98702	0.73	140/147588 (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	30
2	9	0	1
All	All	0	31

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.40	129.59	109.50
16	N	135	VAL	N-CA-C	-10.68	102.64	112.90
19	Q	17	LYS	N-CA-C	-9.57	98.06	109.93
18	P	118	GLN	N-CA-C	-9.35	100.19	111.69
6	D	136	ARG	CA-C-N	8.81	130.85	119.84
6	D	136	ARG	C-N-CA	8.81	130.85	119.84
4	B	157	LYS	N-CA-C	-7.87	104.28	114.04
1	0	1563	G	C4'-C3'-O3'	7.87	121.20	109.40
25	W	143	THR	N-CA-C	-7.79	103.04	112.54
4	B	265	LEU	N-CA-C	7.42	120.56	110.55
15	M	89	THR	N-CA-C	7.36	119.09	111.14
16	N	153	GLN	N-CA-C	-7.34	103.21	113.20
7	E	11	VAL	N-CA-C	7.23	120.31	109.17
3	A	133	ARG	N-CA-C	-7.21	104.48	113.28
3	A	48	ASP	CA-C-N	7.14	127.14	119.28
3	A	48	ASP	C-N-CA	7.14	127.14	119.28
24	V	42	ASN	CA-C-N	6.99	128.58	119.84
24	V	42	ASN	C-N-CA	6.99	128.58	119.84
11	I	96	SER	N-CA-C	-6.95	100.76	110.35
4	B	151	VAL	CA-C-N	6.83	126.64	119.05
4	B	151	VAL	C-N-CA	6.83	126.64	119.05
2	9	39	U	N1-C1'-C2'	6.83	122.24	112.00
5	C	167	ASP	N-CA-C	-6.82	104.22	112.54
1	0	1942	A	C5'-C4'-C3'	6.78	126.17	116.00
16	N	102	LEU	N-CA-C	6.77	118.89	109.15
4	B	114	ASP	N-CA-C	-6.67	100.30	109.71
4	B	222	LYS	N-CA-C	-6.64	100.13	110.42
14	L	7	GLN	N-CA-C	6.61	118.57	111.36
16	N	14	ARG	N-CA-C	-6.61	103.77	110.97
20	R	122	GLN	N-CA-C	-6.54	97.87	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	152	GLU	N-CA-C	-6.54	104.15	111.28
10	H	6	ALA	N-CA-C	-6.46	105.36	113.18
24	V	64	GLY	N-CA-C	-6.46	106.82	115.21
26	X	22	ASN	N-CA-C	6.42	118.81	111.11
16	N	51	GLY	CA-C-N	6.38	126.59	119.32
16	N	51	GLY	C-N-CA	6.38	126.59	119.32
10	H	163	SER	N-CA-C	-6.35	100.22	110.32
3	A	103	VAL	N-CA-C	6.34	115.16	107.61
3	A	236	GLY	N-CA-C	6.25	118.68	111.36
1	0	1504	A	N9-C1'-C2'	6.22	121.34	112.00
12	J	68	GLY	N-CA-C	6.17	120.45	112.18
11	I	89	GLU	N-CA-C	-6.15	105.47	114.39
22	T	54	ASP	N-CA-C	-6.14	105.75	113.18
27	Y	202	ALA	N-CA-C	-6.03	101.53	110.46
17	O	69	VAL	N-CA-C	5.99	118.00	108.89
21	S	27	ALA	N-CA-C	-5.96	99.53	109.24
15	M	74	LYS	N-CA-C	5.88	119.05	109.59
10	H	46	TYR	CA-C-N	5.87	125.25	118.85
10	H	46	TYR	C-N-CA	5.87	125.25	118.85
7	E	112	ALA	CA-C-N	5.87	125.63	119.76
7	E	112	ALA	C-N-CA	5.87	125.63	119.76
1	0	1261	A	N9-C1'-C2'	5.82	120.72	112.00
1	0	834	G	C2'-C3'-O3'	-5.81	104.98	113.70
15	M	42	ARG	CA-C-N	5.80	126.10	119.83
15	M	42	ARG	C-N-CA	5.80	126.10	119.83
4	B	282	GLY	N-CA-C	-5.80	106.52	114.64
14	L	145	LEU	N-CA-C	-5.79	104.97	111.28
16	N	13	ARG	N-CA-C	-5.78	104.42	112.45
17	O	43	VAL	N-CA-C	5.74	116.21	108.17
25	W	69	ARG	N-CA-C	5.74	122.21	113.61
1	0	920	C	C2'-C3'-O3'	-5.71	105.14	113.70
26	X	80	GLU	N-CA-C	-5.70	108.12	114.62
4	B	154	VAL	CA-C-N	5.69	125.16	119.24
4	B	154	VAL	C-N-CA	5.69	125.16	119.24
1	0	1120	U	C5'-C4'-C3'	-5.66	107.51	116.00
4	B	217	ARG	N-CA-C	5.62	117.40	111.28
5	C	239	ALA	N-CA-C	-5.61	104.80	111.03
12	J	107	ASN	CA-C-N	5.60	126.09	120.04
12	J	107	ASN	C-N-CA	5.60	126.09	120.04
23	U	50	GLU	N-CA-C	5.59	118.91	111.75
1	0	2526	C	N1-C1'-C2'	5.59	120.38	112.00
1	0	871	G	C5'-C4'-O4'	-5.59	101.42	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	162	PRO	N-CA-C	5.58	119.45	111.13
1	0	2291	A	N9-C1'-C2'	5.55	120.32	112.00
1	0	2673	U	N1-C1'-C2'	5.54	120.32	112.00
31	3	60	LYS	N-CA-C	-5.54	102.64	110.29
15	M	13	GLU	N-CA-C	-5.53	105.79	112.54
4	B	80	ARG	N-CA-C	5.52	116.45	107.23
19	Q	13	LYS	N-CA-C	5.52	118.06	111.71
16	N	42	HIS	N-CA-C	5.51	116.63	108.86
1	0	1592	G	N9-C1'-C2'	5.51	120.26	112.00
19	Q	68	GLY	N-CA-C	-5.50	101.93	111.50
21	S	4	VAL	N-CA-C	5.50	115.70	110.53
3	A	111	SER	N-CA-C	-5.46	103.19	110.07
20	R	137	ASN	N-CA-C	5.45	118.53	110.46
3	A	213	LYS	N-CA-C	5.43	119.08	112.23
4	B	223	ARG	N-CA-C	-5.43	102.36	110.23
10	H	10	ARG	N-CA-C	5.42	119.00	112.38
24	V	12	THR	N-CA-C	-5.42	103.35	110.39
11	I	116	LEU	N-CA-C	-5.41	105.78	112.38
2	9	39	U	C4'-C3'-O3'	-5.40	104.89	113.00
5	C	219	ASN	N-CA-C	5.38	118.04	109.81
13	K	129	THR	N-CA-C	-5.37	105.34	111.14
27	Y	183	GLU	N-CA-C	-5.37	100.48	109.24
13	K	90	PHE	N-CA-C	5.34	117.99	110.14
4	B	175	LEU	N-CA-C	-5.32	105.38	111.07
1	0	1819	G	C5'-C4'-C3'	5.31	123.97	116.00
12	J	112	ASP	N-CA-C	-5.30	100.53	108.96
5	C	244	ALA	N-CA-C	5.29	118.52	111.75
20	R	141	VAL	N-CA-C	5.29	116.93	108.89
12	J	91	LYS	N-CA-C	-5.28	102.67	110.48
8	F	62	HIS	N-CA-C	5.27	117.93	111.82
5	C	78	ARG	N-CA-C	5.27	115.49	108.38
2	9	65	A	N9-C1'-C2'	5.25	119.88	112.00
12	J	9	ASP	N-CA-C	-5.25	106.38	112.89
1	0	2726	U	N1-C1'-C2'	5.24	119.86	112.00
17	O	82	SER	N-CA-C	-5.24	103.11	110.50
1	0	1504	A	C1'-O4'-C4'	-5.22	104.68	109.90
14	L	12	THR	N-CA-C	5.21	119.62	113.16
16	N	169	PRO	N-CA-C	-5.21	107.63	114.03
16	N	151	ASP	N-CA-C	-5.20	106.89	113.18
31	3	57	GLY	N-CA-C	5.20	118.53	112.50
15	M	36	ALA	N-CA-C	-5.17	106.13	112.90
21	S	57	THR	N-CA-C	5.16	117.36	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	84	ILE	N-CA-C	5.14	115.26	107.80
5	C	192	ILE	N-CA-C	5.14	116.21	109.58
6	D	83	PHE	N-CA-C	-5.13	106.71	113.12
6	D	170	TYR	N-CA-C	5.12	118.19	111.28
27	Y	178	HIS	N-CA-C	-5.12	103.02	110.08
7	E	37	ASP	N-CA-C	5.11	119.09	112.86
20	R	142	ASP	N-CA-C	-5.11	101.55	109.72
5	C	20	ASP	N-CA-C	5.11	117.51	111.33
1	0	2313	C	C5'-C4'-C3'	5.08	123.63	116.00
1	0	922	A	N9-C1'-C2'	5.08	119.62	112.00
27	Y	143	TRP	N-CA-C	5.08	117.52	109.24
1	0	129	A	C2'-C3'-O3'	5.07	121.31	113.70
16	N	170	GLU	N-CA-C	-5.05	105.85	111.36
22	T	47	THR	N-CA-C	-5.05	101.92	109.95
1	0	2316	G	C5'-C4'-C3'	-5.05	107.63	115.20
25	W	68	THR	N-CA-C	5.04	116.77	111.28
20	R	34	GLU	N-CA-C	5.03	116.76	111.28
22	T	34	GLU	N-CA-C	5.03	116.76	111.28
7	E	156	ASP	N-CA-C	5.02	116.44	111.07
8	F	118	LEU	N-CA-C	-5.01	107.22	113.19
14	L	57	VAL	N-CA-C	-5.01	107.82	112.43
21	S	10	VAL	N-CA-C	5.01	114.79	107.37
19	Q	24	SER	CA-C-N	5.01	123.32	119.66
19	Q	24	SER	C-N-CA	5.01	123.32	119.66
20	R	123	GLN	N-CA-C	5.01	117.69	110.28
13	K	54	THR	N-CA-C	-5.00	102.37	110.32

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1599	U	Sidechain
1	0	1758	U	Sidechain
1	0	1809	G	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

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Mol	Chain	Res	Type	Group
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2313	C	Sidechain
1	0	2316	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	324	G	Sidechain
1	0	396	U	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	761	A	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	903	U	Sidechain
2	9	65	A	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	59020	0	29807	1150	0
2	9	2599	0	1325	94	0
3	A	1753	0	1766	158	0
4	B	2625	0	2533	208	0
5	C	1859	0	1816	159	0
6	D	1094	0	1085	132	0
7	E	1357	0	1266	81	0
8	F	890	0	843	76	0
9	G	240	0	231	22	0
10	H	1282	0	1292	100	0
11	I	519	0	500	70	0
12	J	1120	0	1098	83	0
13	K	992	0	1031	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	1118	0	1076	62	0
15	M	1558	0	1566	87	0
16	N	1445	0	1401	142	0
17	O	865	0	873	53	0
18	P	1136	0	1123	79	0
19	Q	735	0	729	37	0
20	R	1149	0	1122	75	0
21	S	641	0	605	37	0
22	T	950	0	923	63	0
23	U	410	0	364	33	0
24	V	499	0	511	40	0
25	W	1196	0	1137	108	0
26	X	654	0	653	57	0
27	Y	1130	0	1133	69	0
28	Z	578	0	540	52	0
29	1	431	0	426	34	0
30	2	396	0	413	26	0
31	3	755	0	729	38	0
32	0	27	0	32	5	0
33	0	110	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	B	1	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	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	3	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	1	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	5892	0	0	234	0
38	1	57	0	0	2	0
38	2	39	0	0	4	0
38	3	74	0	0	9	0
38	9	139	0	0	12	0
38	A	120	0	0	16	0
38	B	146	0	0	27	0
38	C	169	0	0	35	0
38	D	49	0	0	26	0
38	E	41	0	0	11	0
38	F	25	0	0	8	0
38	G	19	0	0	2	0
38	H	68	0	0	15	0
38	I	10	0	0	6	0
38	J	56	0	0	4	0
38	K	60	0	0	9	0
38	L	82	0	0	14	0
38	M	128	0	0	7	0
38	N	64	0	0	11	0
38	O	44	0	0	12	0
38	P	64	0	0	9	0
38	Q	49	0	0	6	0
38	R	79	0	0	8	0
38	S	31	0	0	4	0
38	T	36	0	0	9	0
38	U	27	0	0	3	0
38	V	14	0	0	4	0
38	W	68	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	X	24	0	0	8	0
38	Y	101	0	0	7	0
38	Z	31	0	0	7	0
All	All	99060	0	59949	3216	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 21.

All (3216) 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)
1:0:871:G:H5'	1:0:871:G:H8	1.15	1.12
2:9:6:C:H5''	16:N:37:ARG:HH12	1.16	1.10
13:K:10:GLN:H	13:K:10:GLN:NE2	1.49	1.09
13:K:10:GLN:HE21	13:K:10:GLN:N	1.52	1.07
4:B:62:ARG:HA	4:B:65:MET:HE3	1.36	1.06
1:0:156:C:H5''	15:M:171:ARG:HD3	1.31	1.06
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.21	1.05
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.39	1.05
1:0:2717:C:H2'	1:0:2718:C:H5''	1.40	1.03
8:F:26:THR:HG21	8:F:103:GLU:HB2	1.39	1.02
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.43	1.01
1:0:871:G:H5'	1:0:871:G:C8	1.95	1.01
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.41	1.00
1:0:1559:A:H1'	38:0:5857:HOH:O	1.61	1.00
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.43	0.99
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.41	0.99
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.12	0.98
5:C:1:MET:HG2	5:C:2:GLN:H	1.28	0.98
18:P:59:ARG:HH22	18:P:66:GLN:HE22	0.98	0.98
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.28	0.97
2:9:6:C:H5''	16:N:37:ARG:NH1	1.77	0.97
6:D:25:MET:HE2	6:D:41:LEU:HG	1.44	0.97
21:S:51:GLN:HB3	21:S:67:ARG:HH12	1.30	0.97
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.46	0.97
1:0:1187:U:HO2'	1:0:1189:A:H2	1.08	0.96
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.46	0.96
16:N:93:GLN:HA	16:N:93:GLN:HE21	1.29	0.95
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.45	0.95
5:C:236:THR:HG22	5:C:239:ALA:H	1.30	0.94
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:76:G:H3'	2:9:77:A:H5''	1.51	0.93
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.82	0.93
1:0:21:G:H5'	20:R:2:ILE:HA	1.51	0.93
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.51	0.93
21:S:51:GLN:HE21	21:S:53:ASN:HD21	0.93	0.93
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.49	0.93
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.51	0.92
1:0:870:G:H2'	1:0:871:G:H5''	1.51	0.91
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.51	0.91
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.91
5:C:233:THR:HG22	5:C:234:VAL:H	1.33	0.91
38:0:5210:HOH:O	13:K:39:GLY:HA2	1.71	0.91
1:0:1242:A:H5'	12:J:82:THR:HG23	1.51	0.90
6:D:154:LYS:H	6:D:154:LYS:HD2	1.35	0.90
2:9:56:A:H2'	2:9:57:A:H5''	1.52	0.90
1:0:396:U:H1'	38:0:7599:HOH:O	1.71	0.89
1:0:1116:U:HO2'	1:0:1118:A:H2	0.92	0.89
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.55	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	0.90	0.89
18:P:115:SER:N	18:P:118:GLN:HE21	1.70	0.89
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.37	0.89
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.51	0.89
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
1:0:545:G:H5'	1:0:545:G:H8	1.36	0.88
1:0:960:G:H4'	38:0:7404:HOH:O	1.72	0.88
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.56	0.88
4:B:238:ASN:HD22	4:B:240:GLY:H	0.92	0.87
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.40	0.87
8:F:58:GLU:HA	8:F:61:MET:HE2	1.57	0.87
1:0:21:G:C5'	20:R:2:ILE:HA	2.05	0.87
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.56	0.87
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.58	0.86
23:U:14:GLU:O	23:U:17:THR:HB	1.76	0.86
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.72	0.86
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.57	0.86
5:C:139:VAL:HG13	38:C:8645:HOH:O	1.74	0.86
25:W:149:LEU:HG	25:W:153:MET:HE2	1.57	0.86
4:B:238:ASN:ND2	4:B:240:GLY:H	1.72	0.86
5:C:236:THR:HA	38:C:8648:HOH:O	1.76	0.86
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.58	0.85
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1641:A:H2'	1:0:1642:A:H5'	1.59	0.85
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.85
20:R:39:THR:HB	20:R:42:GLU:HG3	1.58	0.85
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.41	0.85
12:J:76:ASP:HA	38:J:8868:HOH:O	1.74	0.85
1:0:1184:C:H1'	38:0:7437:HOH:O	1.75	0.85
5:C:242:GLU:HG3	38:C:8579:HOH:O	1.75	0.85
30:2:35:ARG:HB2	38:2:2691:HOH:O	1.77	0.85
1:0:1118:A:H62	1:0:1244:U:H3	1.21	0.85
1:0:1160:G:H5'	1:0:1161:A:H5'	1.59	0.85
1:0:381:G:H5''	38:0:4317:HOH:O	1.77	0.84
38:0:5447:HOH:O	9:G:12:ILE:HA	1.76	0.84
1:0:559:U:H6	1:0:559:U:H5'	1.43	0.84
25:W:13:MET:HE1	25:W:21:LEU:HD12	1.59	0.84
1:0:541:C:H2'	1:0:542:A:H5''	1.58	0.84
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.43	0.84
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.43	0.83
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.58	0.83
1:0:1701:A:H5'	38:0:6270:HOH:O	1.77	0.83
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.08	0.83
25:W:142:ASP:HB2	25:W:145:GLY:H	1.44	0.83
1:0:542:A:H5'	1:0:542:A:H8	1.44	0.83
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.26	0.83
14:L:79:ASP:HB3	38:L:8861:HOH:O	1.78	0.83
1:0:1118:A:H8	1:0:1118:A:H3'	1.42	0.83
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.59	0.83
1:0:282:C:H1'	1:0:368:C:N4	1.93	0.83
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.61	0.82
1:0:1118:A:H3'	1:0:1118:A:C8	2.14	0.82
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.60	0.82
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.60	0.82
18:P:115:SER:H	18:P:118:GLN:NE2	1.74	0.82
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.09	0.82
4:B:238:ASN:HD22	4:B:240:GLY:N	1.76	0.82
1:0:2533:C:H5'	1:0:2533:C:H6	1.43	0.82
7:E:100:ASP:HB2	38:E:2789:HOH:O	1.80	0.82
6:D:57:THR:HG23	6:D:63:ILE:HA	1.62	0.82
4:B:179:LEU:O	4:B:183:GLU:HG2	1.78	0.82
30:2:41:HIS:H	30:2:45:ASN:HD22	1.25	0.82
2:9:14:G:H5'	2:9:14:G:H8	1.45	0.81
18:P:143:ALA:HA	38:P:188:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.61	0.81
18:P:59:ARG:HH22	18:P:66:GLN:NE2	1.79	0.81
1:0:1474:C:H6	1:0:1474:C:H5'	1.45	0.81
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.62	0.81
1:0:877:G:H5'	1:0:878:G:OP1	1.81	0.81
2:9:92:G:H2'	2:9:93:A:C8	2.16	0.81
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.19	0.81
2:9:28:U:H5''	16:N:40:ASN:ND2	1.96	0.81
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.62	0.81
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.79	0.81
25:W:26:ILE:O	25:W:26:ILE:HG13	1.80	0.81
1:0:1165:G:H4'	1:0:1174:A:O2'	1.82	0.80
4:B:185:GLY:HA2	38:B:8931:HOH:O	1.79	0.80
16:N:169:PRO:O	16:N:172:PHE:HB3	1.81	0.80
5:C:145:GLU:HG3	38:C:8572:HOH:O	1.82	0.80
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.16	0.80
14:L:77:ALA:HB3	38:L:8832:HOH:O	1.81	0.80
3:A:131:HIS:O	3:A:132:ASP:HB2	1.82	0.80
5:C:236:THR:HG22	5:C:239:ALA:N	1.95	0.80
14:L:67:ARG:O	14:L:71:GLU:HG3	1.81	0.80
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.77	0.80
25:W:65:VAL:HA	25:W:68:THR:HG22	1.63	0.80
26:X:43:VAL:HG12	26:X:44:ASP:H	1.46	0.80
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.12	0.80
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.63	0.80
1:0:2755:G:H1'	38:O:4681:HOH:O	1.81	0.80
7:E:132:THR:HB	38:E:2227:HOH:O	1.81	0.79
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.98	0.79
25:W:13:MET:HE2	25:W:18:GLN:CA	2.12	0.79
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.64	0.79
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.82	0.79
1:0:10:U:H3'	38:O:3326:HOH:O	1.81	0.79
1:0:2756:U:H3	1:0:2896:A:H2	1.31	0.79
3:A:51:ARG:HB2	38:A:8901:HOH:O	1.82	0.79
1:0:2291:A:C8	1:0:2309:C:H5'	2.18	0.78
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.64	0.78
1:0:1667:A:H8	1:0:1667:A:H5'	1.47	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.78
1:0:1701:A:H4'	1:0:1702:U:H5''	1.65	0.78
1:0:1862:C:H1'	38:A:8912:HOH:O	1.83	0.78
4:B:321:PRO:HA	38:B:8957:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.92	0.78
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.66	0.78
31:3:65:THR:HG22	31:3:67:LEU:HG	1.65	0.78
25:W:13:MET:HE2	25:W:18:GLN:HA	1.63	0.78
12:J:131:THR:HG22	12:J:134:GLU:H	1.48	0.77
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.14	0.77
8:F:48:VAL:HG23	8:F:74:PHE:HB3	1.65	0.77
1:0:2908:A:H2'	1:0:2909:G:O4'	1.83	0.77
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.65	0.77
10:H:168:VAL:HG13	38:H:8547:HOH:O	1.83	0.77
24:V:1:THR:HG23	24:V:2:VAL:H	1.50	0.77
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.85	0.77
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.85	0.77
24:V:42:ASN:HB3	38:V:7247:HOH:O	1.84	0.77
1:0:1450:C:H4'	1:0:1451:C:OP2	1.84	0.77
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.78	0.77
7:E:1:PRO:HG2	7:E:59:MET:HE1	1.67	0.77
1:0:541:C:C2'	1:0:542:A:H5''	2.15	0.76
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.65	0.76
1:0:1819:G:H5'	38:0:4709:HOH:O	1.85	0.76
1:0:1835:U:H5	1:0:1840:A:N7	1.82	0.76
1:0:2426:G:H1'	38:0:6082:HOH:O	1.84	0.76
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.66	0.76
4:B:267:LYS:HA	38:B:8827:HOH:O	1.85	0.76
12:J:74:ARG:HH11	12:J:74:ARG:CB	1.96	0.76
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.68	0.76
7:E:166:VAL:HG12	38:E:3134:HOH:O	1.85	0.76
24:V:12:THR:HG22	24:V:15:GLU:CG	2.14	0.76
1:0:2559:C:H4'	38:0:7231:HOH:O	1.85	0.76
1:0:1603:A:H5'	1:0:1605:G:O4'	1.86	0.76
1:0:1666:C:O2'	1:0:1667:A:H5''	1.86	0.76
7:E:37:ASP:OD1	12:J:125:SER:HB3	1.86	0.76
16:N:113:SER:HB2	38:N:8857:HOH:O	1.86	0.76
24:V:56:ILE:O	24:V:60:GLN:HG3	1.86	0.76
21:S:11:THR:H	21:S:14:ALA:HB3	1.49	0.75
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.67	0.75
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.15	0.75
2:9:51:A:H5'	16:N:160:SER:HB3	1.68	0.75
1:0:2716:G:H5''	4:B:206:THR:HG21	1.68	0.75
11:I:101:LYS:O	11:I:105:GLU:HG3	1.86	0.75
1:0:871:G:H8	1:0:871:G:C5'	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:62:ARG:CA	4:B:65:MET:HE3	2.15	0.75
1:O:2420:G:O2'	1:O:2421:G:H5'	1.86	0.75
10:H:88:MET:HA	10:H:139:ALA:HA	1.66	0.75
16:N:164:ASP:CG	16:N:167:ASP:HA	2.12	0.75
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.67	0.75
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.67	0.75
15:M:164:THR:HG22	15:M:166:ALA:H	1.51	0.75
1:O:56:G:H5''	24:V:50:ARG:HH12	1.51	0.75
5:C:214:THR:HG23	38:C:8634:HOH:O	1.87	0.74
1:O:1596:U:H2'	1:O:1598:A:OP2	1.87	0.74
10:H:49:GLN:HB3	10:H:170:ARG:HG3	1.70	0.74
12:J:45:VAL:HG23	12:J:130:VAL:O	1.87	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.81	0.74
25:W:107:LEU:O	25:W:112:LEU:HB2	1.88	0.74
1:O:797:A:H5'	28:Z:10:ARG:N	2.02	0.74
1:O:317:A:H4'	38:O:3770:HOH:O	1.87	0.74
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.88	0.74
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.85	0.74
1:O:338:C:H4'	5:C:174:ILE:HD11	1.69	0.74
1:O:870:G:C2'	1:O:871:G:H5''	2.16	0.74
1:O:902:G:N7	14:L:18:HIS:HD2	1.86	0.74
6:D:67:ASP:O	6:D:69:ILE:HG13	1.88	0.74
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.70	0.74
25:W:88:THR:HB	38:W:6679:HOH:O	1.87	0.74
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.69	0.74
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.70	0.74
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.69	0.74
16:N:151:ASP:OD1	16:N:154:LEU:HD13	1.88	0.74
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.70	0.73
13:K:22:ASP:HB2	38:K:5264:HOH:O	1.86	0.73
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.02	0.73
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.18	0.73
1:O:111:C:O2'	29:1:20:ARG:HG2	1.88	0.73
4:B:62:ARG:HA	4:B:65:MET:CE	2.16	0.73
8:F:96:ALA:HA	38:F:3111:HOH:O	1.87	0.73
1:O:2850:C:H6	1:O:2850:C:H5'	1.54	0.73
1:O:1116:U:H3	1:O:1246:A:H62	1.36	0.73
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.24	0.73
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.71	0.73
1:O:2783:A:H3'	38:O:5219:HOH:O	1.87	0.73
12:J:19:MET:CE	12:J:132:LEU:HD11	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.89	0.73
23:U:9:CYS:HA	23:U:52:THR:HG23	1.70	0.73
1:O:1206:U:H5'	1:O:1206:U:H6	1.53	0.73
1:O:2578:G:H5'	1:O:2578:G:H8	1.54	0.73
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.71	0.73
7:E:119:HIS:O	7:E:140:ALA:HB1	1.88	0.73
10:H:12:ILE:HD12	10:H:57:THR:HG22	1.71	0.73
1:O:506:G:H22	1:O:509:A:C5'	2.02	0.72
1:O:2890:A:H1'	23:U:56:ARG:NH2	2.04	0.72
3:A:8:ARG:HG2	38:A:8846:HOH:O	1.89	0.72
38:O:9692:HOH:O	4:B:254:GLN:HG3	1.87	0.72
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.71	0.72
2:9:56:A:C2'	2:9:57:A:H5''	2.19	0.72
18:P:64:GLU:HG3	38:P:169:HOH:O	1.90	0.72
6:D:163:VAL:HA	38:D:6326:HOH:O	1.88	0.72
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.36	0.72
26:X:78:GLU:HG2	26:X:79:GLU:H	1.54	0.72
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.54	0.72
18:P:103:THR:HA	18:P:106:ARG:NH1	2.04	0.72
1:O:545:G:H5'	1:O:545:G:C8	2.22	0.72
1:O:2421:G:H1'	38:O:6994:HOH:O	1.89	0.72
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.19	0.72
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.72	0.72
10:H:30:LYS:H	10:H:62:HIS:CD2	2.08	0.72
10:H:59:GLN:HE21	10:H:129:ARG:NE	1.86	0.72
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.55	0.72
16:N:38:LYS:HD2	16:N:114:LYS:HE3	1.72	0.71
1:O:1162:G:H1'	11:I:112:LEU:HD11	1.71	0.71
1:O:1632:A:H2'	1:O:1633:C:H5'	1.72	0.71
8:F:58:GLU:HG3	8:F:61:MET:HE2	1.69	0.71
1:O:236:A:H4'	1:O:237:G:H5'	1.72	0.71
14:L:143:THR:HG22	14:L:144:ASP:H	1.55	0.71
1:O:1289:C:H3'	38:O:6391:HOH:O	1.90	0.71
1:O:1666:C:H2'	1:O:1667:A:H5'	1.72	0.71
4:B:66:GLU:OE1	4:B:328:ARG:HD2	1.91	0.71
1:O:338:C:H4'	5:C:174:ILE:CD1	2.21	0.71
1:O:1735:C:OP2	4:B:234:ARG:HG3	1.90	0.71
4:B:56:ASP:OD1	4:B:322:ARG:HB3	1.91	0.71
5:C:140:VAL:HB	38:C:8648:HOH:O	1.89	0.71
27:Y:130:ARG:HB2	27:Y:142:SER:O	1.90	0.71
14:L:138:GLY:HA3	38:L:8856:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:21:SER:OG	17:O:106:PRO:HB2	1.91	0.71
1:O:2827:A:H2'	1:O:2828:G:O4'	1.91	0.71
6:D:25:MET:CE	6:D:37:ALA:HB1	2.20	0.71
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.72	0.71
1:O:1205:U:H2'	1:O:1206:U:C5'	2.21	0.71
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.73	0.71
21:S:51:GLN:HB3	21:S:67:ARG:NH1	2.03	0.71
29:1:10:LYS:HG3	38:1:2979:HOH:O	1.91	0.71
1:O:69:A:H5'	1:O:69:A:C8	2.26	0.70
1:O:272:A:H5'	1:O:273:G:OP2	1.91	0.70
5:C:188:ARG:HD3	38:C:8561:HOH:O	1.91	0.70
1:O:1919:A:H4'	38:O:4845:HOH:O	1.90	0.70
1:O:2004:U:H4'	38:O:5299:HOH:O	1.91	0.70
14:L:136:ALA:HB3	38:L:8875:HOH:O	1.90	0.70
1:O:182:G:H5'	38:O:5146:HOH:O	1.92	0.70
1:O:1450:C:O2'	1:O:1494:A:H5'	1.92	0.70
1:O:2251:G:H2'	1:O:2252:A:C8	2.27	0.70
2:9:73:A:H61	2:9:108:C:H42	1.39	0.70
17:O:14:LEU:HA	17:O:102:ILE:HD11	1.73	0.70
7:E:126:ILE:HB	7:E:131:LEU:HD21	1.74	0.70
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.57	0.70
21:S:33:SER:OG	21:S:36:GLU:HG3	1.92	0.70
8:F:27:GLY:HA3	8:F:101:ALA:O	1.91	0.70
12:J:107:ASN:C	12:J:107:ASN:HD22	2.00	0.70
26:X:25:ARG:HD2	38:X:3861:HOH:O	1.90	0.70
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.74	0.70
16:N:154:LEU:O	16:N:155:GLU:HB3	1.91	0.69
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.22	0.69
38:O:4621:HOH:O	3:A:6:GLY:HA3	1.91	0.69
4:B:305:ASP:O	4:B:306:LYS:HB2	1.90	0.69
5:C:98:ARG:HG2	5:C:98:ARG:HH11	1.57	0.69
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.73	0.69
1:O:2506:A:O2'	1:O:2507:G:H8	1.76	0.69
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.57	0.69
1:O:2414:A:H2'	1:O:2415:A:C8	2.26	0.69
5:C:1:MET:HG2	5:C:2:GLN:N	2.05	0.69
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.74	0.69
1:O:541:C:H2'	1:O:542:A:C5'	2.22	0.69
3:A:11:ARG:HA	38:A:8912:HOH:O	1.93	0.69
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.28	0.69
12:J:52:GLN:HG3	12:J:53:ILE:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1654:U:H2'	3:A:47:HIS:HD2	1.58	0.69
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.40	0.69
21:S:57:THR:HG22	21:S:59:ASP:H	1.57	0.69
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.75	0.69
8:F:91:VAL:HG12	8:F:92:GLY:N	2.07	0.69
12:J:19:MET:HE2	12:J:79:PHE:HA	1.74	0.69
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.58	0.69
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.73	0.69
25:W:80:ASP:HB2	38:W:3312:HOH:O	1.92	0.69
1:O:2637:A:H5'	38:O:9269:HOH:O	1.92	0.69
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.23	0.69
10:H:146:ALA:O	10:H:149:VAL:HG12	1.93	0.68
20:R:39:THR:HB	20:R:42:GLU:CG	2.23	0.68
1:O:69:A:H5'	1:O:69:A:H8	1.58	0.68
1:O:544:G:H2'	1:O:545:G:H5''	1.74	0.68
1:O:1181:A:H5'	11:I:89:GLU:OE2	1.93	0.68
2:9:29:C:H2'	2:9:30:C:H5'	1.74	0.68
3:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.23	0.68
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.93	0.68
1:O:1589:G:N2	1:O:1605:G:H1'	2.07	0.68
1:O:1972:U:H2'	1:O:1973:A:H5'	1.75	0.68
14:L:148:GLU:HA	38:L:8874:HOH:O	1.93	0.68
1:O:272:A:H3'	38:O:7500:HOH:O	1.91	0.68
1:O:2320:U:H4'	1:O:2321:A:O4'	1.93	0.68
3:A:43:VAL:HG21	3:A:59:GLU:HG3	1.76	0.68
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.40	0.68
29:1:25:LYS:HE2	38:2:7213:HOH:O	1.92	0.68
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.08	0.68
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.74	0.68
1:O:200:C:H2'	38:O:3438:HOH:O	1.93	0.68
1:O:1234:U:N3	4:B:244:PRO:HB3	2.09	0.68
2:9:6:C:C5'	16:N:37:ARG:NH1	2.55	0.68
21:S:57:THR:HG22	21:S:59:ASP:N	2.09	0.68
27:Y:212:ARG:HD2	38:Y:8905:HOH:O	1.93	0.68
1:O:1741:U:O2'	1:O:2723:G:H4'	1.93	0.68
1:O:2047:C:H5'	38:O:9811:HOH:O	1.92	0.68
5:C:28:SER:HB2	38:C:8659:HOH:O	1.94	0.68
19:Q:28:ARG:HG2	38:Q:4350:HOH:O	1.93	0.68
1:O:1485:A:H4'	38:O:3277:HOH:O	1.94	0.68
2:9:14:G:H5'	2:9:14:G:C8	2.27	0.68
5:C:236:THR:H	5:C:239:ALA:HB3	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1474:C:H5'	1:0:1474:C:C6	2.28	0.68
38:0:7001:HOH:O	3:A:211:LYS:HG2	1.92	0.68
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.76	0.68
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.24	0.68
1:0:450:C:OP1	5:C:184:ARG:NH2	2.27	0.68
2:9:114:G:O6	16:N:11:ARG:HD3	1.94	0.68
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.19	0.68
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.51	0.68
1:0:2433:A:H2'	1:0:2434:A:C8	2.29	0.67
6:D:50:VAL:O	6:D:71:ALA:HA	1.93	0.67
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.76	0.67
10:H:30:LYS:H	10:H:62:HIS:HD2	1.39	0.67
10:H:66:GLU:HA	38:H:8566:HOH:O	1.94	0.67
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.09	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.29	0.67
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.76	0.67
7:E:169:THR:HG22	7:E:170:ARG:HG3	1.77	0.67
24:V:38:GLY:C	24:V:40:PRO:HD2	2.19	0.67
1:0:1080:C:H4'	1:0:1081:A:OP1	1.94	0.67
2:9:28:U:H5''	16:N:40:ASN:HD21	1.57	0.67
4:B:162:MET:CE	4:B:308:LEU:HD21	2.23	0.67
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.60	0.67
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.23	0.67
1:0:1132:A:N6	1:0:1229:C:H2'	2.10	0.67
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.23	0.67
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.76	0.67
31:3:73:GLU:HB3	38:3:8861:HOH:O	1.94	0.67
3:A:191:GLY:HA2	3:A:194:MET:CE	2.23	0.67
10:H:49:GLN:NE2	10:H:140:TYR:HE2	1.92	0.67
1:0:338:C:H3'	38:0:3799:HOH:O	1.94	0.67
11:I:120:ALA:O	11:I:124:VAL:HG23	1.94	0.67
1:0:2812:A:H2	1:0:2814:A:H62	1.43	0.67
2:9:6:C:C5'	16:N:37:ARG:HH12	2.03	0.67
4:B:125:GLU:O	4:B:129:ARG:HG3	1.95	0.67
8:F:26:THR:HG21	8:F:103:GLU:CB	2.22	0.67
19:Q:94:GLN:O	19:Q:95:GLU:HB2	1.95	0.67
25:W:52:VAL:HG22	25:W:53:ALA:H	1.59	0.67
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.93	0.67
1:0:2237:G:H1'	38:0:4849:HOH:O	1.93	0.67
12:J:107:ASN:ND2	12:J:109:TYR:H	1.92	0.67
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.76	0.66
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.92	0.66
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.10	0.66
25:W:13:MET:CE	25:W:18:GLN:HA	2.25	0.66
10:H:12:ILE:HG23	10:H:129:ARG:CZ	2.25	0.66
22:T:48:VAL:HG22	22:T:98:VAL:HA	1.76	0.66
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.77	0.66
9:G:64:ASN:HD22	9:G:64:ASN:N	1.91	0.66
10:H:69:ARG:NH2	10:H:70:LEU:HD12	2.11	0.66
17:O:32:ARG:O	17:O:32:ARG:HD3	1.93	0.66
4:B:119:HIS:O	4:B:121:PRO:HD3	1.96	0.66
4:B:141:ARG:HD2	4:B:163:GLU:OE2	1.95	0.66
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.77	0.66
23:U:9:CYS:SG	23:U:11:THR:HG23	2.35	0.66
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.96	0.66
5:C:2:GLN:HB3	38:C:8535:HOH:O	1.95	0.66
1:O:2054:A:N3	20:R:128:ARG:NH2	2.44	0.66
38:9:8664:HOH:O	16:N:147:ILE:HB	1.95	0.66
3:A:94:LEU:HD23	3:A:94:LEU:N	2.10	0.66
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.61	0.66
38:0:4964:HOH:O	10:H:61:ARG:HG3	1.94	0.66
38:0:9351:HOH:O	29:1:1:THR:HA	1.96	0.66
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.24	0.66
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.59	0.66
28:Z:10:ARG:HG3	28:Z:11:SER:H	1.61	0.66
1:O:470:U:O2'	29:1:16:HIS:HD2	1.79	0.66
1:O:1372:A:H3'	38:0:7165:HOH:O	1.95	0.66
1:O:1589:G:H22	1:O:1605:G:H1'	1.60	0.66
4:B:140:LEU:HD23	38:B:8874:HOH:O	1.96	0.66
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.60	0.66
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.77	0.66
20:R:39:THR:HG23	20:R:107:GLU:O	1.96	0.66
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.95	0.66
1:O:1097:A:H5''	25:W:125:HIS:NE2	2.11	0.66
38:0:5522:HOH:O	15:M:58:GLN:HG3	1.95	0.66
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.61	0.66
15:M:164:THR:HG22	15:M:166:ALA:N	2.10	0.66
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.11	0.66
24:V:4:HIS:HB3	38:V:6622:HOH:O	1.95	0.66
1:O:308:U:H5'	1:O:309:C:OP1	1.96	0.65
1:O:2502:C:C2'	1:O:2503:A:H5'	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:C2'	1:0:2770:G:H5'	2.26	0.65
38:0:9891:HOH:O	12:J:18:ILE:HG23	1.95	0.65
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.78	0.65
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.77	0.65
1:0:1160:G:H5'	1:0:1161:A:C5'	2.25	0.65
1:0:2502:C:H2'	1:0:2503:A:H5'	1.78	0.65
14:L:145:LEU:O	14:L:148:GLU:HG3	1.96	0.65
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.78	0.65
1:0:1741:U:H5'	1:0:1742:A:OP1	1.97	0.65
1:0:156:C:H5''	15:M:171:ARG:CD	2.19	0.65
4:B:86:ALA:HA	38:B:8874:HOH:O	1.96	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.96	0.65
1:0:1505:U:H6	1:0:1505:U:H5'	1.60	0.65
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.78	0.65
1:0:2491:G:H1'	38:0:6841:HOH:O	1.97	0.65
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.79	0.65
1:0:2281:C:H2'	1:0:2282:U:H5'	1.78	0.65
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.78	0.65
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.94	0.65
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.79	0.65
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.12	0.65
1:0:513:A:N3	38:0:3656:HOH:O	2.29	0.65
1:0:2679:G:H2'	1:0:2681:A:OP2	1.95	0.65
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.60	0.65
10:H:165:ARG:HD2	38:H:8568:HOH:O	1.96	0.64
20:R:99:ALA:HB1	20:R:109:MET:CE	2.27	0.64
1:0:681:G:N3	1:0:681:G:H5'	2.13	0.64
1:0:2411:C:H4'	38:0:4946:HOH:O	1.97	0.64
3:A:194:MET:HE3	3:A:199:HIS:HB2	1.79	0.64
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.79	0.64
14:L:149:ARG:O	14:L:150:GLN:HB2	1.96	0.64
1:0:396:U:OP2	31:3:38:ARG:HD2	1.97	0.64
25:W:65:VAL:HA	25:W:68:THR:CG2	2.27	0.64
1:0:2459:G:H3'	38:0:6980:HOH:O	1.97	0.64
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.32	0.64
21:S:81:ILE:HG12	38:S:8534:HOH:O	1.97	0.64
24:V:39:ALA:C	24:V:41:GLU:H	2.06	0.64
3:A:41:THR:HG23	3:A:77:GLY:O	1.98	0.64
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.78	0.64
1:O:281:U:H2'	1:O:282:C:O4'	1.97	0.64
1:O:459:A:H4'	38:O:9445:HOH:O	1.97	0.64
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.38	0.64
1:O:1164:U:H3	1:O:1192:A:H2	1.44	0.64
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.80	0.64
4:B:98:THR:HG22	4:B:99:GLU:H	1.63	0.64
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.79	0.64
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.79	0.64
1:O:1733:A:H4'	4:B:212:GLN:HA	1.80	0.64
1:O:1834:C:H2'	1:O:1840:A:N6	2.12	0.64
38:O:4483:HOH:O	18:P:37:ARG:HB2	1.97	0.64
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.13	0.64
1:O:2445:U:H2'	1:O:2446:G:C8	2.33	0.63
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.80	0.63
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.80	0.63
6:D:128:LEU:N	38:D:3349:HOH:O	2.30	0.63
23:U:52:THR:HG22	23:U:54:THR:H	1.63	0.63
1:O:558:C:C2'	1:O:559:U:H5''	2.28	0.63
1:O:1679:C:H5'	38:O:9318:HOH:O	1.98	0.63
3:A:65:ARG:O	3:A:66:ARG:HG3	1.98	0.63
3:A:88:ILE:O	3:A:88:ILE:HG22	1.97	0.63
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.44	0.63
13:K:26:ALA:HB2	13:K:64:MET:HE3	1.79	0.63
16:N:86:LEU:O	16:N:90:LEU:HG	1.98	0.63
26:X:43:VAL:HG12	26:X:44:ASP:N	2.12	0.63
1:O:1204:C:H1'	38:O:4742:HOH:O	1.98	0.63
1:O:2638:G:H1'	38:O:7729:HOH:O	1.98	0.63
4:B:248:ARG:O	4:B:251:VAL:HG13	1.98	0.63
6:D:136:ARG:HD2	6:D:155:HIS:O	1.99	0.63
6:D:154:LYS:H	6:D:154:LYS:CD	2.10	0.63
9:G:69:ARG:HD2	38:G:4619:HOH:O	1.98	0.63
11:I:108:HIS:N	11:I:109:PRO:HD2	2.13	0.63
17:O:44:ASN:OD1	17:O:65:LEU:HB2	1.99	0.63
1:O:558:C:H2'	1:O:559:U:C5'	2.28	0.63
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.79	0.63
5:C:77:ALA:O	5:C:78:ARG:HG3	1.99	0.63
13:K:37:TYR:HB3	38:K:7169:HOH:O	1.98	0.63
19:Q:26:PRO:O	19:Q:30:VAL:HG23	1.98	0.63
1:O:2111:G:H1'	38:O:9045:HOH:O	1.96	0.63
2:9:39:U:H3	2:9:42:C:H5''	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:196:THR:HG23	38:C:8599:HOH:O	1.97	0.63
11:I:87:PRO:O	11:I:89:GLU:HG3	1.99	0.63
21:S:32:ALA:HA	21:S:36:GLU:OE1	1.99	0.63
12:J:52:GLN:HG3	12:J:53:ILE:H	1.63	0.63
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.34	0.63
1:O:553:G:P	27:Y:204:ARG:HH22	2.22	0.63
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.99	0.63
1:O:558:C:O2'	1:O:559:U:H5''	1.98	0.63
1:O:2281:C:C2'	1:O:2282:U:H5'	2.28	0.63
1:O:2670:G:O2'	1:O:2671:U:H5'	1.98	0.63
4:B:297:VAL:HB	38:B:8901:HOH:O	1.98	0.63
1:O:1205:U:H2'	1:O:1206:U:H5'	1.80	0.62
7:E:68:HIS:O	7:E:72:MET:HG3	1.99	0.62
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	1.98	0.62
22:T:106:GLU:HG3	38:T:4913:HOH:O	1.99	0.62
1:O:506:G:H3'	38:O:3769:HOH:O	1.99	0.62
5:C:2:GLN:HB3	38:C:8582:HOH:O	1.98	0.62
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.29	0.62
16:N:80:SER:HB2	38:N:8835:HOH:O	1.99	0.62
1:O:371:U:H2'	1:O:372:A:H8	1.64	0.62
4:B:41:PHE:HA	4:B:79:MET:HE2	1.80	0.62
7:E:137:ASP:O	7:E:141:VAL:HG23	1.99	0.62
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.64	0.62
15:M:28:GLN:O	15:M:32:ARG:HG3	1.99	0.62
1:O:558:C:H5'	38:O:5247:HOH:O	1.98	0.62
1:O:711:G:H1'	38:O:7068:HOH:O	1.98	0.62
1:O:1119:G:N2	1:O:1246:A:C2	2.65	0.62
1:O:2276:U:H2'	1:O:2277:U:C6	2.34	0.62
3:A:194:MET:HE3	3:A:199:HIS:CB	2.30	0.62
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.34	0.62
10:H:12:ILE:HD12	10:H:57:THR:CG2	2.30	0.62
11:I:95:LEU:HD23	11:I:99:GLN:OE1	1.99	0.62
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.82	0.62
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.81	0.62
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.79	0.62
25:W:88:THR:HG22	25:W:89:ASP:H	1.63	0.62
28:Z:46:ARG:O	28:Z:57:CYS:HA	1.99	0.62
1:O:1266:U:H4'	27:Y:115:ARG:HH21	1.62	0.62
7:E:6:GLU:HA	7:E:46:THR:HG22	1.80	0.62
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.82	0.62
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:21:HIS:HB2	38:N:8831:HOH:O	1.99	0.62
16:N:93:GLN:HA	16:N:93:GLN:NE2	2.07	0.62
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.34	0.62
1:O:558:C:H2'	1:O:559:U:H5'	1.82	0.62
1:O:2748:G:H2'	38:O:7511:HOH:O	2.00	0.62
6:D:24:HIS:HB2	6:D:71:ALA:O	1.98	0.62
6:D:140:ARG:O	6:D:144:ARG:HG2	2.00	0.62
9:G:71:LEU:C	9:G:73:ASP:H	2.08	0.62
12:J:108:PRO:HG2	12:J:109:TYR:HD1	1.64	0.62
1:O:1118:A:C8	1:O:1118:A:C3'	2.80	0.62
1:O:1189:A:H1'	1:O:1209:C:O4'	1.99	0.62
2:9:39:U:H3'	2:9:40:C:H5''	1.81	0.62
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.26	0.62
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.29	0.62
10:H:72:ALA:HB2	10:H:156:ALA:HB2	1.82	0.62
11:I:94:ASP:O	11:I:95:LEU:HG	1.99	0.62
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.81	0.62
25:W:52:VAL:HG22	25:W:53:ALA:N	2.14	0.62
1:O:1130:U:H5'	38:O:7641:HOH:O	1.99	0.62
5:C:221:GLU:HG3	38:C:8548:HOH:O	2.00	0.62
11:I:96:SER:H	11:I:99:GLN:NE2	1.97	0.62
28:Z:57:CYS:O	28:Z:61:ASP:HA	2.00	0.62
3:A:109:GLU:HG2	3:A:116:GLY:H	1.65	0.61
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.29	0.61
38:C:8566:HOH:O	22:T:2:LYS:HE2	1.99	0.61
24:V:5:VAL:HG23	38:V:2271:HOH:O	2.00	0.61
25:W:4:LEU:HD23	25:W:54:PHE:CB	2.27	0.61
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.82	0.61
1:O:245:C:H2'	38:O:5562:HOH:O	1.99	0.61
1:O:1654:U:H2'	3:A:47:HIS:CD2	2.35	0.61
1:O:2715:G:N2	4:B:264:GLU:OE1	2.32	0.61
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.65	0.61
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.80	0.61
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.82	0.61
1:O:2769:C:H2'	1:O:2770:G:H5'	1.82	0.61
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.29	0.61
1:O:657:G:OP1	5:C:27:ARG:NH2	2.34	0.61
1:O:2840:A:H3'	38:O:7617:HOH:O	2.00	0.61
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.29	0.61
4:B:27:ASN:HD22	4:B:27:ASN:H	1.49	0.61
15:M:46:LEU:HG	38:M:8918:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:97:VAL:HG12	16:N:127:LEU:HD11	1.82	0.61
1:O:820:G:C6	3:A:171:LYS:HB2	2.34	0.61
1:O:1162:G:H1'	11:I:112:LEU:CD1	2.29	0.61
1:O:2346:C:O2'	6:D:52:THR:HG21	1.99	0.61
3:A:33:GLU:H	3:A:33:GLU:CD	2.07	0.61
6:D:35:ALA:C	6:D:37:ALA:H	2.09	0.61
6:D:64:ARG:NE	6:D:67:ASP:HB3	2.15	0.61
6:D:65:GLU:HA	38:D:6752:HOH:O	2.00	0.61
6:D:94:ALA:HA	6:D:174:VAL:O	2.01	0.61
11:I:108:HIS:HE1	11:I:116:LEU:HD22	1.64	0.61
38:O:7426:HOH:O	4:B:211:THR:HG21	2.00	0.61
4:B:43:GLY:O	4:B:308:LEU:HD12	2.00	0.61
8:F:46:GLU:OE1	8:F:100:ASP:HA	1.99	0.61
38:O:9660:HOH:O	17:O:112:ARG:HD2	2.00	0.61
11:I:96:SER:H	11:I:99:GLN:CD	2.08	0.61
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.83	0.61
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.33	0.61
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.61
5:C:111:VAL:HB	38:C:8521:HOH:O	2.01	0.61
7:E:11:VAL:HG12	7:E:12:ASP:N	2.16	0.61
15:M:125:ARG:HD3	38:M:8894:HOH:O	2.00	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.82	0.61
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.83	0.61
27:Y:184:GLU:OE2	27:Y:204:ARG:HD2	2.01	0.61
1:O:316:A:H5'	22:T:54:ASP:OD2	2.01	0.61
1:O:1118:A:H8	1:O:1119:G:H5''	1.66	0.61
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.83	0.61
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.16	0.61
12:J:107:ASN:HD22	12:J:109:TYR:H	1.48	0.61
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.83	0.61
21:S:51:GLN:CB	21:S:67:ARG:HH12	2.11	0.61
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.66	0.61
1:O:544:G:C2'	1:O:545:G:H5''	2.31	0.61
1:O:2795:C:O2'	1:O:2796:U:H5'	2.00	0.61
4:B:98:THR:HG22	4:B:99:GLU:N	2.15	0.61
5:C:233:THR:HG22	5:C:234:VAL:N	2.13	0.61
25:W:38:THR:HG22	38:W:3580:HOH:O	2.00	0.61
27:Y:205:ILE:HB	27:Y:230:ASN:HD21	1.66	0.61
1:O:2505:G:O2'	1:O:2506:A:H5'	2.01	0.60
10:H:41:LYS:HE2	10:H:45:ASP:HB3	1.82	0.60
17:O:105:ASN:HD21	17:O:109:SER:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:98:VAL:HG11	22:T:101:LEU:CD2	2.31	0.60
1:0:1165:G:H1'	1:0:1174:A:H1'	1.82	0.60
1:0:1477:C:H5'	1:0:1868:G:C5'	2.31	0.60
1:0:2359:G:H3'	38:0:5682:HOH:O	2.01	0.60
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.82	0.60
26:X:43:VAL:HG11	26:X:82:GLU:HA	1.82	0.60
4:B:145:HIS:HD2	4:B:146:THR:O	1.84	0.60
5:C:236:THR:HG21	38:C:8572:HOH:O	2.00	0.60
6:D:25:MET:HE2	6:D:41:LEU:CG	2.27	0.60
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.36	0.60
24:V:39:ALA:N	24:V:40:PRO:HD2	2.16	0.60
29:1:28:HIS:HD2	29:1:30:LYS:H	1.50	0.60
1:0:328:U:O4'	5:C:202:THR:HG22	2.02	0.60
38:0:6271:HOH:O	27:Y:158:LYS:HD3	2.01	0.60
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.82	0.60
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.30	0.60
1:0:21:G:H4'	20:R:2:ILE:HG22	1.83	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.01	0.60
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.28	0.60
1:0:1180:U:H1'	38:I:1549:HOH:O	2.02	0.60
1:0:1667:A:H5'	1:0:1667:A:C8	2.34	0.60
1:0:2404:G:H5''	38:0:5200:HOH:O	2.02	0.60
2:9:44:A:O4'	6:D:76:ARG:NE	2.34	0.60
3:A:192:VAL:HB	38:A:8889:HOH:O	2.01	0.60
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.32	0.60
4:B:177:HIS:O	4:B:181:ILE:HG13	2.02	0.60
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.36	0.60
15:M:60:VAL:C	15:M:61:ILE:HD12	2.27	0.60
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.33	0.60
1:0:1205:U:H2'	1:0:1206:U:H5''	1.84	0.60
1:0:2724:U:H2'	1:0:2725:G:O4'	2.01	0.60
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.17	0.60
4:B:84:LEU:HD23	4:B:178:ALA:HB1	1.83	0.60
20:R:104:PHE:HB2	20:R:109:MET:HE2	1.82	0.60
1:0:1118:A:C8	1:0:1119:G:H5''	2.36	0.60
1:0:1187:U:H2'	38:0:6870:HOH:O	2.01	0.60
1:0:1702:U:H5'	38:0:3420:HOH:O	2.01	0.60
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.32	0.60
15:M:102:GLU:CD	15:M:164:THR:HG21	2.26	0.60
1:0:1641:A:C2'	1:0:1642:A:H5'	2.31	0.60
1:0:2604:A:H5'	38:0:5778:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.83	0.60
29:1:25:LYS:HD2	30:2:49:GLU:H	1.65	0.60
1:0:820:G:O2'	1:0:856:G:H4'	2.01	0.60
1:0:1182:C:H1'	1:0:1192:A:H8	1.67	0.60
1:0:1278:A:H4'	1:0:1279:U:C4	2.37	0.60
1:0:1593:C:H5'	18:P:116:SER:O	2.02	0.60
4:B:53:LEU:HD21	4:B:270:ILE:HD12	1.84	0.60
10:H:157:TYR:CD1	10:H:157:TYR:C	2.79	0.60
10:H:157:TYR:C	10:H:157:TYR:HD1	2.10	0.60
23:U:9:CYS:CA	23:U:52:THR:HG23	2.31	0.60
23:U:52:THR:HG22	23:U:54:THR:N	2.17	0.60
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.84	0.60
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.31	0.60
1:0:1189:A:H1'	1:0:1209:C:C1'	2.31	0.59
1:0:1632:A:C2'	1:0:1633:C:H5'	2.31	0.59
11:I:108:HIS:N	11:I:109:PRO:CD	2.65	0.59
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.02	0.59
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.83	0.59
1:0:644:G:H5'	1:0:644:G:N3	2.16	0.59
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.83	0.59
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.59
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.59
1:0:2365:G:H4'	19:Q:45:PRO:O	2.01	0.59
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.85	0.59
11:I:95:LEU:CD2	11:I:99:GLN:HB3	2.32	0.59
16:N:154:LEU:C	16:N:156:GLU:H	2.08	0.59
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.32	0.59
1:0:399:C:H5'	15:M:179:GLY:O	2.02	0.59
1:0:506:G:H22	1:0:509:A:H5''	1.66	0.59
1:0:559:U:H2'	1:0:560:U:O4'	2.01	0.59
1:0:952:G:N3	1:0:2302:A:H2'	2.17	0.59
1:0:2103:A:C6	32:0:9000:CLY:H92	2.38	0.59
6:D:166:ILE:HB	38:D:6326:HOH:O	2.02	0.59
38:E:2512:HOH:O	12:J:127:ILE:HD11	2.02	0.59
10:H:49:GLN:HB2	10:H:170:ARG:HD2	1.85	0.59
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.17	0.59
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.02	0.59
1:0:1213:C:O2'	1:0:1214:G:H5'	2.01	0.59
1:0:2036:C:O4'	13:K:44:LEU:HG	2.02	0.59
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.84	0.59
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.01	0.59
24:V:49:LEU:O	24:V:53:ILE:HG13	2.02	0.59
1:0:704:C:H2'	1:0:705:C:H6	1.68	0.59
1:0:737:A:H2'	1:0:738:G:O4'	2.03	0.59
1:0:820:G:H3'	38:0:3042:HOH:O	2.03	0.59
1:0:1872:C:H5	3:A:20:SER:HB3	1.66	0.59
3:A:192:VAL:HG12	3:A:192:VAL:O	2.03	0.59
4:B:41:PHE:HA	4:B:79:MET:CE	2.32	0.59
5:C:107:ARG:NE	38:C:8653:HOH:O	2.29	0.59
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.32	0.59
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.84	0.59
30:2:41:HIS:N	30:2:45:ASN:HD22	1.98	0.59
1:0:2862:G:H4'	4:B:336:GLN:O	2.02	0.59
2:9:40:C:H42	6:D:53:LYS:HE3	1.67	0.59
13:K:89:LYS:HA	38:K:7064:HOH:O	2.00	0.59
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.03	0.59
1:0:138:U:OP2	1:0:139:C:H5	1.85	0.59
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.59
1:0:1634:G:H2'	1:0:1635:U:C6	2.37	0.59
1:0:1768:C:H2'	1:0:1769:C:O4'	2.02	0.59
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.84	0.59
8:F:56:PRO:HG2	15:M:43:PRO:O	2.01	0.59
8:F:99:THR:HA	38:F:3461:HOH:O	2.02	0.59
15:M:164:THR:HG22	15:M:165:GLY:N	2.16	0.59
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.33	0.59
15:M:57:LYS:HE2	15:M:140:ALA:O	2.03	0.59
20:R:40:ALA:O	20:R:44:VAL:HG23	2.02	0.59
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.43	0.59
1:0:1060:C:H6	1:0:1060:C:H5'	1.68	0.58
1:0:1168:C:H4'	38:I:5128:HOH:O	2.02	0.58
1:0:1500:U:P	18:P:41:ARG:HH22	2.26	0.58
2:9:13:A:O2'	2:9:14:G:H5''	2.02	0.58
2:9:34:A:H2'	2:9:35:C:O4'	2.03	0.58
3:A:48:ASP:HB3	38:A:8901:HOH:O	2.02	0.58
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.85	0.58
7:E:77:THR:OG1	7:E:78:GLU:N	2.36	0.58
12:J:46:ILE:HD11	12:J:53:ILE:HG23	1.85	0.58
23:U:9:CYS:HA	23:U:52:THR:CG2	2.32	0.58
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.17	0.58
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.18	0.58
1:0:289:G:O2'	1:0:290:C:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:129:LEU:HD12	3:A:145:MET:HE1	1.85	0.58
3:A:200:PRO:HD3	38:A:8816:HOH:O	2.03	0.58
4:B:85:ARG:NH1	38:B:8932:HOH:O	2.36	0.58
8:F:34:ASN:HA	15:M:4:ALA:HB2	1.83	0.58
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.85	0.58
16:N:132:ASN:O	16:N:135:VAL:HG12	2.03	0.58
20:R:33:ARG:NH1	38:R:8841:HOH:O	2.27	0.58
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.19	0.58
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.03	0.58
31:3:3:MET:O	31:3:90:PHE:HA	2.02	0.58
1:0:138:U:H5''	1:0:139:C:OP2	2.02	0.58
1:0:2821:C:H4'	4:B:116:PRO:HB3	1.84	0.58
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.18	0.58
15:M:80:GLY:O	15:M:81:ARG:HD2	2.03	0.58
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.85	0.58
1:0:21:G:H5''	20:R:1:GLY:O	2.04	0.58
1:0:945:U:H2'	1:0:946:C:C6	2.38	0.58
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.31	0.58
22:T:98:VAL:HG11	22:T:101:LEU:HD23	1.84	0.58
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.33	0.58
1:0:871:G:C8	1:0:871:G:C5'	2.77	0.58
1:0:1164:U:OP1	11:I:69:PRO:HA	2.04	0.58
1:0:1625:U:H4'	38:0:4667:HOH:O	2.03	0.58
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.58
38:0:5288:HOH:O	3:A:210:GLY:HA3	2.02	0.58
1:0:588:G:O6	25:W:154:ARG:NH1	2.37	0.58
1:0:1189:A:H3'	38:0:7649:HOH:O	2.04	0.58
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.14	0.58
5:C:168:ARG:NH2	5:C:190:ALA:O	2.37	0.58
10:H:174:LEU:HA	38:H:8557:HOH:O	2.04	0.58
3:A:88:ILE:CD1	3:A:100:PRO:HD3	2.31	0.58
20:R:39:THR:O	20:R:40:ALA:C	2.47	0.58
26:X:76:ARG:O	26:X:77:PHE:HB3	2.03	0.58
28:Z:54:ILE:HD12	38:Z:8716:HOH:O	2.04	0.58
1:0:1116:U:O2'	1:0:1118:A:H2	1.73	0.58
13:K:82:ARG:HH21	13:K:115:ARG:HG2	1.69	0.58
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.69	0.58
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.33	0.58
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.37	0.58
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.38	0.58
1:0:56:G:H5''	24:V:50:ARG:NH1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1383:U:H5''	38:0:6636:HOH:O	2.03	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.58
2:9:6:C:OP1	16:N:37:ARG:NH1	2.37	0.58
4:B:7:ARG:NH1	4:B:11:LEU:HD21	2.18	0.58
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.38	0.58
14:L:55:GLN:HA	14:L:58:GLN:HE21	1.69	0.58
14:L:133:VAL:HB	38:L:8859:HOH:O	2.03	0.58
28:Z:10:ARG:HA	38:Z:8715:HOH:O	2.04	0.58
1:0:659:A:H5''	38:0:7071:HOH:O	2.04	0.57
1:0:2667:G:H1'	1:0:2914:A:N3	2.18	0.57
2:9:20:G:H3'	38:9:8634:HOH:O	2.04	0.57
3:A:129:LEU:CD1	3:A:145:MET:HE1	2.33	0.57
7:E:84:MET:HE2	7:E:133:VAL:HG22	1.84	0.57
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.69	0.57
12:J:84:ARG:HB2	12:J:98:PHE:CE1	2.39	0.57
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.86	0.57
1:0:1160:G:O2'	1:0:1190:G:H1'	2.03	0.57
5:C:18:LEU:HD12	5:C:19:PRO:HD2	1.85	0.57
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.38	0.57
15:M:157:ASP:HB3	15:M:160:PHE:HD1	1.69	0.57
20:R:104:PHE:CB	20:R:109:MET:HE2	2.33	0.57
27:Y:197:ASP:OD2	27:Y:200:THR:HB	2.04	0.57
31:3:69:TYR:O	31:3:77:ALA:HA	2.04	0.57
1:0:1972:U:H2'	1:0:1973:A:C5'	2.35	0.57
1:0:2265:U:H2'	1:0:2266:A:C8	2.39	0.57
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.70	0.57
6:D:99:ASP:HB3	6:D:103:ASN:H	1.69	0.57
14:L:55:GLN:HA	14:L:58:GLN:NE2	2.20	0.57
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.19	0.57
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.04	0.57
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.20	0.57
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.85	0.57
38:0:3985:HOH:O	22:T:82:THR:HA	2.05	0.57
2:9:35:C:H5''	38:9:8654:HOH:O	2.04	0.57
2:9:48:C:H4'	16:N:141:ARG:HH21	1.69	0.57
5:C:103:ASN:HA	38:C:8588:HOH:O	2.03	0.57
13:K:55:VAL:HG12	13:K:56:SER:N	2.18	0.57
1:0:246:G:H5'	38:0:5562:HOH:O	2.03	0.57
1:0:1544:U:H2'	1:0:1545:C:H6	1.69	0.57
2:9:64:C:H2'	2:9:65:A:H5'	1.86	0.57
14:L:61:ALA:HA	38:L:8866:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.19	0.57
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57
1:0:1015:C:H2'	1:0:1016:U:H6	1.68	0.57
1:0:2361:A:H5'	1:0:2361:A:H8	1.70	0.57
1:0:2401:A:H5'	38:0:9486:HOH:O	2.04	0.57
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.69	0.57
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.86	0.57
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.35	0.57
16:N:42:HIS:HA	16:N:75:THR:O	2.05	0.57
18:P:138:GLU:HA	18:P:141:ILE:HD12	1.86	0.57
22:T:19:ARG:NH1	22:T:68:ASP:O	2.37	0.57
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.67	0.57
22:T:73:HIS:HB3	38:T:6320:HOH:O	2.04	0.57
29:1:28:HIS:ND1	29:1:31:LYS:HE2	2.18	0.57
1:0:1154:A:H2'	1:0:1155:G:C8	2.39	0.57
1:0:1393:A:H2'	1:0:1394:C:C6	2.40	0.57
38:0:6490:HOH:O	30:2:1:GLY:HA3	2.05	0.57
13:K:125:ALA:C	13:K:127:ALA:H	2.12	0.57
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.19	0.57
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.69	0.57
1:0:447:A:OP1	22:T:2:LYS:HG2	2.05	0.57
1:0:2469:A:H1'	38:0:3233:HOH:O	2.04	0.57
38:0:9530:HOH:O	18:P:81:LYS:HG2	2.03	0.57
4:B:223:ARG:HG3	4:B:232:TRP:O	2.04	0.57
4:B:275:GLY:O	4:B:291:ASP:HA	2.05	0.57
14:L:143:THR:HG22	14:L:144:ASP:N	2.20	0.57
1:0:1170:U:H2'	1:0:1172:G:OP2	2.05	0.57
1:0:1562:C:O2	1:0:1562:C:H2'	2.05	0.57
1:0:2851:G:O2'	1:0:2852:A:H5'	2.05	0.57
8:F:101:ALA:HA	38:F:5413:HOH:O	2.04	0.57
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.05	0.57
16:N:114:LYS:O	16:N:117:ALA:HB3	2.04	0.57
18:P:14:LEU:HD13	18:P:51:ALA:HB2	1.87	0.57
21:S:57:THR:C	21:S:59:ASP:H	2.13	0.57
22:T:64:ASN:HA	38:T:5927:HOH:O	2.04	0.57
1:0:1535:G:H2'	1:0:1536:C:C6	2.40	0.56
1:0:2003:U:H4'	1:0:2004:U:H5	1.70	0.56
1:0:2055:A:H4'	20:R:132:ARG:NH2	2.19	0.56
4:B:162:MET:HG3	4:B:310:ARG:NH1	2.19	0.56
6:D:172:VAL:HG12	6:D:173:GLU:N	2.19	0.56
26:X:85:VAL:HG12	26:X:86:GLU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:660:A:H4'	1:0:661:G:O5'	2.05	0.56
2:9:49:G:H5''	38:9:8664:HOH:O	2.04	0.56
3:A:66:ARG:HB2	3:A:66:ARG:NH1	2.17	0.56
15:M:164:THR:CG2	15:M:165:GLY:N	2.67	0.56
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.86	0.56
25:W:65:VAL:CA	25:W:68:THR:HG22	2.35	0.56
1:0:106:A:H1'	38:0:9491:HOH:O	2.05	0.56
1:0:777:U:O2'	29:1:11:LYS:HG2	2.05	0.56
1:0:1377:C:H5'	1:0:1377:C:H6	1.70	0.56
1:0:1446:U:H2'	21:S:55:GLN:NE2	2.19	0.56
1:0:1771:U:H5'	28:Z:20:ARG:HH21	1.69	0.56
38:0:7039:HOH:O	20:R:33:ARG:HD3	2.04	0.56
3:A:186:TRP:CG	3:A:187:PRO:HA	2.40	0.56
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.35	0.56
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.41	0.56
11:I:95:LEU:HD22	11:I:99:GLN:HB3	1.86	0.56
20:R:39:THR:HB	20:R:42:GLU:CD	2.30	0.56
23:U:47:ARG:HG3	38:U:4381:HOH:O	2.04	0.56
1:0:1185:U:H5'	38:0:7437:HOH:O	2.05	0.56
1:0:2781:U:O2'	1:0:2782:G:H5'	2.05	0.56
6:D:23:VAL:HG23	6:D:23:VAL:O	2.05	0.56
15:M:61:ILE:HA	38:M:8920:HOH:O	2.05	0.56
16:N:93:GLN:HG2	38:N:8855:HOH:O	2.06	0.56
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.41	0.56
25:W:69:ARG:NH2	38:W:4276:HOH:O	2.38	0.56
1:0:1805:G:H2'	1:0:1806:G:H8	1.68	0.56
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.40	0.56
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.69	0.56
2:9:54:A:O2'	2:9:55:U:H5'	2.05	0.56
3:A:76:VAL:HG23	28:Z:63:LYS:O	2.05	0.56
5:C:107:ARG:O	5:C:111:VAL:HG23	2.05	0.56
5:C:236:THR:O	5:C:237:GLU:C	2.48	0.56
8:F:37:THR:O	8:F:41:GLU:HG3	2.05	0.56
11:I:127:CYS:N	38:I:7330:HOH:O	2.39	0.56
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.87	0.56
18:P:115:SER:O	18:P:117:SER:N	2.38	0.56
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.87	0.56
27:Y:219:GLU:HG3	27:Y:220:GLU:N	2.21	0.56
1:0:42:C:H1'	38:0:4675:HOH:O	2.06	0.56
1:0:221:G:H2'	1:0:222:A:C8	2.40	0.56
1:0:1603:A:H5''	1:0:1605:G:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2510:C:H42	1:0:2564:G:H22	1.53	0.56
1:0:2850:C:H5'	1:0:2850:C:C6	2.40	0.56
1:0:2910:A:H5''	38:0:4126:HOH:O	2.04	0.56
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.35	0.56
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.05	0.56
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.33	0.56
20:R:132:ARG:HG2	20:R:133:ALA:N	2.20	0.56
30:2:39:ARG:HG2	38:2:3143:HOH:O	2.04	0.56
1:0:2578:G:H5'	1:0:2578:G:C8	2.39	0.56
2:9:57:A:H8	6:D:141:VAL:HG21	1.71	0.56
2:9:96:C:H2'	2:9:97:U:C6	2.40	0.56
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.87	0.56
1:0:396:U:O2'	1:0:418:C:H4'	2.06	0.56
2:9:1:U:H5''	2:9:3:A:OP1	2.06	0.56
2:9:95:C:O2'	2:9:96:C:H5'	2.05	0.56
10:H:79:GLU:C	10:H:80:LEU:HD23	2.31	0.56
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.36	0.56
19:Q:14:LEU:HD21	19:Q:43:ILE:HD12	1.88	0.56
21:S:33:SER:O	21:S:37:VAL:HG23	2.06	0.56
21:S:43:GLU:HB3	38:S:8540:HOH:O	2.05	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.05	0.56
1:0:2435:U:H1'	38:0:5419:HOH:O	2.06	0.56
5:C:72:LYS:HD2	38:C:8622:HOH:O	2.06	0.56
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.87	0.56
12:J:88:PRO:HA	36:J:8802:CL:CL	2.42	0.56
1:0:281:U:H3'	38:0:7182:HOH:O	2.05	0.56
1:0:710:G:OP1	17:O:24:ALA:HB3	2.07	0.56
1:0:1701:A:H4'	1:0:1702:U:C5'	2.36	0.56
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.06	0.56
38:0:7415:HOH:O	3:A:211:LYS:NZ	2.37	0.56
3:A:51:ARG:NH1	3:A:120:ARG:O	2.38	0.56
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.19	0.56
6:D:146:LYS:HZ1	16:N:107:ASN:ND2	2.03	0.56
7:E:7:ILE:HD11	7:E:11:VAL:C	2.32	0.56
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.56
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.21	0.56
26:X:78:GLU:HG2	26:X:79:GLU:N	2.21	0.56
1:0:383:A:H2'	1:0:384:G:O4'	2.06	0.55
1:0:1120:U:H5''	1:0:1120:U:C6	2.41	0.55
1:0:2421:G:H2'	38:0:4074:HOH:O	2.05	0.55
7:E:69:ILE:HA	7:E:72:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:23:LEU:HD22	24:V:49:LEU:HD23	1.87	0.55
1:0:285:A:H2'	1:0:286:U:O4'	2.06	0.55
1:0:539:G:H2'	1:0:540:A:C8	2.41	0.55
1:0:820:G:H5'	1:0:821:U:H5'	1.88	0.55
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.88	0.55
16:N:115:VAL:HG23	16:N:116:PHE:H	1.70	0.55
25:W:122:ARG:HG3	25:W:122:ARG:HH11	1.71	0.55
1:0:960:G:N3	1:0:960:G:H2'	2.21	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
1:0:2884:G:H5'	38:0:4125:HOH:O	2.06	0.55
4:B:280:VAL:HG13	4:B:333:GLU:O	2.07	0.55
4:B:294:TYR:HE2	38:B:8950:HOH:O	1.89	0.55
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.20	0.55
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.07	0.55
11:I:73:LEU:HD12	11:I:107:LYS:NZ	2.20	0.55
20:R:132:ARG:CZ	38:R:8878:HOH:O	2.53	0.55
1:0:1015:C:H2'	1:0:1016:U:C6	2.41	0.55
1:0:1416:G:H2'	1:0:1417:G:H5'	1.88	0.55
1:0:2831:C:H2'	1:0:2832:C:H5'	1.89	0.55
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.36	0.55
12:J:131:THR:HB	12:J:134:GLU:OE1	2.05	0.55
14:L:104:ASP:O	14:L:105:TYR:HB3	2.06	0.55
18:P:115:SER:HB2	38:P:176:HOH:O	2.06	0.55
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.89	0.55
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.07	0.55
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.07	0.55
1:0:1682:A:H5''	38:0:9448:HOH:O	2.05	0.55
1:0:2073:G:OP2	1:0:2490:A:H5'	2.06	0.55
5:C:132:ASP:HB3	38:C:8562:HOH:O	2.07	0.55
6:D:10:PHE:CG	6:D:11:HIS:N	2.74	0.55
28:Z:51:GLY:HA3	38:Z:8716:HOH:O	2.05	0.55
1:0:1242:A:H5'	12:J:82:THR:CG2	2.30	0.55
1:0:1636:G:O2'	1:0:1637:A:H5'	2.06	0.55
4:B:60:SER:C	4:B:62:ARG:H	2.13	0.55
7:E:81:GLU:O	7:E:172:PRO:HD3	2.07	0.55
11:I:95:LEU:O	11:I:134:ILE:HG23	2.07	0.55
16:N:176:ARG:O	16:N:180:LEU:HD13	2.06	0.55
20:R:114:VAL:HG13	20:R:114:VAL:O	2.06	0.55
22:T:18:GLU:O	22:T:21:LYS:HG2	2.06	0.55
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.06	0.55
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:24:G:N2	1:0:518:G:H1'	2.21	0.55
1:0:346:U:H4'	38:0:6817:HOH:O	2.05	0.55
1:0:474:C:O3'	5:C:73:LEU:HD21	2.06	0.55
1:0:945:U:O2'	25:W:43:GLY:HA3	2.06	0.55
1:0:1183:C:H2'	38:0:6232:HOH:O	2.05	0.55
1:0:2834:G:OP1	26:X:39:LYS:HE2	2.06	0.55
3:A:35:GLY:O	3:A:36:ASP:CB	2.53	0.55
5:C:236:THR:O	5:C:239:ALA:N	2.40	0.55
6:D:55:LYS:HB2	38:D:5708:HOH:O	2.05	0.55
9:G:64:ASN:N	9:G:64:ASN:ND2	2.53	0.55
10:H:23:ILE:HG23	10:H:123:ILE:CD1	2.36	0.55
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.05	0.55
16:N:100:ALA:O	16:N:129:ILE:HG23	2.06	0.55
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.88	0.55
1:0:2241:C:O2'	1:0:2242:U:H5'	2.07	0.55
1:0:2443:C:H1'	14:L:56:LYS:HE3	1.89	0.55
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.55
2:9:43:G:H5'	38:9:8608:HOH:O	2.07	0.55
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.06	0.55
12:J:6:PHE:O	12:J:8:ALA:N	2.39	0.55
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.89	0.55
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.36	0.55
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.06	0.55
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.88	0.55
28:Z:46:ARG:CD	28:Z:59:TYR:HB2	2.28	0.55
1:0:120:A:H2'	1:0:120:A:N3	2.22	0.55
1:0:383:A:H4'	38:0:5319:HOH:O	2.06	0.55
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.06	0.55
1:0:944:G:H21	25:W:44:MET:CE	2.20	0.55
3:A:179:MET:HA	3:A:179:MET:HE3	1.88	0.55
5:C:130:GLU:OE1	5:C:130:GLU:HA	2.07	0.55
9:G:64:ASN:O	9:G:68:GLU:HG3	2.07	0.55
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.88	0.55
16:N:91:ARG:HD3	38:N:8814:HOH:O	2.05	0.55
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.89	0.55
25:W:76:ASP:O	25:W:77:ALA:C	2.50	0.55
1:0:652:G:H8	38:0:3005:HOH:O	1.90	0.55
1:0:2768:A:H2'	1:0:2769:C:O4'	2.07	0.55
38:0:4607:HOH:O	3:A:206:ARG:HG2	2.06	0.55
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.07	0.55
10:H:69:ARG:HD3	38:H:8566:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:88:GLN:HA	11:I:91:PHE:CE2	2.41	0.55
1:O:1507:C:H4'	38:O:3598:HOH:O	2.05	0.54
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.37	0.54
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.40	0.54
3:A:206:ARG:HH11	3:A:208:HIS:CD2	2.25	0.54
10:H:12:ILE:O	10:H:12:ILE:HG22	2.05	0.54
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.22	0.54
14:L:42:ASN:HB2	38:L:8877:HOH:O	2.05	0.54
17:O:73:ASP:HA	17:O:92:VAL:O	2.06	0.54
27:Y:189:ASN:HD22	27:Y:191:ASP:N	2.05	0.54
29:1:25:LYS:O	29:1:25:LYS:HG2	2.06	0.54
30:2:48:ASP:O	30:2:49:GLU:HB2	2.07	0.54
1:O:67:A:H5''	1:O:69:A:C8	2.43	0.54
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.89	0.54
6:D:86:THR:HG23	38:D:7477:HOH:O	2.06	0.54
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.37	0.54
12:J:133:GLY:O	12:J:137:GLU:HG3	2.07	0.54
19:Q:24:SER:HB3	19:Q:28:ARG:HH21	1.72	0.54
1:O:1175:G:H1'	1:O:1193:A:H2'	1.90	0.54
1:O:2105:C:H2'	1:O:2106:C:C6	2.42	0.54
2:9:57:A:C8	6:D:141:VAL:HG21	2.43	0.54
5:C:154:VAL:O	5:C:158:GLU:HG3	2.07	0.54
10:H:12:ILE:HG23	10:H:129:ARG:NE	2.22	0.54
12:J:103:VAL:HG12	38:J:8868:HOH:O	2.06	0.54
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.72	0.54
1:O:705:C:O2	1:O:705:C:H2'	2.07	0.54
1:O:797:A:C4'	28:Z:10:ARG:N	2.70	0.54
1:O:1373:G:H1'	38:O:6128:HOH:O	2.06	0.54
1:O:2769:C:H2'	1:O:2770:G:C5'	2.38	0.54
4:B:41:PHE:HB3	4:B:190:MET:CE	2.36	0.54
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.42	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
1:O:933:C:H4'	1:O:1297:U:H4'	1.89	0.54
1:O:1787:C:H4'	1:O:2883:A:O4'	2.08	0.54
1:O:2336:G:H1'	38:D:5675:HOH:O	2.07	0.54
1:O:2730:G:O2'	1:O:2731:G:H5'	2.08	0.54
4:B:305:ASP:O	4:B:306:LYS:CB	2.55	0.54
7:E:21:THR:HG23	7:E:30:THR:OG1	2.08	0.54
1:O:1163:G:H5'	11:I:110:ASP:O	2.08	0.54
1:O:1235:G:C1'	12:J:63:ILE:HG23	2.37	0.54
1:O:2474:A:N7	1:O:2621:PSU:H4'	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:109:LEU:HD12	5:C:109:LEU:O	2.07	0.54
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.08	0.54
15:M:139:PRO:HA	15:M:142:GLN:HB2	1.89	0.54
16:N:152:GLU:OE1	16:N:152:GLU:HA	2.07	0.54
16:N:171:HIS:CE1	38:N:8864:HOH:O	2.61	0.54
25:W:1:MET:HE3	25:W:101:LEU:HD23	1.90	0.54
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.08	0.54
27:Y:234:VAL:HG12	27:Y:235:GLU:H	1.73	0.54
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.90	0.54
1:0:902:G:N7	14:L:18:HIS:CD2	2.71	0.54
1:0:1634:G:H3'	38:0:3894:HOH:O	2.08	0.54
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.54
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.90	0.54
31:3:55:VAL:HG22	38:3:8809:HOH:O	2.08	0.54
1:0:2897:C:H2'	1:0:2898:G:H8	1.72	0.54
1:0:2900:G:H2'	1:0:2901:C:O4'	2.08	0.54
4:B:132:HIS:NE2	4:B:171:VAL:HG23	2.23	0.54
9:G:63:ARG:N	38:G:2569:HOH:O	2.40	0.54
13:K:113:ILE:HG22	13:K:114:ALA:N	2.21	0.54
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.90	0.54
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.90	0.54
24:V:64:GLY:O	24:V:65:ASP:HB2	2.06	0.54
25:W:80:ASP:O	25:W:84:VAL:HG23	2.08	0.54
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.90	0.54
1:0:564:G:H1'	38:0:6293:HOH:O	2.07	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.82	0.54
1:0:1943:C:O4'	3:A:212:PRO:HA	2.06	0.54
1:0:2468:A:H61	31:3:48:ASN:HD21	1.56	0.54
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.54
1:0:2577:A:H5'	38:0:7721:HOH:O	2.08	0.54
1:0:2748:G:H1'	38:0:7873:HOH:O	2.08	0.54
3:A:22:ARG:HB3	38:A:8874:HOH:O	2.07	0.54
4:B:280:VAL:HG12	4:B:334:SER:HA	1.89	0.54
5:C:49:ASP:HB3	5:C:52:ALA:HB2	1.90	0.54
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.38	0.54
6:D:167:GLU:C	6:D:169:THR:H	2.16	0.54
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.90	0.54
12:J:104:TYR:HA	38:J:8835:HOH:O	2.08	0.54
16:N:58:LEU:N	16:N:58:LEU:HD12	2.23	0.54
30:2:19:SER:O	30:2:36:ASN:ND2	2.41	0.54
1:0:558:C:C2'	1:0:559:U:C5'	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:958:G:H2'	1:0:959:C:C6	2.42	0.54
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.09	0.54
1:0:1160:G:H5''	1:0:1161:A:H5'	1.90	0.54
1:0:2836:G:H1'	38:0:6813:HOH:O	2.07	0.54
38:0:6235:HOH:O	23:U:56:ARG:HD3	2.07	0.54
5:C:88:SER:O	5:C:91:PRO:HD3	2.08	0.54
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.14	0.54
11:I:118:ASN:HA	11:I:121:LYS:CD	2.38	0.54
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.56	0.54
14:L:57:VAL:O	14:L:57:VAL:HG12	2.08	0.54
1:0:542:A:H5'	1:0:542:A:C8	2.32	0.53
1:0:1471:A:H2'	1:0:1472:C:C6	2.42	0.53
1:0:2672:C:O2'	1:0:2673:U:H5'	2.08	0.53
1:0:2878:U:H2'	1:0:2879:A:O4'	2.08	0.53
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.89	0.53
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.88	0.53
8:F:119:ARG:HD3	8:F:119:ARG:C	2.34	0.53
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.90	0.53
18:P:89:ASN:HA	38:P:164:HOH:O	2.08	0.53
25:W:21:LEU:CD1	25:W:26:ILE:HD11	2.30	0.53
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.66	0.53
1:0:110:C:H1'	38:0:6680:HOH:O	2.08	0.53
1:0:2115:U:H2'	1:0:2116:U:C6	2.43	0.53
1:0:2421:G:H3'	1:0:2422:U:H5''	1.91	0.53
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.53
38:0:9322:HOH:O	25:W:9:GLY:HA3	2.07	0.53
3:A:33:GLU:O	3:A:34:ASP:HB2	2.07	0.53
10:H:17:TYR:HB2	38:H:8540:HOH:O	2.08	0.53
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.74	0.53
1:0:101:C:H2'	1:0:102:A:H8	1.73	0.53
1:0:835:U:H3'	38:0:9367:HOH:O	2.08	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.43	0.53
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.89	0.53
5:C:246:ARG:NH2	38:C:8621:HOH:O	2.42	0.53
6:D:144:ARG:NH2	38:D:3839:HOH:O	2.40	0.53
8:F:28:ALA:CB	8:F:99:THR:HG23	2.38	0.53
10:H:41:LYS:HE2	10:H:45:ASP:CB	2.39	0.53
13:K:49:LEU:HD23	13:K:73:VAL:O	2.07	0.53
15:M:46:LEU:HD22	15:M:50:ARG:HD2	1.91	0.53
1:0:2256:G:O2'	1:0:2257:G:H5'	2.09	0.53
1:0:2748:G:H5'	38:0:7511:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:87:GLU:HB3	38:A:8919:HOH:O	2.06	0.53
3:A:199:HIS:HD2	3:A:201:PHE:HB2	1.72	0.53
13:K:34:VAL:HB	38:K:7169:HOH:O	2.08	0.53
16:N:167:ASP:O	16:N:168:LEU:HD23	2.09	0.53
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.09	0.53
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.06	0.53
38:O:5935:HOH:O	18:P:87:ARG:HG2	2.07	0.53
3:A:72:GLU:OE1	28:Z:72:GLU:HA	2.09	0.53
4:B:54:VAL:HB	38:B:8909:HOH:O	2.07	0.53
5:C:104:ASP:O	5:C:108:GLN:HG3	2.09	0.53
5:C:246:ARG:NE	38:C:8621:HOH:O	2.42	0.53
14:L:35:ARG:C	14:L:35:ARG:HD3	2.33	0.53
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.26	0.53
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.53
22:T:47:THR:HB	22:T:100:ASP:HB3	1.91	0.53
1:O:709:G:O2'	17:O:25:VAL:HG12	2.08	0.53
1:O:2270:G:O3'	3:A:223:ARG:NH1	2.40	0.53
38:O:9891:HOH:O	12:J:46:ILE:HA	2.08	0.53
5:C:16:VAL:HG12	5:C:17:ASP:N	2.24	0.53
5:C:246:ARG:HB3	5:C:246:ARG:HH11	1.72	0.53
9:G:16:LYS:O	9:G:20:VAL:HG23	2.09	0.53
10:H:149:VAL:HG22	38:H:8563:HOH:O	2.07	0.53
1:O:290:C:H2'	1:O:291:C:O4'	2.09	0.53
1:O:1849:G:H1'	1:O:2011:A:N1	2.24	0.53
5:C:40:ALA:O	5:C:43:LYS:HB2	2.09	0.53
6:D:81:GLU:C	6:D:83:PHE:H	2.17	0.53
10:H:53:ILE:HG23	10:H:134:GLU:O	2.08	0.53
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.72	0.53
20:R:83:LYS:HG3	38:R:8871:HOH:O	2.09	0.53
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.91	0.53
25:W:29:VAL:O	25:W:30:ASN:HB2	2.07	0.53
1:O:2028:U:H2'	1:O:2029:C:C6	2.43	0.53
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.38	0.53
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.08	0.53
8:F:68:ASP:C	8:F:70:LYS:H	2.17	0.53
1:O:168:C:O5'	1:O:168:C:H6	1.92	0.53
1:O:1973:A:H2'	1:O:1974:G:O4'	2.09	0.53
1:O:2540:G:H1'	32:O:9000:CLY:H4	1.91	0.53
1:O:2780:C:H2'	1:O:2781:U:C6	2.44	0.53
8:F:4:VAL:HA	8:F:76:PHE:CE1	2.44	0.53
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.72	0.53
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.91	0.53
1:0:65:C:O2'	1:0:66:G:H5'	2.08	0.53
1:0:694:A:H2'	1:0:695:C:H5'	1.91	0.53
1:0:920:C:H5''	1:0:921:G:O5'	2.09	0.53
1:0:1086:A:C6	25:W:11:VAL:HG11	2.43	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.42	0.53
1:0:2635:A:O2'	1:0:2636:C:H5'	2.10	0.53
1:0:2781:U:C2'	1:0:2782:G:H5'	2.39	0.53
3:A:89:ALA:HB3	38:A:8919:HOH:O	2.08	0.53
10:H:32:ALA:HB3	10:H:69:ARG:NH1	2.18	0.53
10:H:39:LYS:HD3	38:H:8564:HOH:O	2.07	0.53
13:K:87:ARG:NE	38:K:4854:HOH:O	2.38	0.53
24:V:39:ALA:N	24:V:40:PRO:CD	2.71	0.53
1:0:1783:A:O2'	1:0:1784:U:H5'	2.09	0.52
1:0:1811:A:C2	1:0:2752:C:H1'	2.44	0.52
38:0:9071:HOH:O	4:B:214:PRO:HD2	2.09	0.52
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.39	0.52
5:C:236:THR:H	5:C:239:ALA:CB	2.23	0.52
10:H:91:ARG:NH1	10:H:138:THR:OG1	2.41	0.52
11:I:129:SER:O	11:I:130:LEU:HD23	2.09	0.52
14:L:30:ARG:NH2	38:L:8823:HOH:O	2.41	0.52
16:N:151:ASP:O	16:N:154:LEU:HB2	2.08	0.52
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.52
1:0:1878:G:H1'	38:0:6112:HOH:O	2.08	0.52
1:0:2300:A:H4'	1:0:2301:A:O5'	2.10	0.52
2:9:56:A:C3'	2:9:57:A:H5''	2.39	0.52
3:A:134:ASN:O	3:A:150:PRO:HD3	2.10	0.52
4:B:332:ASN:HB3	38:B:8859:HOH:O	2.08	0.52
8:F:111:ILE:O	8:F:115:VAL:HG23	2.09	0.52
16:N:110:THR:HB	16:N:113:SER:OG	2.09	0.52
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.57	0.52
31:3:87:ARG:HD2	31:3:89:GLU:OE2	2.09	0.52
1:0:598:C:H2'	1:0:599:G:H8	1.72	0.52
1:0:1183:C:N4	1:0:1184:C:H41	2.07	0.52
1:0:1940:C:H4'	38:0:7321:HOH:O	2.09	0.52
1:0:2001:G:O2'	1:0:2002:C:H5'	2.09	0.52
3:A:64:ASP:OD1	3:A:66:ARG:HD2	2.08	0.52
3:A:206:ARG:NH1	3:A:208:HIS:NE2	2.57	0.52
8:F:91:VAL:CG1	8:F:92:GLY:N	2.73	0.52
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:25:ASP:OD2	23:U:26:GLY:N	2.43	0.52
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.52
2:9:26:C:H2'	2:9:27:C:H6	1.74	0.52
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.09	0.52
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.37	0.52
27:Y:169:ARG:NH2	38:Y:8834:HOH:O	2.37	0.52
1:0:100:C:H4'	22:T:16:LEU:HB2	1.90	0.52
1:0:282:C:O2'	1:0:283:U:H5'	2.09	0.52
3:A:57:ALA:HA	3:A:67:LEU:HD23	1.91	0.52
3:A:66:ARG:HH11	3:A:66:ARG:CB	2.20	0.52
3:A:81:GLN:HG3	3:A:92:ASN:HD21	1.74	0.52
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.91	0.52
9:G:23:ILE:O	9:G:27:ILE:HG13	2.10	0.52
9:G:71:LEU:C	9:G:73:ASP:N	2.65	0.52
11:I:118:ASN:HA	11:I:121:LYS:HD2	1.90	0.52
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.91	0.52
17:O:60:VAL:HB	17:O:78:ALA:HB2	1.92	0.52
1:0:1874:U:P	3:A:51:ARG:HD2	2.49	0.52
1:0:2092:G:H2'	1:0:2613:G:OP1	2.09	0.52
2:9:40:C:N4	6:D:53:LYS:HE3	2.24	0.52
2:9:64:C:C2'	2:9:65:A:H5'	2.40	0.52
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.91	0.52
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.92	0.52
5:C:173:LYS:HD3	5:C:187:ARG:HG2	1.92	0.52
15:M:102:GLU:OE2	15:M:164:THR:HG21	2.10	0.52
20:R:39:THR:O	20:R:42:GLU:N	2.42	0.52
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.27	0.52
28:Z:21:VAL:HG12	38:Z:8713:HOH:O	2.10	0.52
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.44	0.52
1:0:797:A:H4'	28:Z:10:ARG:N	2.24	0.52
1:0:1624:A:H4'	1:0:1626:A:H5''	1.91	0.52
2:9:26:C:H2'	2:9:27:C:C6	2.44	0.52
3:A:199:HIS:CE1	3:A:225:VAL:HG11	2.44	0.52
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.91	0.52
5:C:20:ASP:O	5:C:23:GLU:HB2	2.10	0.52
8:F:58:GLU:HG3	8:F:61:MET:CE	2.40	0.52
12:J:47:THR:N	38:J:8844:HOH:O	2.42	0.52
16:N:115:VAL:HG23	16:N:116:PHE:N	2.25	0.52
18:P:114:LEU:HD22	18:P:118:GLN:HB2	1.92	0.52
26:X:31:ILE:O	26:X:35:GLU:HG3	2.10	0.52
1:0:371:U:H2'	1:0:372:A:C8	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H22	1:0:1246:A:H2	1.50	0.52
1:0:1174:A:C6	1:0:1201:C:H4'	2.44	0.52
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.23	0.52
4:B:274:GLU:HA	4:B:292:GLY:O	2.10	0.52
8:F:78:GLU:HG3	38:F:5966:HOH:O	2.09	0.52
12:J:74:ARG:O	12:J:78:ILE:HG12	2.09	0.52
13:K:72:VAL:O	13:K:95:ALA:HA	2.10	0.52
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.45	0.52
23:U:6:CYS:C	23:U:8:TYR:H	2.18	0.52
1:0:797:A:C5'	28:Z:10:ARG:N	2.71	0.52
1:0:1189:A:H1'	1:0:1209:C:H1'	1.91	0.52
1:0:1702:U:H1'	38:0:5763:HOH:O	2.09	0.52
1:0:2002:C:H2'	1:0:2003:U:H5'	1.91	0.52
1:0:2433:A:H2'	1:0:2434:A:H8	1.73	0.52
38:0:6679:HOH:O	27:Y:165:GLU:HB3	2.08	0.52
10:H:66:GLU:OE2	10:H:70:LEU:HD13	2.09	0.52
18:P:80:ARG:HG2	18:P:87:ARG:NH1	2.25	0.52
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.45	0.52
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.92	0.52
1:0:136:C:H2'	1:0:137:U:O4'	2.10	0.52
1:0:2737:C:H2'	38:0:6133:HOH:O	2.10	0.52
4:B:82:VAL:O	4:B:82:VAL:HG12	2.10	0.52
11:I:87:PRO:C	11:I:89:GLU:H	2.18	0.52
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.52
21:S:37:VAL:O	21:S:41:VAL:HG23	2.09	0.52
23:U:6:CYS:HA	23:U:13:ILE:HD11	1.92	0.52
25:W:110:GLN:HA	25:W:110:GLN:NE2	2.25	0.52
1:0:926:A:O2'	14:L:41:HIS:CD2	2.63	0.51
1:0:1853:C:H3'	38:0:6904:HOH:O	2.08	0.51
1:0:2824:C:H5''	1:0:2825:C:H5'	1.92	0.51
2:9:55:U:H4'	2:9:56:A:C8	2.45	0.51
5:C:61:PHE:HB3	38:C:8642:HOH:O	2.09	0.51
7:E:1:PRO:HG2	7:E:59:MET:CE	2.38	0.51
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.90	0.51
10:H:141:CYS:HB2	38:H:8531:HOH:O	2.10	0.51
10:H:174:LEU:CA	38:H:8557:HOH:O	2.57	0.51
14:L:35:ARG:HB2	14:L:43:HIS:CD2	2.45	0.51
16:N:154:LEU:CD1	16:N:157:PRO:HA	2.41	0.51
18:P:94:TRP:CH2	18:P:98:ILE:HG13	2.45	0.51
21:S:77:VAL:O	21:S:80:ARG:HG2	2.10	0.51
22:T:43:ASN:HD22	22:T:108:ARG:CZ	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:73:ARG:O	26:X:85:VAL:HG13	2.10	0.51
1:0:922:A:N7	1:0:2281:C:H5'	2.25	0.51
3:A:65:ARG:C	3:A:66:ARG:HG3	2.35	0.51
3:A:109:GLU:HG2	3:A:116:GLY:N	2.24	0.51
6:D:35:ALA:N	38:D:5576:HOH:O	2.43	0.51
10:H:80:LEU:HD12	10:H:86:TYR:CD2	2.46	0.51
16:N:115:VAL:HG23	38:N:8857:HOH:O	2.10	0.51
20:R:53:GLY:HA2	20:R:80:TYR:CD2	2.45	0.51
25:W:56:GLU:O	25:W:143:THR:HG23	2.10	0.51
1:0:281:U:H5	38:0:7565:HOH:O	1.93	0.51
1:0:407:A:H5'	38:0:6017:HOH:O	2.10	0.51
1:0:447:A:O2'	1:0:448:G:H5'	2.10	0.51
1:0:1496:A:H5'	1:0:1572:A:H1'	1.91	0.51
1:0:2265:U:H2'	1:0:2266:A:H8	1.76	0.51
2:9:55:U:H4'	2:9:56:A:H8	1.74	0.51
10:H:32:ALA:C	10:H:33:GLN:HG3	2.35	0.51
12:J:77:GLY:O	12:J:78:ILE:C	2.53	0.51
26:X:70:ILE:HG23	26:X:70:ILE:O	2.09	0.51
27:Y:220:GLU:HG2	38:Y:8850:HOH:O	2.10	0.51
1:0:29:C:H5'	1:0:1342:C:OP1	2.11	0.51
1:0:284:C:H4'	1:0:285:A:O5'	2.11	0.51
1:0:821:U:H2'	1:0:822:C:H6	1.76	0.51
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.45	0.51
1:0:1641:A:H2'	1:0:1642:A:C5'	2.37	0.51
4:B:5:ARG:HD2	4:B:8:LYS:HE2	1.90	0.51
4:B:152:PRO:HD2	38:B:8928:HOH:O	2.09	0.51
6:D:35:ALA:C	6:D:37:ALA:N	2.68	0.51
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.36	0.51
13:K:75:ARG:HH12	13:K:111:GLY:HA3	1.75	0.51
15:M:109:PHE:HB3	15:M:112:LEU:HD12	1.92	0.51
20:R:39:THR:CB	20:R:42:GLU:HG3	2.35	0.51
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.51
1:0:968:G:O2'	1:0:969:G:H5'	2.10	0.51
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.51
1:0:1896:G:H1'	38:0:4257:HOH:O	2.11	0.51
3:A:36:ASP:OD2	3:A:85:SER:HB2	2.11	0.51
4:B:82:VAL:HG12	4:B:101:TRP:CE3	2.46	0.51
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.41	0.51
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	0.51
18:P:83:LYS:O	18:P:86:ALA:HB3	2.11	0.51
19:Q:75:ILE:HB	38:Q:6286:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:14:GLU:OE1	23:U:15:PRO:CD	2.59	0.51
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.10	0.51
1:0:380:A:OP2	15:M:9:ARG:HD2	2.11	0.51
1:0:860:U:H2'	1:0:861:A:C8	2.46	0.51
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
8:F:46:GLU:O	8:F:73:PRO:HD2	2.10	0.51
11:I:95:LEU:HD13	11:I:100:VAL:HG22	1.92	0.51
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.40	0.51
1:0:317:A:OP1	22:T:52:ARG:O	2.27	0.51
1:0:1055:G:OP2	10:H:99:ARG:NH1	2.44	0.51
1:0:1184:C:O2'	1:0:1185:U:OP2	2.27	0.51
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.51
6:D:63:ILE:HG13	6:D:64:ARG:N	2.25	0.51
6:D:170:TYR:CD1	6:D:170:TYR:N	2.78	0.51
10:H:43:ALA:O	10:H:170:ARG:NH1	2.43	0.51
10:H:92:LYS:HG3	10:H:130:VAL:HG22	1.92	0.51
12:J:14:ALA:O	12:J:15:ARG:C	2.53	0.51
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.92	0.51
1:0:656:G:OP2	17:O:37:ARG:HD2	2.11	0.51
1:0:2540:G:H1'	32:O:9000:CLY:CL1	2.47	0.51
1:0:2869:G:H2'	1:0:2870:C:C6	2.46	0.51
2:9:2:U:OP2	2:9:3:A:H5'	2.11	0.51
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.51
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.92	0.51
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.40	0.51
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.76	0.51
12:J:107:ASN:C	12:J:107:ASN:ND2	2.67	0.51
18:P:137:LEU:O	18:P:141:ILE:HG13	2.11	0.51
1:0:581:G:O2'	1:0:582:U:H5'	2.11	0.51
1:0:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
1:0:1157:C:H2'	1:0:1158:G:H8	1.74	0.51
1:0:2437:A:H2'	1:0:2438:G:C8	2.45	0.51
38:O:5339:HOH:O	22:T:3:GLN:HG2	2.11	0.51
4:B:23:THR:CG2	4:B:162:MET:HE3	2.41	0.51
4:B:55:ASN:CB	4:B:63:GLU:HA	2.40	0.51
4:B:307:ARG:HD3	38:B:8823:HOH:O	2.09	0.51
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.26	0.51
6:D:51:ARG:HH11	6:D:68:PRO:HB3	1.75	0.51
7:E:116:THR:CG2	7:E:151:LEU:HD22	2.40	0.51
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:32:PRO:HD2	16:N:99:GLU:O	2.11	0.51
1:O:1882:C:O2'	1:O:2012:U:OP2	2.29	0.51
2:9:44:A:H1'	6:D:76:ARG:NH2	2.26	0.51
3:A:186:TRP:CD1	3:A:187:PRO:HA	2.45	0.51
4:B:88:GLU:HG3	4:B:88:GLU:O	2.10	0.51
4:B:267:LYS:HD3	38:B:8827:HOH:O	2.11	0.51
5:C:138:VAL:O	5:C:234:VAL:HA	2.11	0.51
8:F:30:LYS:HA	38:F:5719:HOH:O	2.11	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.51
26:X:47:ALA:HB1	26:X:82:GLU:HB3	1.93	0.51
1:O:189:A:OP1	15:M:171:ARG:NH2	2.43	0.50
1:O:292:G:H2'	1:O:358:G:N2	2.26	0.50
1:O:816:G:C6	1:O:817:G:N1	2.79	0.50
1:O:945:U:H2'	1:O:946:C:H6	1.76	0.50
1:O:951:A:C2'	1:O:952:G:H5'	2.41	0.50
1:O:1787:C:O2'	1:O:1788:U:H5'	2.11	0.50
1:O:1926:G:H2'	1:O:1927:A:H8	1.75	0.50
1:O:2039:A:OP2	4:B:234:ARG:NH2	2.44	0.50
2:9:2:U:H4'	38:9:8679:HOH:O	2.11	0.50
3:A:36:ASP:O	3:A:38:ILE:N	2.43	0.50
4:B:162:MET:SD	4:B:310:ARG:HD3	2.51	0.50
4:B:243:ASN:HA	4:B:244:PRO:C	2.36	0.50
9:G:20:VAL:O	9:G:24:VAL:HG23	2.11	0.50
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.09	0.50
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.41	0.50
25:W:110:GLN:HA	25:W:110:GLN:HE21	1.75	0.50
1:O:101:C:H2'	1:O:102:A:C8	2.46	0.50
1:O:1120:U:H5''	1:O:1120:U:H6	1.76	0.50
1:O:1167:G:H2'	1:O:1168:C:O4'	2.11	0.50
1:O:1973:A:H5'	1:O:1973:A:H8	1.76	0.50
1:O:2088:C:H1'	1:O:2841:A:N1	2.26	0.50
1:O:2911:C:H2'	1:O:2912:C:C6	2.46	0.50
38:O:3753:HOH:O	22:T:9:LYS:CD	2.59	0.50
4:B:51:VAL:HG23	4:B:329:TYR:O	2.11	0.50
10:H:76:LEU:HD21	10:H:149:VAL:HA	1.93	0.50
10:H:165:ARG:HD3	38:H:8569:HOH:O	2.12	0.50
11:I:71:ALA:O	11:I:75:LYS:HG3	2.11	0.50
15:M:57:LYS:NZ	15:M:144:ASP:OD2	2.39	0.50
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.92	0.50
1:O:746:A:C6	17:O:65:LEU:HD13	2.46	0.50
1:O:962:C:H2'	1:O:963:C:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1087:G:H4'	1:0:1088:A:OP1	2.12	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.46	0.50
1:0:1624:A:H5'	1:0:1626:A:O4'	2.11	0.50
1:0:2103:A:N6	32:0:9000:CLY:H92	2.27	0.50
1:0:2478:U:O2'	1:0:2479:A:H5'	2.11	0.50
1:0:2507:G:H5'	38:0:3744:HOH:O	2.12	0.50
2:9:34:A:O5'	2:9:34:A:H8	1.94	0.50
5:C:150:THR:HA	5:C:203:ALA:O	2.11	0.50
16:N:37:ARG:NE	38:N:8832:HOH:O	2.45	0.50
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.27	0.50
25:W:4:LEU:O	25:W:32:CYS:HA	2.12	0.50
1:0:812:A:H2'	1:0:813:C:O4'	2.11	0.50
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.10	0.50
1:0:2893:C:O2'	1:0:2894:C:H5'	2.11	0.50
5:C:7:ASP:C	5:C:9:ASP:H	2.20	0.50
5:C:46:TYR:HE2	5:C:98:ARG:HH12	1.57	0.50
6:D:128:LEU:C	6:D:128:LEU:HD23	2.37	0.50
8:F:14:ASP:O	8:F:18:GLU:HG3	2.11	0.50
11:I:74:ILE:C	11:I:76:ASP:H	2.19	0.50
16:N:47:LEU:HD12	16:N:92:ALA:CB	2.41	0.50
25:W:130:HIS:O	25:W:136:GLY:HA3	2.11	0.50
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.50
31:3:56:PRO:N	38:3:8849:HOH:O	2.44	0.50
31:3:83:TRP:HA	38:3:8845:HOH:O	2.11	0.50
1:0:137:U:OP1	1:0:259:G:O2'	2.29	0.50
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.11	0.50
1:0:1926:G:H2'	1:0:1927:A:C8	2.47	0.50
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.45	0.50
13:K:113:ILE:CG2	13:K:114:ALA:N	2.75	0.50
25:W:154:ARG:C	38:W:4276:HOH:O	2.54	0.50
1:0:93:C:H5''	24:V:1:THR:HB	1.94	0.50
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	0.50
1:0:2506:A:O2'	1:0:2507:G:C8	2.61	0.50
38:0:6768:HOH:O	21:S:63:LYS:HE3	2.11	0.50
3:A:45:ILE:HG22	28:Z:54:ILE:HG12	1.93	0.50
12:J:27:ALA:HB1	12:J:87:LEU:HD21	1.94	0.50
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.94	0.50
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.10	0.50
1:0:105:G:O2'	1:0:106:A:H5'	2.11	0.50
1:0:512:G:O3'	1:0:513:A:H8	1.95	0.50
1:0:667:C:H2'	1:0:668:C:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:C2'	1:0:2257:G:H5'	2.41	0.50
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.10	0.50
1:0:2821:C:H4'	4:B:116:PRO:CB	2.41	0.50
3:A:61:GLU:C	3:A:63:GLY:H	2.20	0.50
4:B:234:ARG:NH1	38:B:8915:HOH:O	2.44	0.50
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.94	0.50
5:C:165:ASP:O	5:C:168:ARG:HB3	2.10	0.50
8:F:23:ALA:HB1	8:F:98:VAL:HG13	1.93	0.50
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.26	0.50
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.40	0.50
24:V:55:ARG:O	24:V:59:ILE:HG12	2.12	0.50
25:W:151:GLU:O	25:W:154:ARG:HB3	2.11	0.50
1:0:638:C:H2'	1:0:639:A:C8	2.47	0.50
1:0:703:G:O2'	1:0:704:C:H5'	2.12	0.50
1:0:1761:U:H5'	18:P:81:LYS:O	2.11	0.50
1:0:1773:G:C8	28:Z:16:ALA:HA	2.47	0.50
4:B:215:VAL:O	4:B:219:GLY:HA2	2.12	0.50
5:C:133:ARG:HE	5:C:138:VAL:HG22	1.77	0.50
5:C:180:SER:HB3	38:C:8643:HOH:O	2.11	0.50
20:R:59:PHE:HZ	20:R:81:PRO:HG3	1.75	0.50
24:V:17:GLU:HG3	38:V:874:HOH:O	2.10	0.50
1:0:628:1MA:H4'	38:0:3136:HOH:O	2.11	0.50
1:0:1602:C:H5'	38:0:6465:HOH:O	2.11	0.50
1:0:1839:A:H5'	1:0:2643:G:H4'	1.94	0.50
1:0:2421:G:H3'	1:0:2422:U:C5'	2.41	0.50
4:B:195:ARG:CG	4:B:323:LEU:HD22	2.40	0.50
8:F:4:VAL:HG13	8:F:76:PHE:CE1	2.47	0.50
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.77	0.50
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.93	0.50
22:T:80:GLU:HG2	38:T:2885:HOH:O	2.11	0.50
27:Y:133:HIS:HD2	38:Y:8886:HOH:O	1.95	0.50
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:1189:A:O2'	1:0:1208:C:H2'	2.12	0.49
1:0:1566:C:H2'	1:0:1567:G:H8	1.77	0.49
1:0:1909:A:H2'	1:0:1910:A:C8	2.47	0.49
6:D:10:PHE:N	38:D:7345:HOH:O	2.43	0.49
6:D:35:ALA:HB3	38:D:3279:HOH:O	2.11	0.49
11:I:116:LEU:O	11:I:119:ALA:HB3	2.12	0.49
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.93	0.49
17:O:100:GLN:O	17:O:101:ALA:C	2.55	0.49
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.94	0.49
23:U:13:ILE:HG12	23:U:32:CYS:CB	2.42	0.49
1:O:820:G:C5	3:A:171:LYS:HB2	2.46	0.49
1:O:1766:U:O2	1:O:1778:A:H5'	2.12	0.49
14:L:134:GLU:HG3	38:L:8859:HOH:O	2.10	0.49
18:P:35:ILE:HA	38:P:198:HOH:O	2.11	0.49
23:U:36:CYS:O	23:U:37:GLU:C	2.55	0.49
1:O:1545:C:H2'	1:O:1546:G:O4'	2.13	0.49
1:O:1753:C:H4'	38:O:5990:HOH:O	2.12	0.49
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.27	0.49
4:B:235:ARG:HA	38:B:8889:HOH:O	2.12	0.49
12:J:127:ILE:N	36:J:8801:CL:CL	2.69	0.49
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.94	0.49
1:O:745:G:O6	17:O:68:GLY:HA3	2.12	0.49
1:O:2039:A:H2'	1:O:2040:C:C6	2.47	0.49
1:O:2443:C:H3'	38:O:3468:HOH:O	2.11	0.49
1:O:2712:G:H5'	38:O:5210:HOH:O	2.11	0.49
38:O:9127:HOH:O	5:C:55:ARG:HB2	2.13	0.49
2:9:75:G:H1	2:9:106:U:H3	1.59	0.49
5:C:7:ASP:OD1	5:C:11:ASN:O	2.30	0.49
6:D:36:ASN:C	38:D:7500:HOH:O	2.55	0.49
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.12	0.49
16:N:34:LEU:HD13	16:N:47:LEU:CD2	2.42	0.49
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.94	0.49
24:V:4:HIS:HB2	24:V:7:GLU:HG3	1.95	0.49
1:O:90:A:H2'	1:O:91:G:O4'	2.11	0.49
1:O:363:C:O2'	1:O:364:U:H5'	2.12	0.49
1:O:926:A:H5'	14:L:39:GLU:OE2	2.12	0.49
1:O:941:G:C5	1:O:942:U:C4	3.01	0.49
1:O:1762:C:H2'	1:O:1763:C:H6	1.77	0.49
38:O:6018:HOH:O	19:Q:50:GLY:HA2	2.13	0.49
4:B:298:LYS:HD3	38:B:8920:HOH:O	2.13	0.49
14:L:143:THR:HG21	38:L:8840:HOH:O	2.11	0.49
19:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.12	0.49
25:W:129:LYS:HG2	38:W:1990:HOH:O	2.12	0.49
28:Z:30:GLU:HA	28:Z:33:MET:HE2	1.95	0.49
1:O:407:A:H2'	1:O:408:A:C8	2.47	0.49
1:O:559:U:H5'	1:O:559:U:C6	2.34	0.49
1:O:1086:A:N6	25:W:11:VAL:HG11	2.27	0.49
1:O:1845:A:OP2	3:A:190:ARG:NH1	2.46	0.49
1:O:2787:C:H2'	1:O:2788:A:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2880:A:H2'	1:0:2881:C:H5'	1.95	0.49
38:0:4797:HOH:O	8:F:31:LYS:HD2	2.12	0.49
4:B:96:PRO:HG3	38:B:8932:HOH:O	2.11	0.49
6:D:139:TYR:CE2	6:D:143:LYS:HE2	2.47	0.49
13:K:18:ILE:HG22	13:K:93:ASN:HB2	1.94	0.49
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.43	0.49
17:O:49:GLU:HG2	38:O:5191:HOH:O	2.13	0.49
25:W:64:THR:O	25:W:68:THR:HG22	2.13	0.49
1:0:794:U:H3	1:0:819:A:H61	1.60	0.49
1:0:886:A:OP2	1:0:2113:G:H5'	2.12	0.49
1:0:2256:G:H2'	1:0:2257:G:C5'	2.43	0.49
1:0:2839:C:H2'	1:0:2840:A:H5''	1.94	0.49
38:0:9210:HOH:O	3:A:11:ARG:HD3	2.12	0.49
4:B:55:ASN:CG	4:B:63:GLU:HA	2.38	0.49
5:C:21:VAL:C	5:C:23:GLU:H	2.19	0.49
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.77	0.49
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.38	0.49
1:0:536:A:H3'	38:0:5042:HOH:O	2.13	0.49
1:0:625:U:H5''	1:0:1044:C:N4	2.28	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
1:0:2374:G:H2'	1:0:2375:A:C8	2.48	0.49
1:0:2807:U:P	4:B:27:ASN:HD21	2.35	0.49
1:0:2846:C:H4'	4:B:156:LYS:HB3	1.94	0.49
2:9:20:G:O2'	2:9:21:G:H5'	2.13	0.49
3:A:36:ASP:CG	3:A:85:SER:HB2	2.38	0.49
5:C:4:THR:HB	5:C:135:GLU:OE1	2.13	0.49
5:C:157:LEU:HD11	5:C:194:PHE:HZ	1.78	0.49
7:E:145:ALA:HB1	7:E:168:ILE:HD11	1.95	0.49
10:H:49:GLN:HB3	10:H:170:ARG:CG	2.41	0.49
15:M:182:LYS:NZ	38:M:8825:HOH:O	2.46	0.49
16:N:82:TYR:C	16:N:82:TYR:CD2	2.91	0.49
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.12	0.49
25:W:73:LEU:HD22	25:W:111:GLY:HA2	1.94	0.49
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.49
1:0:1330:A:H5''	1:0:1331:G:OP2	2.13	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.43	0.49
1:0:1657:A:H2'	1:0:1658:A:C8	2.48	0.49
1:0:2301:A:H5''	1:0:2302:A:H5'	1.95	0.49
6:D:105:SER:HB2	6:D:131:THR:HG23	1.94	0.49
8:F:91:VAL:HG12	8:F:92:GLY:H	1.76	0.49
9:G:23:ILE:HG22	9:G:27:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:133:THR:HG22	11:I:134:ILE:H	1.78	0.49
15:M:27:ARG:O	15:M:30:GLU:N	2.46	0.49
17:O:59:VAL:HG23	17:O:111:VAL:HG21	1.95	0.49
1:O:2899:A:O2'	1:O:2900:G:H5'	2.13	0.49
4:B:1:PRO:O	4:B:2:GLN:HB2	2.13	0.49
4:B:180:ASP:O	4:B:181:ILE:C	2.54	0.49
7:E:2:ARG:NH2	7:E:48:VAL:HG21	2.28	0.49
7:E:93:MET:HE1	7:E:165:GLY:N	2.27	0.49
13:K:98:VAL:CG1	13:K:99:ASP:N	2.76	0.49
15:M:47:ASP:CG	15:M:48:LYS:H	2.21	0.49
15:M:47:ASP:CG	15:M:48:LYS:N	2.71	0.49
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.48	0.49
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.11	0.49
26:X:71:ARG:HD2	38:X:7542:HOH:O	2.12	0.49
1:O:952:G:OP1	19:Q:42:LYS:HE2	2.13	0.48
1:O:999:C:N3	38:O:5070:HOH:O	2.35	0.48
1:O:1163:G:N2	38:O:4724:HOH:O	2.45	0.48
1:O:2110:G:H4'	38:O:7675:HOH:O	2.13	0.48
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.94	0.48
14:L:24:ALA:HB2	14:L:30:ARG:HD2	1.94	0.48
17:O:7:LEU:HD22	38:O:5650:HOH:O	2.12	0.48
21:S:67:ARG:HB3	21:S:67:ARG:HH11	1.78	0.48
26:X:30:MET:CE	26:X:55:ASN:HA	2.43	0.48
1:O:282:C:H2'	1:O:283:U:O4'	2.13	0.48
1:O:1008:C:H5''	10:H:19:ARG:HH12	1.77	0.48
1:O:1398:G:H2'	1:O:1399:A:C8	2.48	0.48
1:O:1684:A:O2'	1:O:1685:A:H5''	2.13	0.48
1:O:2072:G:C6	1:O:2533:C:H1'	2.49	0.48
2:9:39:U:H1'	2:9:44:A:H61	1.77	0.48
6:D:128:LEU:N	38:D:6007:HOH:O	2.46	0.48
7:E:23:GLU:HG2	7:E:28:SER:HB2	1.95	0.48
7:E:81:GLU:N	38:E:6931:HOH:O	2.46	0.48
8:F:31:LYS:HG2	8:F:87:ALA:HB1	1.95	0.48
8:F:46:GLU:N	38:F:3461:HOH:O	2.46	0.48
20:R:47:LEU:O	20:R:51:ILE:HG13	2.13	0.48
21:S:11:THR:H	21:S:14:ALA:CB	2.20	0.48
1:O:31:C:H4'	38:T:7242:HOH:O	2.12	0.48
1:O:285:A:C2	1:O:368:C:H4'	2.48	0.48
1:O:1886:A:H4'	38:Z:8706:HOH:O	2.12	0.48
1:O:2050:G:H5''	20:R:80:TYR:O	2.13	0.48
1:O:2132:C:H2'	38:O:7529:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:48:C:H4'	16:N:141:ARG:NH2	2.27	0.48
2:9:49:G:O2'	2:9:50:G:H5'	2.12	0.48
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.96	0.48
7:E:69:ILE:HA	7:E:72:MET:HE2	1.94	0.48
1:0:962:C:H5''	38:0:4909:HOH:O	2.12	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.13	0.48
38:0:7117:HOH:O	29:1:1:THR:HB	2.13	0.48
2:9:41:C:O4'	6:D:50:VAL:HG22	2.13	0.48
38:9:8664:HOH:O	16:N:147:ILE:HD12	2.13	0.48
5:C:13:ASP:OD1	5:C:13:ASP:O	2.30	0.48
6:D:136:ARG:O	6:D:138:GLY:N	2.45	0.48
11:I:94:ASP:OD1	11:I:133:THR:HB	2.12	0.48
25:W:72:PRO:CG	25:W:77:ALA:HB3	2.39	0.48
1:0:204:A:H2'	1:0:205:U:H5'	1.94	0.48
1:0:2538:A:H8	32:0:9000:CLY:O8	1.97	0.48
10:H:50:ILE:HD12	10:H:149:VAL:HG11	1.95	0.48
12:J:45:VAL:HG22	12:J:46:ILE:N	2.27	0.48
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.81	0.48
29:1:25:LYS:HB2	30:2:48:ASP:HB3	1.95	0.48
1:0:792:G:H4'	38:0:3412:HOH:O	2.13	0.48
1:0:1299:G:N7	14:L:6:ARG:NH1	2.62	0.48
1:0:1815:A:H2'	1:0:1816:C:O4'	2.13	0.48
4:B:248:ARG:NH2	38:B:8824:HOH:O	2.45	0.48
5:C:237:GLU:HB2	38:C:8628:HOH:O	2.13	0.48
9:G:71:LEU:O	9:G:73:ASP:N	2.46	0.48
11:I:88:GLN:NE2	11:I:128:THR:CG2	2.76	0.48
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.13	0.48
20:R:126:LYS:O	20:R:126:LYS:HG3	2.14	0.48
24:V:1:THR:O	24:V:4:HIS:CE1	2.67	0.48
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.49	0.48
1:0:10:U:O4	1:0:532:A:OP2	2.32	0.48
1:0:204:A:C2'	1:0:205:U:H5'	2.43	0.48
1:0:1173:A:H2	38:0:6267:HOH:O	1.96	0.48
1:0:1416:G:C2'	1:0:1417:G:H5'	2.43	0.48
1:0:1622:G:C2'	1:0:1623:C:H5'	2.43	0.48
1:0:2821:C:H4'	4:B:116:PRO:HG3	1.95	0.48
2:9:51:A:H5'	16:N:160:SER:CB	2.40	0.48
4:B:279:THR:HG22	4:B:280:VAL:N	2.27	0.48
5:C:156:LEU:HD12	5:C:156:LEU:O	2.14	0.48
7:E:137:ASP:OD1	7:E:137:ASP:C	2.55	0.48
8:F:110:ASP:O	8:F:114:LYS:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:28:GLN:HA	15:M:31:TRP:HB2	1.96	0.48
26:X:9:VAL:HG11	38:X:2171:HOH:O	2.13	0.48
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.42	0.48
1:0:106:A:H2'	1:0:107:U:O4'	2.14	0.48
1:0:682:A:H2'	1:0:683:G:O4'	2.13	0.48
1:0:745:G:H5''	1:0:746:A:OP1	2.14	0.48
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.46	0.48
1:0:1279:U:O2	1:0:1279:U:H2'	2.13	0.48
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.14	0.48
1:0:2756:U:N3	1:0:2896:A:H2	2.06	0.48
38:0:4034:HOH:O	5:C:149:LYS:HE3	2.13	0.48
2:9:1:U:H4'	2:9:3:A:OP1	2.14	0.48
5:C:218:VAL:HG12	38:C:8621:HOH:O	2.12	0.48
16:N:119:GLN:O	16:N:123:ILE:HG13	2.14	0.48
16:N:154:LEU:C	16:N:156:GLU:N	2.72	0.48
17:O:47:ARG:HD3	17:O:115:ARG:O	2.14	0.48
25:W:90:TYR:N	25:W:90:TYR:CD1	2.81	0.48
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.49	0.48
1:0:407:A:H8	38:0:4458:HOH:O	1.97	0.48
1:0:681:G:H1'	1:0:683:G:O6	2.14	0.48
1:0:1180:U:H4'	11:I:86:GLU:HG2	1.94	0.48
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.48
3:A:37:VAL:HG22	38:A:8891:HOH:O	2.13	0.48
6:D:138:GLY:N	38:D:7597:HOH:O	2.46	0.48
12:J:117:ASP:O	12:J:119:THR:HG23	2.14	0.48
16:N:144:GLY:O	16:N:147:ILE:CG2	2.62	0.48
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.78	0.48
27:Y:97:LEU:HA	27:Y:234:VAL:O	2.14	0.48
1:0:584:U:H3'	38:0:6085:HOH:O	2.13	0.48
1:0:1120:U:H5'	1:0:1121:G:OP2	2.14	0.48
1:0:1191:A:H2'	1:0:1193:A:H5'	1.95	0.48
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.48
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.94	0.48
1:0:1527:A:H1'	1:0:1528:A:C8	2.49	0.48
1:0:1644:C:H2'	1:0:1645:U:H6	1.79	0.48
1:0:2594:C:O2'	1:0:2595:U:H5'	2.13	0.48
38:0:4651:HOH:O	30:2:36:ASN:HA	2.13	0.48
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.96	0.48
10:H:24:THR:O	10:H:123:ILE:HD12	2.14	0.48
10:H:48:VAL:HG21	10:H:143:VAL:HA	1.96	0.48
13:K:22:ASP:HB3	13:K:96:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:30:MET:HE3	26:X:55:ASN:OD1	2.14	0.48
1:O:134:U:C2	1:O:145:A:C2	3.02	0.47
1:O:1829:A:H2'	1:O:1830:C:H5'	1.96	0.47
1:O:2717:C:H5'	4:B:302:PRO:HA	1.94	0.47
1:O:2786:G:H2'	38:O:7163:HOH:O	2.14	0.47
38:9:8644:HOH:O	6:D:139:TYR:N	2.47	0.47
3:A:134:ASN:O	3:A:150:PRO:CD	2.61	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.47	0.47
9:G:63:ARG:O	9:G:67:LEU:HG	2.14	0.47
10:H:49:GLN:CB	10:H:170:ARG:HG3	2.39	0.47
11:I:119:ALA:O	11:I:123:VAL:HG23	2.14	0.47
13:K:72:VAL:HG11	13:K:121:PHE:CD1	2.48	0.47
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.48	0.47
16:N:15:GLU:HB3	16:N:17:ARG:HD2	1.95	0.47
21:S:11:THR:O	21:S:14:ALA:HB3	2.14	0.47
25:W:69:ARG:NE	38:W:4276:HOH:O	2.47	0.47
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.13	0.47
1:O:1213:C:C2'	1:O:1214:G:H5'	2.44	0.47
1:O:2467:A:H3'	38:O:5445:HOH:O	2.13	0.47
3:A:217:ARG:CG	3:A:217:ARG:NH1	2.77	0.47
5:C:40:ALA:HB3	5:C:100:LEU:HD12	1.96	0.47
5:C:98:ARG:HG2	5:C:98:ARG:NH1	2.26	0.47
8:F:117:GLU:C	8:F:119:ARG:H	2.20	0.47
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.44	0.47
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.14	0.47
1:O:694:A:H4'	1:O:2441:U:OP1	2.14	0.47
1:O:1434:A:H2'	1:O:1436:C:C5	2.49	0.47
1:O:1622:G:H2'	1:O:1623:C:H5'	1.97	0.47
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.44	0.47
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.97	0.47
5:C:19:PRO:CD	5:C:240:LEU:HD22	2.44	0.47
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.95	0.47
6:D:140:ARG:HH11	6:D:140:ARG:HG3	1.78	0.47
11:I:70:THR:HA	11:I:107:LYS:NZ	2.29	0.47
11:I:87:PRO:HB3	38:I:6825:HOH:O	2.14	0.47
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.95	0.47
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.79	0.47
1:O:232:A:H4'	38:O:6074:HOH:O	2.13	0.47
1:O:583:C:H2'	1:O:584:U:H6	1.79	0.47
1:O:792:G:O2'	1:O:793:A:H5'	2.13	0.47
1:O:1181:A:C2'	1:O:1182:C:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1241:G:H2'	1:0:1242:A:O4'	2.14	0.47
1:0:1352:A:N1	5:C:48:SER:HB3	2.29	0.47
1:0:1664:A:H8	1:0:1664:A:OP1	1.97	0.47
1:0:2135:A:O2'	1:0:2136:G:H5'	2.14	0.47
1:0:2787:C:H5	38:0:4632:HOH:O	1.98	0.47
38:0:4187:HOH:O	27:Y:186:ARG:HD2	2.13	0.47
15:M:44:THR:O	15:M:44:THR:HG22	2.13	0.47
16:N:27:LEU:HD13	16:N:50:LEU:HD21	1.96	0.47
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.50	0.47
1:0:671:A:O2'	1:0:672:G:H2'	2.15	0.47
1:0:695:C:O2'	1:0:696:C:H5'	2.14	0.47
1:0:834:G:H5''	1:0:835:U:O5'	2.15	0.47
1:0:1625:U:H6	1:0:1625:U:H3'	1.80	0.47
1:0:1834:C:H2'	1:0:1840:A:H62	1.78	0.47
2:9:8:G:O6	16:N:11:ARG:NH1	2.47	0.47
6:D:101:THR:O	6:D:101:THR:HG22	2.15	0.47
11:I:102:GLN:HA	11:I:105:GLU:OE2	2.13	0.47
12:J:46:ILE:HD11	12:J:53:ILE:CG2	2.44	0.47
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.44	0.47
18:P:41:ARG:O	18:P:44:VAL:HB	2.15	0.47
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.44	0.47
25:W:48:VAL:O	25:W:48:VAL:HG12	2.15	0.47
31:3:62:THR:HB	38:3:8850:HOH:O	2.14	0.47
1:0:295:C:H2'	1:0:296:G:O4'	2.15	0.47
1:0:466:A:H2'	1:0:467:G:O4'	2.14	0.47
1:0:589:U:H2'	1:0:590:A:H8	1.78	0.47
1:0:827:A:H2'	1:0:828:G:O4'	2.14	0.47
1:0:1687:C:O2	29:1:9:GLY:HA2	2.14	0.47
1:0:1930:A:H2'	1:0:1931:A:C8	2.50	0.47
2:9:59:C:H5'	38:9:8677:HOH:O	2.14	0.47
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.95	0.47
4:B:109:LEU:HG	4:B:113:LEU:HD12	1.97	0.47
5:C:22:PHE:HA	5:C:116:ALA:HA	1.96	0.47
5:C:27:ARG:NH1	5:C:30:LEU:HG	2.30	0.47
5:C:127:ARG:HD3	5:C:129:HIS:HE1	1.79	0.47
8:F:63:ILE:HB	8:F:64:PRO:CD	2.39	0.47
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.45	0.47
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.50	0.47
17:O:105:ASN:HD21	17:O:109:SER:N	2.13	0.47
18:P:134:VAL:O	18:P:137:LEU:HB3	2.15	0.47
1:0:157:G:H4'	15:M:95:LYS:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:553:G:O4'	1:0:1325:G:H5'	2.14	0.47
1:0:685:C:O2	1:0:748:C:H4'	2.13	0.47
1:0:832:U:H2'	1:0:833:G:C8	2.50	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.96	0.47
1:0:1181:A:H2'	1:0:1182:C:H5'	1.96	0.47
1:0:1185:U:H2'	1:0:1186:C:C6	2.50	0.47
1:0:1419:U:H2'	1:0:1685:A:C2	2.50	0.47
1:0:1679:C:O2'	1:0:1685:A:N1	2.46	0.47
1:0:1883:U:O2'	1:0:1884:G:H5'	2.14	0.47
1:0:2654:C:H5'	38:B:8961:HOH:O	2.15	0.47
1:0:2714:U:H4'	4:B:10:SER:HB2	1.96	0.47
1:0:2758:G:H2'	1:0:2759:C:C6	2.50	0.47
1:0:2812:A:N7	38:0:7487:HOH:O	2.36	0.47
1:0:2840:A:OP1	4:B:211:THR:HG23	2.15	0.47
4:B:13:PHE:CD1	4:B:13:PHE:N	2.82	0.47
4:B:129:ARG:O	4:B:133:GLU:HG3	2.14	0.47
4:B:313:PRO:O	4:B:314:ALA:C	2.57	0.47
6:D:54:ALA:HB3	6:D:69:ILE:HD12	1.97	0.47
6:D:56:ARG:N	38:D:6752:HOH:O	2.47	0.47
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.95	0.47
6:D:81:GLU:C	6:D:83:PHE:N	2.70	0.47
7:E:158:ASP:HA	38:E:2712:HOH:O	2.14	0.47
13:K:13:GLU:OE2	13:K:44:LEU:HB2	2.14	0.47
17:O:44:ASN:HB2	36:O:8808:CL:CL	2.52	0.47
17:O:105:ASN:ND2	17:O:109:SER:H	2.13	0.47
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.97	0.47
22:T:55:PHE:O	22:T:56:ALA:C	2.57	0.47
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.47
24:V:26:GLU:HB3	24:V:49:LEU:HD21	1.97	0.47
28:Z:60:CYS:SG	28:Z:62:TYR:HB2	2.54	0.47
1:0:730:G:P	38:0:4021:HOH:O	2.73	0.47
1:0:932:U:H2'	1:0:933:C:C6	2.50	0.47
1:0:1813:U:O2'	18:P:81:LYS:HE3	2.14	0.47
1:0:1852:A:H4'	3:A:230:SER:HB2	1.95	0.47
38:0:4724:HOH:O	11:I:125:GLY:C	2.57	0.47
4:B:278:PRO:HD3	4:B:294:TYR:CE2	2.50	0.47
5:C:200:PRO:HB3	5:C:212:VAL:CG2	2.43	0.47
8:F:43:GLY:C	8:F:45:ALA:H	2.23	0.47
8:F:70:LYS:C	8:F:72:VAL:H	2.22	0.47
16:N:37:ARG:HH21	16:N:105:GLY:CA	2.28	0.47
17:O:107:GLU:O	17:O:108:GLY:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:27:ARG:HA	38:P:174:HOH:O	2.14	0.47
24:V:39:ALA:C	24:V:41:GLU:N	2.73	0.47
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.24	0.47
25:W:142:ASP:HB2	25:W:145:GLY:N	2.23	0.47
27:Y:110:SER:O	27:Y:111:ASP:C	2.57	0.47
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.29	0.47
1:0:199:A:H5''	38:0:3523:HOH:O	2.14	0.47
1:0:545:G:H2'	1:0:546:C:O4'	2.13	0.47
1:0:1098:A:H2'	1:0:1099:G:O4'	2.15	0.47
1:0:1477:C:H5'	1:0:1868:G:H5''	1.97	0.47
1:0:1762:C:H2'	1:0:1763:C:C6	2.50	0.47
38:0:7173:HOH:O	29:1:38:GLY:HA3	2.15	0.47
4:B:202:VAL:HG11	4:B:301:VAL:HG13	1.97	0.47
5:C:14:GLY:O	5:C:15:GLU:HB3	2.13	0.47
5:C:26:VAL:N	38:C:8555:HOH:O	2.47	0.47
5:C:194:PHE:HA	5:C:234:VAL:HG13	1.95	0.47
7:E:84:MET:HA	7:E:167:TYR:O	2.15	0.47
13:K:10:GLN:H	13:K:10:GLN:HE21	0.69	0.47
14:L:134:GLU:O	14:L:137:GLY:N	2.48	0.47
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.97	0.47
31:3:10:TYR:HB2	31:3:17:HIS:CE1	2.49	0.47
1:0:598:C:H2'	1:0:599:G:C8	2.50	0.47
1:0:1753:C:O2	4:B:229:ARG:NH2	2.47	0.47
1:0:2320:U:OP2	31:3:1:MET:HA	2.15	0.47
5:C:146:ASP:O	5:C:147:LEU:C	2.58	0.47
5:C:188:ARG:NH2	38:C:8523:HOH:O	2.42	0.47
7:E:80:TRP:O	7:E:134:SER:HA	2.15	0.47
21:S:4:VAL:HG23	38:S:8521:HOH:O	2.14	0.47
26:X:25:ARG:NH1	38:X:3861:HOH:O	2.45	0.47
1:0:1172:G:H5''	38:0:7234:HOH:O	2.16	0.46
1:0:1209:C:H2'	1:0:1210:G:H8	1.80	0.46
1:0:1681:G:H5''	1:0:1682:A:H5'	1.96	0.46
1:0:2584:G:H4'	38:0:7090:HOH:O	2.15	0.46
7:E:32:ARG:O	7:E:33:LEU:HD23	2.15	0.46
12:J:57:TYR:O	12:J:61:VAL:HG23	2.15	0.46
13:K:49:LEU:HD21	13:K:74:VAL:O	2.15	0.46
18:P:103:THR:HA	18:P:106:ARG:HH12	1.80	0.46
27:Y:186:ARG:HG2	38:Y:8883:HOH:O	2.15	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.79	0.46
1:0:157:G:H4'	15:M:95:LYS:HE3	1.95	0.46
1:0:426:G:H2'	1:0:427:C:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:622:G:P	27:Y:148:GLY:HA3	2.55	0.46
1:0:1172:G:H1'	38:0:4966:HOH:O	2.15	0.46
1:0:1587:U:H2'	1:0:1588:G:O4'	2.14	0.46
38:0:3688:HOH:O	7:E:143:GLN:HG2	2.15	0.46
5:C:236:THR:CG2	5:C:239:ALA:H	2.16	0.46
10:H:117:ARG:HB3	38:H:8576:HOH:O	2.14	0.46
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.50	0.46
24:V:1:THR:HG23	24:V:2:VAL:N	2.26	0.46
1:0:638:C:H2'	1:0:639:A:H8	1.81	0.46
1:0:2831:C:H2'	1:0:2832:C:C5'	2.44	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.80	0.46
3:A:164:ARG:HA	28:Z:69:TYR:CE1	2.51	0.46
5:C:26:VAL:HG21	5:C:123:LEU:HD11	1.98	0.46
5:C:39:GLN:O	5:C:43:LYS:HD3	2.16	0.46
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.43	0.46
6:D:89:PRO:C	6:D:91:ALA:H	2.23	0.46
6:D:135:VAL:HG22	6:D:136:ARG:N	2.30	0.46
10:H:174:LEU:C	38:H:8557:HOH:O	2.59	0.46
12:J:24:SER:HA	12:J:86:MET:SD	2.56	0.46
17:O:32:ARG:HB2	38:O:4656:HOH:O	2.15	0.46
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.46	0.46
22:T:113:GLU:O	22:T:114:SER:C	2.57	0.46
24:V:7:GLU:O	24:V:11:MET:HG3	2.15	0.46
27:Y:146:PRO:HB2	27:Y:154:ARG:HB2	1.96	0.46
1:0:17:G:H2'	1:0:18:C:C6	2.50	0.46
1:0:1200:A:H3'	38:0:5744:HOH:O	2.16	0.46
1:0:1747:A:C8	13:K:44:LEU:HD13	2.51	0.46
1:0:1845:A:P	3:A:190:ARG:HH11	2.39	0.46
1:0:2000:G:O2'	1:0:2001:G:H5'	2.15	0.46
1:0:2256:G:H2'	1:0:2257:G:H5'	1.97	0.46
1:0:2570:G:H5''	38:0:4907:HOH:O	2.14	0.46
1:0:2668:G:H2'	1:0:2669:U:C6	2.51	0.46
2:9:39:U:N3	2:9:42:C:H5''	2.29	0.46
3:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.96	0.46
5:C:7:ASP:O	5:C:9:ASP:N	2.46	0.46
6:D:69:ILE:HG22	6:D:69:ILE:O	2.15	0.46
6:D:170:TYR:O	6:D:171:ASP:HB3	2.15	0.46
10:H:12:ILE:HD11	10:H:58:VAL:O	2.16	0.46
10:H:86:TYR:C	10:H:86:TYR:CD1	2.93	0.46
13:K:23:ASN:HD21	13:K:107:THR:HB	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:24:THR:HB	13:K:64:MET:HE2	1.97	0.46
18:P:110:ASP:C	18:P:112:GLY:H	2.23	0.46
19:Q:93:ARG:HG3	19:Q:93:ARG:HH11	1.80	0.46
24:V:12:THR:O	24:V:13:PRO:C	2.59	0.46
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.30	0.46
27:Y:197:ASP:O	27:Y:199:ASP:N	2.49	0.46
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.16	0.46
1:O:119:A:H2'	1:O:120:A:H5''	1.98	0.46
1:O:316:A:N3	1:O:336:G:O2'	2.47	0.46
1:O:1201:C:H2'	1:O:1202:A:H5'	1.98	0.46
1:O:1801:A:H3'	38:O:7586:HOH:O	2.15	0.46
1:O:2015:A:H2'	1:O:2016:U:O4'	2.15	0.46
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:O:2239:C:H2'	1:O:2240:U:C6	2.51	0.46
1:O:2453:G:H3'	38:O:5909:HOH:O	2.16	0.46
1:O:2533:C:O2'	1:O:2534:C:H5'	2.16	0.46
1:O:2597:U:H2'	1:O:2598:U:H5'	1.97	0.46
1:O:2718:C:H6	1:O:2718:C:H5'	1.79	0.46
1:O:2780:C:C1'	7:E:143:GLN:HE21	2.27	0.46
3:A:34:ASP:OD1	3:A:35:GLY:N	2.48	0.46
4:B:175:LEU:C	4:B:175:LEU:CD2	2.88	0.46
7:E:7:ILE:HD11	7:E:11:VAL:O	2.16	0.46
8:F:107:ASP:O	8:F:108:VAL:C	2.59	0.46
16:N:49:THR:HB	16:N:58:LEU:HD11	1.98	0.46
19:Q:91:LEU:O	19:Q:92:ARG:HD2	2.16	0.46
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.22	0.46
21:S:67:ARG:NH1	21:S:67:ARG:HB3	2.29	0.46
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.46	0.46
1:O:1293:U:H5'	27:Y:154:ARG:HH21	1.79	0.46
1:O:2468:A:H5'	38:3:8821:HOH:O	2.15	0.46
3:A:130:THR:HG22	3:A:131:HIS:O	2.14	0.46
3:A:173:GLY:O	3:A:176:HIS:HB3	2.16	0.46
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.97	0.46
4:B:52:VAL:C	4:B:53:LEU:HD12	2.40	0.46
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.80	0.46
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.98	0.46
8:F:58:GLU:HA	8:F:61:MET:HG3	1.96	0.46
10:H:49:GLN:OE1	10:H:169:GLU:HG3	2.16	0.46
15:M:146:ASP:O	15:M:147:LEU:HD23	2.15	0.46
16:N:67:ALA:C	16:N:69:TYR:H	2.23	0.46
17:O:57:THR:HB	17:O:111:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:7:LYS:HG2	18:P:23:PHE:CE2	2.51	0.46
26:X:51:ASP:OD2	26:X:52:PRO:HD2	2.16	0.46
1:0:482:G:H4'	1:0:508:A:N1	2.31	0.46
1:0:1003:U:H4'	10:H:91:ARG:O	2.16	0.46
1:0:1154:A:H2'	1:0:1155:G:O4'	2.16	0.46
1:0:1159:G:H1	1:0:1208:C:H42	1.63	0.46
1:0:1384:C:H5'	26:X:30:MET:HG2	1.97	0.46
1:0:1441:G:O2'	1:0:1442:A:H5'	2.15	0.46
1:0:1666:C:C2'	1:0:1667:A:H5'	2.43	0.46
38:O:3753:HOH:O	22:T:9:LYS:HD3	2.15	0.46
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.97	0.46
3:A:164:ARG:HB2	28:Z:68:SER:OG	2.16	0.46
4:B:18:ARG:HE	4:B:256:GLN:HE21	1.63	0.46
8:F:100:ASP:O	8:F:101:ALA:O	2.34	0.46
15:M:95:LYS:HG2	15:M:99:ARG:HB3	1.96	0.46
16:N:35:VAL:HB	16:N:46:GLN:HB2	1.97	0.46
18:P:55:LYS:HA	38:P:181:HOH:O	2.14	0.46
22:T:41:ARG:NH1	22:T:42:VAL:O	2.48	0.46
22:T:80:GLU:HA	38:T:6653:HOH:O	2.14	0.46
26:X:71:ARG:HB2	38:X:6590:HOH:O	2.15	0.46
28:Z:10:ARG:HB2	28:Z:27:ALA:CB	2.46	0.46
1:0:214:U:H5'	38:O:6131:HOH:O	2.14	0.46
1:0:401:C:O2'	15:M:92:THR:HB	2.16	0.46
1:0:506:G:N2	1:0:508:A:H3'	2.30	0.46
1:0:947:U:O2'	1:0:948:G:H5'	2.15	0.46
1:0:1477:C:H5'	1:0:1868:G:H5'	1.96	0.46
1:0:1544:U:H2'	1:0:1545:C:C6	2.49	0.46
1:0:1805:G:H2'	1:0:1806:G:C8	2.49	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.46
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.46
2:9:28:U:H2'	2:9:29:C:C6	2.51	0.46
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.98	0.46
15:M:61:ILE:CG2	15:M:62:VAL:N	2.78	0.46
16:N:178:THR:O	16:N:181:ASP:HB3	2.15	0.46
19:Q:62:THR:O	19:Q:64:GLU:HG2	2.15	0.46
20:R:89:LEU:HD23	20:R:89:LEU:HA	1.78	0.46
28:Z:23:ARG:NH1	38:Z:8704:HOH:O	2.49	0.46
1:0:20:G:H21	20:R:117:HIS:HD2	1.64	0.46
1:0:523:C:H2'	1:0:524:A:C8	2.51	0.46
1:0:1713:G:H1'	38:O:5065:HOH:O	2.16	0.46
1:0:2784:A:H1'	7:E:60:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:50:G:H5''	16:N:159:TYR:HE1	1.80	0.46
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.13	0.46
4:B:275:GLY:C	4:B:291:ASP:HA	2.41	0.46
5:C:178:GLN:O	5:C:179:GLY:C	2.59	0.46
7:E:107:PHE:C	7:E:109:GLY:N	2.72	0.46
10:H:87:LYS:HB2	10:H:87:LYS:NZ	2.30	0.46
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.46	0.46
12:J:54:VAL:HG12	12:J:58:GLU:HG3	1.98	0.46
16:N:143:ARG:HH12	16:N:173:ASP:CG	2.24	0.46
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.80	0.46
17:O:87:THR:O	17:O:91:GLN:HG3	2.16	0.46
25:W:35:VAL:HG22	25:W:36:PRO:O	2.15	0.46
1:0:236:A:H4'	1:0:237:G:OP1	2.15	0.46
1:0:241:A:C2	1:0:378:A:H4'	2.51	0.46
1:0:424:C:H2'	1:0:425:U:C6	2.51	0.46
1:0:710:G:O2'	1:0:711:G:H5'	2.15	0.46
1:0:1334:C:H2'	1:0:1335:C:H6	1.81	0.46
1:0:1617:C:C4	1:0:1643:C:H4'	2.51	0.46
1:0:2684:A:H2'	1:0:2685:C:C6	2.51	0.46
38:0:6560:HOH:O	2:9:83:G:H4'	2.15	0.46
2:9:2:U:C4'	38:9:8679:HOH:O	2.63	0.46
3:A:66:ARG:NH1	3:A:66:ARG:CB	2.77	0.46
4:B:104:GLU:HG3	38:B:8887:HOH:O	2.16	0.46
5:C:46:TYR:HE2	5:C:98:ARG:NH1	2.11	0.46
6:D:65:GLU:HG3	38:D:6752:HOH:O	2.16	0.46
7:E:2:ARG:HH21	7:E:48:VAL:HG21	1.80	0.46
10:H:29:SER:HA	10:H:62:HIS:HD2	1.80	0.46
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.98	0.46
1:0:303:C:H2'	1:0:304:G:O4'	2.16	0.45
1:0:319:A:H4'	1:0:338:C:C4	2.52	0.45
1:0:470:U:O2'	29:1:16:HIS:CD2	2.65	0.45
1:0:613:C:H2'	1:0:614:U:H6	1.81	0.45
1:0:1345:A:H2'	1:0:1346:U:C6	2.51	0.45
1:0:2353:A:H4'	1:0:2354:A:O5'	2.16	0.45
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.16	0.45
1:0:2445:U:H2'	1:0:2446:G:H8	1.77	0.45
5:C:5:ILE:HG13	5:C:15:GLU:HA	1.98	0.45
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.98	0.45
7:E:23:GLU:HG2	7:E:28:SER:CB	2.46	0.45
15:M:68:ARG:O	15:M:68:ARG:HD3	2.16	0.45
15:M:134:ILE:O	15:M:136:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:140:GLN:CD	16:N:143:ARG:HD3	2.40	0.45
17:O:35:LYS:HB3	17:O:36:PRO:HD2	1.97	0.45
18:P:36:THR:O	18:P:39:ASP:HB2	2.16	0.45
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.63	0.45
1:0:263:U:C4	8:F:54:VAL:HG13	2.51	0.45
1:0:2909:G:H2'	1:0:2910:A:H8	1.82	0.45
3:A:76:VAL:HG21	28:Z:63:LYS:HB3	1.96	0.45
3:A:184:THR:N	38:A:8844:HOH:O	2.50	0.45
4:B:14:GLY:HA2	4:B:15:PRO:C	2.42	0.45
4:B:279:THR:OG1	4:B:290:VAL:HB	2.16	0.45
5:C:101:ASP:HA	38:C:8646:HOH:O	2.16	0.45
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.98	0.45
7:E:84:MET:HG2	7:E:168:ILE:HD13	1.98	0.45
7:E:156:ASP:OD2	7:E:157:LYS:NZ	2.41	0.45
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.98	0.45
11:I:107:LYS:C	11:I:109:PRO:HD2	2.42	0.45
11:I:114:TYR:CD1	11:I:114:TYR:N	2.84	0.45
12:J:14:ALA:O	12:J:17:CYS:HB2	2.15	0.45
12:J:95:ARG:NE	12:J:99:GLU:OE2	2.49	0.45
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.49	0.45
14:L:7:GLN:HB3	14:L:13:HIS:CE1	2.52	0.45
20:R:32:ALA:O	20:R:33:ARG:C	2.59	0.45
22:T:89:ARG:HD2	22:T:89:ARG:C	2.40	0.45
23:U:38:ASN:O	23:U:42:LEU:HG	2.17	0.45
24:V:42:ASN:N	24:V:43:PRO:HD3	2.31	0.45
1:0:661:G:C5	1:0:686:A:C2	3.05	0.45
1:0:776:A:OP1	29:1:28:HIS:HE1	2.00	0.45
1:0:790:A:H2'	1:0:791:A:O4'	2.17	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.16	0.45
1:0:2866:U:H4'	1:0:2867:G:H5'	1.99	0.45
4:B:54:VAL:O	4:B:55:ASN:C	2.59	0.45
4:B:62:ARG:HH21	4:B:67:GLU:HG3	1.81	0.45
4:B:82:VAL:O	4:B:82:VAL:CG1	2.63	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.46	0.45
6:D:94:ALA:HB3	6:D:97:GLN:HE21	1.81	0.45
10:H:100:GLU:HB3	10:H:124:VAL:HG11	1.98	0.45
13:K:72:VAL:HG11	13:K:121:PHE:HD1	1.81	0.45
23:U:53:ASP:O	23:U:54:THR:C	2.59	0.45
1:0:243:A:H61	1:0:269:G:H1'	1.81	0.45
1:0:419:A:H1'	1:0:1921:A:C2	2.51	0.45
1:0:580:A:H5''	38:0:5572:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:920:C:H4'	1:0:921:G:C2	2.51	0.45
1:0:1603:A:C5'	1:0:1605:G:H5'	2.47	0.45
1:0:1942:A:H2'	1:0:1943:C:H6	1.80	0.45
1:0:2102:G:C2	1:0:2103:A:N6	2.84	0.45
3:A:99:ILE:O	3:A:131:HIS:HE1	2.00	0.45
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.46	0.45
12:J:36:VAL:HG12	12:J:37:ALA:N	2.32	0.45
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.15	0.45
18:P:20:ARG:HH12	18:P:54:LYS:HD3	1.80	0.45
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.46	0.45
25:W:35:VAL:HA	25:W:36:PRO:HD3	1.83	0.45
25:W:108:ARG:C	25:W:110:GLN:H	2.24	0.45
1:0:1427:A:H61	1:0:1440:U:H1'	1.82	0.45
1:0:1461:U:H2'	1:0:1462:C:C6	2.52	0.45
1:0:2002:C:C2'	1:0:2003:U:H5'	2.46	0.45
38:0:7429:HOH:O	5:C:188:ARG:HD3	2.16	0.45
4:B:304:PRO:CG	4:B:307:ARG:NH1	2.80	0.45
5:C:51:TYR:CE2	29:1:53:LYS:HB3	2.51	0.45
5:C:133:ARG:NH2	38:C:8623:HOH:O	2.48	0.45
8:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.45
14:L:145:LEU:HD23	14:L:145:LEU:C	2.42	0.45
18:P:115:SER:OG	18:P:118:GLN:HG3	2.17	0.45
22:T:48:VAL:CG1	22:T:49:GLU:N	2.78	0.45
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.16	0.45
1:0:596:C:H2'	1:0:597:A:C8	2.52	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.32	0.45
1:0:1116:U:O2'	1:0:1118:A:C2	2.57	0.45
1:0:1154:A:H2'	1:0:1155:G:H8	1.82	0.45
1:0:1406:A:H4'	1:0:1407:A:H5''	1.98	0.45
3:A:93:THR:HG23	3:A:154:ALA:O	2.17	0.45
3:A:125:ASN:ND2	38:A:8829:HOH:O	2.46	0.45
4:B:138:GLY:O	4:B:139:ASP:C	2.59	0.45
6:D:86:THR:C	6:D:89:PRO:HD2	2.41	0.45
18:P:110:ASP:C	18:P:112:GLY:N	2.74	0.45
19:Q:50:GLY:O	19:Q:86:VAL:HG23	2.16	0.45
24:V:27:LEU:HA	24:V:49:LEU:HD13	1.99	0.45
25:W:38:THR:HG22	25:W:39:ASP:N	2.32	0.45
27:Y:190:VAL:HG23	38:Y:8829:HOH:O	2.16	0.45
28:Z:81:ARG:O	28:Z:82:SER:C	2.60	0.45
29:1:5:THR:N	29:1:6:PRO:HD2	2.31	0.45
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:303:C:O2'	1:0:304:G:H5'	2.17	0.45
1:0:653:U:H2'	1:0:654:A:C8	2.52	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45
1:0:2870:C:H2'	1:0:2871:G:H8	1.82	0.45
38:0:3845:HOH:O	10:H:14:LYS:HE2	2.15	0.45
5:C:84:VAL:O	5:C:85:LYS:HB2	2.17	0.45
8:F:38:LYS:NZ	15:M:3:SER:HA	2.32	0.45
11:I:87:PRO:CB	11:I:129:SER:C	2.89	0.45
14:L:89:PHE:N	38:L:8873:HOH:O	2.50	0.45
15:M:107:ARG:HD2	38:M:8873:HOH:O	2.17	0.45
16:N:67:ALA:C	16:N:69:TYR:N	2.73	0.45
20:R:69:LYS:HE2	20:R:78:GLY:O	2.16	0.45
21:S:57:THR:HG22	21:S:58:MET:N	2.32	0.45
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.14	0.45
25:W:91:ASP:HB2	38:W:5425:HOH:O	2.16	0.45
25:W:108:ARG:C	25:W:110:GLN:N	2.73	0.45
27:Y:177:LYS:HD3	27:Y:181:GLY:O	2.17	0.45
31:3:60:LYS:CG	31:3:61:PRO:HD2	2.41	0.45
1:0:111:C:H2'	1:0:112:G:O4'	2.16	0.45
1:0:484:A:N1	1:0:506:G:H4'	2.32	0.45
1:0:714:U:H4'	38:0:5729:HOH:O	2.17	0.45
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
1:0:2613:G:O2'	1:0:2614:C:H5'	2.16	0.45
2:9:3:A:H2	2:9:21:G:N3	2.14	0.45
3:A:192:VAL:O	3:A:192:VAL:CG1	2.64	0.45
3:A:211:LYS:HB2	38:A:8915:HOH:O	2.15	0.45
4:B:138:GLY:O	4:B:139:ASP:O	2.34	0.45
4:B:307:ARG:HH11	4:B:307:ARG:HB2	1.81	0.45
5:C:136:VAL:HA	5:C:137:PRO:C	2.41	0.45
6:D:44:ILE:HG23	6:D:45:THR:N	2.31	0.45
7:E:91:PHE:HA	7:E:92:PRO:HD3	1.81	0.45
13:K:28:GLU:HG2	13:K:58:THR:HB	1.98	0.45
13:K:74:VAL:HG21	13:K:96:VAL:HG23	1.98	0.45
15:M:109:PHE:CB	15:M:112:LEU:HD12	2.46	0.45
16:N:64:SER:C	16:N:66:LEU:H	2.24	0.45
1:0:449:A:N7	5:C:43:LYS:HG2	2.31	0.45
4:B:41:PHE:HB3	4:B:190:MET:HE1	1.99	0.45
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.97	0.45
6:D:95:THR:C	6:D:97:GLN:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:173:GLU:O	6:D:174:VAL:C	2.59	0.45
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.98	0.45
9:G:12:ILE:N	9:G:13:PRO:HD3	2.32	0.45
10:H:48:VAL:HA	10:H:170:ARG:O	2.17	0.45
15:M:159:VAL:HG13	15:M:160:PHE:N	2.32	0.45
17:O:35:LYS:HD3	38:O:3360:HOH:O	2.16	0.45
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.46	0.45
20:R:6:VAL:HG21	20:R:113:HIS:CD2	2.51	0.45
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.32	0.45
1:O:162:C:H2'	1:O:163:U:H5'	1.99	0.45
1:O:1524:U:OP1	1:O:1524:U:H4'	2.16	0.45
1:O:1568:G:O2'	1:O:1569:U:H5'	2.16	0.45
1:O:1942:A:O2'	1:O:1943:C:H5'	2.17	0.45
1:O:2434:A:O3'	31:3:28:GLY:HA3	2.17	0.45
1:O:2761:A:C4	1:O:2763:G:C8	3.05	0.45
4:B:60:SER:C	4:B:62:ARG:N	2.75	0.45
11:I:95:LEU:HA	11:I:99:GLN:OE1	2.16	0.45
14:L:75:LEU:HD21	38:O:7543:HOH:O	2.16	0.45
16:N:37:ARG:CZ	38:N:8832:HOH:O	2.65	0.45
16:N:132:ASN:N	38:N:8853:HOH:O	2.45	0.45
16:N:170:GLU:HA	16:N:173:ASP:OD2	2.16	0.45
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.17	0.45
25:W:3:ALA:O	25:W:54:PHE:HA	2.17	0.45
25:W:62:LEU:HD12	25:W:62:LEU:O	2.17	0.45
1:O:230:C:H2'	1:O:231:G:C8	2.52	0.44
1:O:350:G:O2'	1:O:351:A:H5'	2.16	0.44
1:O:517:U:H2'	1:O:518:G:H5'	1.99	0.44
1:O:825:U:H5''	1:O:826:U:OP1	2.17	0.44
1:O:1421:C:O2'	1:O:1422:U:H5'	2.16	0.44
1:O:2252:A:C5	1:O:2253:G:H1'	2.52	0.44
1:O:2524:G:H5''	38:O:4728:HOH:O	2.16	0.44
3:A:135:VAL:HG11	3:A:147:ARG:NH2	2.32	0.44
3:A:199:HIS:CD2	3:A:201:PHE:H	2.35	0.44
3:A:206:ARG:NH1	3:A:208:HIS:CD2	2.85	0.44
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.83	0.44
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.44
8:F:32:GLY:N	38:F:3111:HOH:O	2.49	0.44
10:H:30:LYS:N	10:H:62:HIS:HD2	2.11	0.44
11:I:87:PRO:C	11:I:89:GLU:N	2.73	0.44
11:I:109:PRO:HG2	11:I:110:ASP:H	1.82	0.44
13:K:75:ARG:HH21	13:K:94:ALA:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.17	0.44
20:R:17:MET:HG2	20:R:144:GLU:HA	1.99	0.44
25:W:31:HIS:HB3	38:W:5420:HOH:O	2.17	0.44
26:X:74:ALA:HB2	26:X:85:VAL:HG22	1.99	0.44
27:Y:105:LYS:HE2	27:Y:198:GLY:O	2.18	0.44
28:Z:49:ARG:HH21	28:Z:52:THR:HA	1.81	0.44
29:1:29:THR:O	29:1:32:LYS:NZ	2.47	0.44
31:3:24:LYS:HE3	31:3:90:PHE:HE1	1.82	0.44
1:0:213:G:HO2'	1:0:214:U:P	2.40	0.44
1:0:656:G:H5'	17:O:3:THR:HG22	2.00	0.44
1:0:711:G:C2	1:0:718:C:C2	3.05	0.44
1:0:721:A:H5''	17:O:51:TYR:CE2	2.52	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.52	0.44
1:0:1132:A:H3'	38:0:4815:HOH:O	2.16	0.44
1:0:1328:A:N7	1:0:1329:G:C5	2.86	0.44
1:0:2728:C:H4'	1:0:2894:C:HO2'	1.83	0.44
1:0:2754:G:O2'	1:0:2755:G:H5'	2.17	0.44
1:0:2897:C:O2'	1:0:2898:G:H5'	2.18	0.44
2:9:91:C:H2'	2:9:92:G:O4'	2.17	0.44
2:9:107:C:O2'	2:9:108:C:H5'	2.17	0.44
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.31	0.44
4:B:38:VAL:HG22	4:B:142:LEU:HD12	1.98	0.44
4:B:84:LEU:HD23	4:B:142:LEU:CD2	2.46	0.44
4:B:109:LEU:HD11	4:B:113:LEU:HD12	1.99	0.44
5:C:173:LYS:HB3	5:C:187:ARG:HG3	1.97	0.44
6:D:11:HIS:CG	6:D:12:GLU:N	2.84	0.44
8:F:107:ASP:O	8:F:111:ILE:HG13	2.17	0.44
10:H:34:HIS:HD2	10:H:90:LEU:O	1.99	0.44
15:M:69:LYS:O	15:M:73:ARG:NH2	2.50	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.84	0.44
24:V:39:ALA:O	24:V:41:GLU:N	2.50	0.44
26:X:25:ARG:HD3	26:X:64:ALA:O	2.17	0.44
26:X:30:MET:CE	26:X:58:ALA:HB3	2.47	0.44
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.50	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.17	0.44
1:0:137:U:O5'	1:0:137:U:H6	1.99	0.44
1:0:394:G:H1	15:M:181:GLU:CD	2.26	0.44
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.98	0.44
1:0:1505:U:H5'	1:0:1505:U:C6	2.48	0.44
1:0:1566:C:H2'	1:0:1567:G:C8	2.53	0.44
1:0:1667:A:H2'	1:0:1668:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H5''	1:0:1702:U:H3'	1.99	0.44
38:0:6151:HOH:O	3:A:223:ARG:HG3	2.17	0.44
38:0:7064:HOH:O	14:L:2:SER:HB2	2.18	0.44
2:9:37:C:H4'	16:N:110:THR:HG23	1.98	0.44
3:A:140:LEU:HB3	3:A:141:PRO:HD2	1.99	0.44
5:C:126:ASP:C	5:C:128:GLY:N	2.75	0.44
9:G:23:ILE:HG22	9:G:27:ILE:CD1	2.48	0.44
12:J:17:CYS:HA	12:J:119:THR:O	2.18	0.44
13:K:97:ILE:HG22	13:K:98:VAL:N	2.32	0.44
17:O:2:LYS:NZ	38:O:3002:HOH:O	2.50	0.44
17:O:43:VAL:HG21	17:O:115:ARG:HA	1.99	0.44
18:P:138:GLU:O	18:P:139:ARG:C	2.59	0.44
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.97	0.44
26:X:73:ARG:HB2	26:X:88:GLU:HG2	1.99	0.44
1:0:88:G:H8	1:0:88:G:H5'	1.83	0.44
1:0:549:A:O2'	1:0:550:C:H5'	2.18	0.44
1:0:843:A:C2	1:0:846:A:C8	3.05	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
1:0:962:C:H2'	1:0:963:C:C5'	2.47	0.44
1:0:1162:G:O2'	11:I:112:LEU:HG	2.17	0.44
1:0:1850:U:H2'	1:0:1851:G:H8	1.82	0.44
1:0:2716:G:H1'	38:B:8842:HOH:O	2.17	0.44
1:0:2766:A:O2'	1:0:2767:C:H5'	2.17	0.44
1:0:2831:C:C2'	1:0:2832:C:H5'	2.48	0.44
2:9:9:C:H2'	2:9:10:C:H5'	2.00	0.44
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.81	0.44
5:C:21:VAL:C	5:C:23:GLU:N	2.76	0.44
6:D:18:ILE:HD13	6:D:84:LEU:HD11	1.98	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.44
8:F:26:THR:HG21	8:F:102:GLY:C	2.43	0.44
12:J:88:PRO:CA	36:J:8802:CL:CL	3.02	0.44
14:L:149:ARG:NH2	38:L:8889:HOH:O	2.45	0.44
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.44
1:0:875:A:C2	3:A:194:MET:SD	3.11	0.44
1:0:1173:A:H4'	1:0:1174:A:C8	2.53	0.44
1:0:1407:A:O2'	1:0:1408:U:H3'	2.17	0.44
1:0:1419:U:H5'	1:0:1420:C:OP2	2.18	0.44
1:0:1755:A:H2'	1:0:1756:G:O4'	2.17	0.44
1:0:2419:U:H5''	1:0:2420:G:H5'	2.00	0.44
1:0:2511:A:H2'	1:0:2512:U:O4'	2.17	0.44
38:0:5852:HOH:O	12:J:74:ARG:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:11:A:O2'	2:9:12:C:H3'	2.18	0.44
10:H:5:PRO:HB2	10:H:7:SER:OG	2.18	0.44
11:I:91:PHE:HA	11:I:131:GLY:CA	2.47	0.44
20:R:96:VAL:O	20:R:99:ALA:HB3	2.17	0.44
1:0:195:C:H2'	1:0:196:G:H5'	1.98	0.44
1:0:398:U:H2'	1:0:399:C:C6	2.53	0.44
1:0:1185:U:H2'	1:0:1186:C:O4'	2.17	0.44
1:0:1205:U:C2'	1:0:1206:U:C5'	2.94	0.44
1:0:1669:G:O2'	1:0:1670:A:H5'	2.17	0.44
1:0:1771:U:O2	28:Z:19:GLY:HA2	2.18	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.53	0.44
1:0:2032:U:H2'	1:0:2033:G:C5'	2.48	0.44
1:0:2291:A:N9	1:0:2309:C:H5'	2.32	0.44
1:0:2320:U:H3'	31:3:2:GLN:HB2	2.00	0.44
1:0:2453:G:H4'	14:L:50:GLY:C	2.43	0.44
1:0:2551:C:O2'	1:0:2552:C:H5'	2.17	0.44
1:0:2589:U:H2'	1:0:2590:U:C6	2.52	0.44
1:0:2709:G:N2	38:0:7592:HOH:O	2.51	0.44
38:0:3516:HOH:O	21:S:13:LYS:HE2	2.17	0.44
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.34	0.44
6:D:36:ASN:HA	38:D:7500:HOH:O	2.17	0.44
10:H:146:ALA:HA	10:H:149:VAL:HG12	2.00	0.44
12:J:19:MET:HE1	12:J:78:ILE:CG2	2.45	0.44
13:K:49:LEU:HA	13:K:73:VAL:HG12	1.99	0.44
13:K:113:ILE:HG22	13:K:114:ALA:O	2.16	0.44
19:Q:53:HIS:CE1	19:Q:55:ARG:HG3	2.53	0.44
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.52	0.44
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.26	0.44
1:0:59:A:H5'	38:0:4329:HOH:O	2.18	0.44
1:0:228:C:H2'	1:0:229:G:H5'	1.99	0.44
1:0:499:G:O2'	1:0:500:G:H5'	2.17	0.44
1:0:645:U:OP2	14:L:4:LYS:HE3	2.17	0.44
1:0:2582:G:O3'	13:K:41:LYS:HA	2.18	0.44
1:0:2838:A:H2	38:0:3517:HOH:O	2.00	0.44
3:A:211:LYS:NZ	38:A:8867:HOH:O	2.50	0.44
4:B:162:MET:CE	4:B:310:ARG:HD3	2.46	0.44
4:B:278:PRO:HD3	4:B:294:TYR:CZ	2.52	0.44
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.18	0.44
7:E:69:ILE:HA	7:E:72:MET:HE3	1.99	0.44
8:F:117:GLU:C	8:F:119:ARG:N	2.76	0.44
10:H:122:LYS:O	10:H:124:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:78:ALA:HB1	11:I:93:ALA:CB	2.48	0.44
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.16	0.44
13:K:75:ARG:O	13:K:93:ASN:HA	2.17	0.44
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.83	0.44
16:N:183:ASP:O	16:N:184:ILE:O	2.35	0.44
20:R:82:GLU:O	20:R:86:LYS:HG3	2.17	0.44
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.81	0.44
1:O:158:A:H2'	1:O:159:G:O4'	2.18	0.44
1:O:368:C:H2'	1:O:369:G:H5'	1.99	0.44
1:O:440:C:H2'	1:O:441:A:C8	2.52	0.44
1:O:534:C:N3	1:O:2083:A:H2'	2.32	0.44
1:O:1342:C:H2'	1:O:1343:C:H5'	1.99	0.44
1:O:1494:A:C4	1:O:1495:C:C5	3.06	0.44
1:O:2598:U:O2	1:O:2600:A:C8	2.71	0.44
1:O:2601:A:N1	13:K:38:SER:HB2	2.32	0.44
1:O:2781:U:H2'	1:O:2782:G:H5'	2.00	0.44
1:O:2890:A:H1'	23:U:56:ARG:HH21	1.78	0.44
4:B:62:ARG:NH2	4:B:66:GLU:O	2.50	0.44
6:D:97:GLN:O	6:D:104:PHE:HB2	2.18	0.44
8:F:110:ASP:O	8:F:114:LYS:HG3	2.17	0.44
10:H:12:ILE:HG12	10:H:59:GLN:CG	2.47	0.44
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.43	0.44
16:N:143:ARG:HA	16:N:172:PHE:CE2	2.53	0.44
18:P:103:THR:O	18:P:107:GLU:HG3	2.18	0.44
22:T:20:HIS:CE1	22:T:67:LEU:HD11	2.53	0.44
28:Z:39:CYS:HA	28:Z:47:VAL:CG2	2.48	0.44
1:O:183:A:H1'	15:M:161:ARG:NH1	2.33	0.44
1:O:262:A:C6	8:F:89:LEU:HD21	2.52	0.44
1:O:297:U:H2'	1:O:298:C:C6	2.53	0.44
1:O:333:G:O2'	1:O:334:G:H5'	2.18	0.44
1:O:1313:A:H5''	27:Y:210:GLY:N	2.32	0.44
1:O:1398:G:O2'	1:O:1399:A:H5'	2.17	0.44
1:O:2134:G:N2	1:O:2242:U:C2	2.85	0.44
1:O:2489:G:H1'	38:O:7250:HOH:O	2.17	0.44
38:O:3502:HOH:O	5:C:81:PRO:HD3	2.18	0.44
38:O:3753:HOH:O	22:T:9:LYS:HD2	2.18	0.44
5:C:141:SER:C	5:C:143:ASP:N	2.76	0.44
7:E:83:GLY:O	7:E:169:THR:N	2.37	0.44
8:F:26:THR:CG2	8:F:103:GLU:HB2	2.29	0.44
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.48	0.44
12:J:27:ALA:HB1	12:J:87:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:32:ILE:HD11	13:K:56:SER:HB3	2.00	0.44
15:M:82:ARG:NH1	15:M:84:LYS:HB2	2.33	0.44
18:P:90:SER:O	18:P:91:LYS:C	2.60	0.44
18:P:115:SER:OG	18:P:118:GLN:CG	2.66	0.44
18:P:120:ARG:HG3	18:P:120:ARG:O	2.18	0.44
25:W:38:THR:HG22	25:W:39:ASP:H	1.83	0.44
25:W:83:TRP:HD1	38:W:4859:HOH:O	2.01	0.44
26:X:80:GLU:N	38:X:5564:HOH:O	2.50	0.44
1:0:230:C:H2'	1:0:231:G:H8	1.82	0.43
1:0:553:G:O2'	1:0:554:G:H5'	2.18	0.43
1:0:1016:U:O2'	1:0:2303:A:N7	2.50	0.43
1:0:1972:U:C2'	1:0:1973:A:C5'	2.96	0.43
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.18	0.43
4:B:148:PRO:HD2	38:B:8875:HOH:O	2.17	0.43
4:B:185:GLY:C	4:B:187:GLU:H	2.26	0.43
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.53	0.43
6:D:82:GLU:HA	6:D:85:GLN:HE21	1.82	0.43
16:N:73:ALA:N	38:N:8864:HOH:O	2.50	0.43
19:Q:88:ALA:O	19:Q:91:LEU:N	2.40	0.43
19:Q:93:ARG:HG3	19:Q:93:ARG:NH1	2.33	0.43
26:X:41:PHE:O	26:X:43:VAL:HG23	2.18	0.43
1:0:837:U:H4'	38:0:3388:HOH:O	2.18	0.43
1:0:1160:G:H5'	1:0:1161:A:O4'	2.19	0.43
1:0:1205:U:C2'	1:0:1206:U:H5''	2.48	0.43
1:0:1463:U:H2'	1:0:1464:C:C6	2.53	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.18	0.43
1:0:2114:C:O2'	1:0:2115:U:H5'	2.18	0.43
1:0:2637:A:H5'	38:0:4362:HOH:O	2.18	0.43
38:0:6573:HOH:O	31:3:79:LEU:HB2	2.18	0.43
3:A:125:ASN:HB2	3:A:158:VAL:HG12	1.97	0.43
4:B:176:ASP:O	4:B:177:HIS:C	2.61	0.43
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.66	0.43
4:B:279:THR:CG2	4:B:280:VAL:N	2.80	0.43
5:C:140:VAL:HG12	5:C:141:SER:N	2.33	0.43
5:C:235:PHE:CE2	5:C:243:VAL:HG21	2.52	0.43
6:D:39:ASP:HB2	38:D:5583:HOH:O	2.16	0.43
6:D:51:ARG:HD3	38:D:7636:HOH:O	2.18	0.43
7:E:26:ASN:HB3	7:E:76:VAL:O	2.18	0.43
8:F:4:VAL:HG13	8:F:76:PHE:CD1	2.53	0.43
11:I:74:ILE:C	11:I:76:ASP:N	2.76	0.43
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:13:VAL:HG13	18:P:14:LEU:N	2.33	0.43
20:R:132:ARG:NH2	38:R:8878:HOH:O	2.51	0.43
23:U:34:SER:HA	23:U:37:GLU:OE1	2.18	0.43
1:0:684:G:H2'	1:0:685:C:C6	2.53	0.43
1:0:1319:G:H1'	38:0:4690:HOH:O	2.18	0.43
1:0:1746:A:O4'	1:0:1747:A:C2	2.71	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.48	0.43
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.18	0.43
4:B:106:HIS:CE1	4:B:147:VAL:HG13	2.53	0.43
5:C:160:LEU:O	5:C:161:ASP:HB2	2.18	0.43
5:C:162:VAL:CG1	5:C:192:ILE:HD11	2.47	0.43
6:D:18:ILE:HD13	6:D:84:LEU:CD1	2.48	0.43
7:E:118:ILE:HG23	7:E:144:THR:HG21	2.01	0.43
10:H:12:ILE:HG12	10:H:59:GLN:HG3	2.00	0.43
13:K:53:ILE:HG13	13:K:55:VAL:CG2	2.49	0.43
15:M:30:GLU:O	15:M:34:GLU:HG3	2.18	0.43
16:N:61:ALA:HB2	16:N:88:ALA:HB2	2.00	0.43
17:O:9:SER:O	17:O:10:LEU:C	2.61	0.43
17:O:69:VAL:HG12	17:O:70:LEU:N	2.32	0.43
18:P:27:ARG:O	18:P:28:GLN:C	2.61	0.43
18:P:63:ARG:O	18:P:64:GLU:C	2.61	0.43
19:Q:15:LYS:HG2	19:Q:16:ASN:N	2.34	0.43
20:R:132:ARG:NH1	38:R:8878:HOH:O	2.51	0.43
22:T:23:VAL:C	22:T:93:THR:HG21	2.44	0.43
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.17	0.43
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
1:0:1543:G:N1	1:0:1641:A:OP2	2.41	0.43
38:0:4094:HOH:O	26:X:18:ARG:HD3	2.18	0.43
38:0:4225:HOH:O	30:2:38:LYS:HE3	2.17	0.43
2:9:11:A:P	19:Q:19:ARG:HH21	2.41	0.43
3:A:30:ARG:HD3	3:A:60:PHE:CZ	2.53	0.43
3:A:99:ILE:O	3:A:131:HIS:CE1	2.71	0.43
6:D:10:PHE:CD1	6:D:11:HIS:N	2.87	0.43
6:D:95:THR:C	6:D:97:GLN:N	2.76	0.43
11:I:94:ASP:HA	11:I:133:THR:O	2.18	0.43
15:M:152:ALA:HA	38:M:8934:HOH:O	2.18	0.43
16:N:13:ARG:O	16:N:13:ARG:NH1	2.47	0.43
18:P:83:LYS:NZ	38:P:199:HOH:O	2.52	0.43
25:W:140:LYS:C	25:W:141:HIS:HD2	2.26	0.43
27:Y:97:LEU:CD2	27:Y:235:GLU:HG3	2.48	0.43
30:2:31:ARG:NH1	38:2:7177:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:348:C:H5	38:0:6313:HOH:O	2.02	0.43
1:0:583:C:H2'	1:0:584:U:C6	2.53	0.43
1:0:655:U:O2'	17:O:3:THR:HB	2.18	0.43
1:0:696:C:O2'	1:0:697:G:H5'	2.18	0.43
1:0:876:A:H2'	1:0:876:A:N3	2.34	0.43
1:0:907:A:H4'	1:0:1328:A:C2	2.54	0.43
1:0:939:A:H5'	38:0:5400:HOH:O	2.18	0.43
1:0:962:C:C2'	1:0:963:C:H5'	2.49	0.43
1:0:1488:U:H4'	1:0:1489:G:OP1	2.19	0.43
1:0:1548:U:H5''	18:P:59:ARG:NE	2.33	0.43
1:0:2690:U:O2'	7:E:111:LYS:HE3	2.19	0.43
1:0:2765:C:H2'	1:0:2766:A:H8	1.83	0.43
1:0:2821:C:H4'	4:B:116:PRO:CG	2.49	0.43
38:0:9980:HOH:O	14:L:22:ARG:HG2	2.17	0.43
3:A:206:ARG:HH11	3:A:206:ARG:CG	2.31	0.43
4:B:71:VAL:HG13	4:B:297:VAL:O	2.19	0.43
4:B:140:LEU:HD13	4:B:175:LEU:HA	2.00	0.43
4:B:217:ARG:CG	4:B:257:THR:HG22	2.46	0.43
4:B:329:TYR:HE2	23:U:15:PRO:HG2	1.79	0.43
5:C:141:SER:C	5:C:143:ASP:H	2.25	0.43
14:L:66:VAL:HG23	14:L:67:ARG:N	2.34	0.43
23:U:52:THR:CG2	23:U:54:THR:HB	2.49	0.43
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.18	0.43
25:W:131:PRO:O	25:W:136:GLY:N	2.50	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.53	0.43
29:1:36:SER:O	29:1:46:ARG:HD3	2.18	0.43
1:0:21:G:H1'	38:0:9750:HOH:O	2.17	0.43
1:0:152:A:O2'	1:0:153:C:H5'	2.18	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:363:C:H1'	38:0:5272:HOH:O	2.19	0.43
1:0:932:U:H1'	1:0:1296:A:H1'	2.00	0.43
1:0:2505:G:H8	38:0:5632:HOH:O	2.02	0.43
38:0:6848:HOH:O	15:M:178:LYS:HB2	2.17	0.43
6:D:60:GLU:HG3	6:D:60:GLU:O	2.19	0.43
8:F:118:LEU:O	8:F:119:ARG:OXT	2.37	0.43
13:K:41:LYS:O	13:K:42:ASN:HB2	2.18	0.43
16:N:163:PHE:O	16:N:164:ASP:CG	2.62	0.43
18:P:10:ALA:O	18:P:13:VAL:HG12	2.18	0.43
21:S:39:ASP:O	21:S:40:ALA:C	2.62	0.43
22:T:48:VAL:O	22:T:59:GLU:HG3	2.18	0.43
24:V:43:PRO:O	24:V:46:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:75:ALA:O	26:X:83:ALA:HA	2.18	0.43
1:0:154:C:H2'	1:0:155:C:H6	1.84	0.43
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.43
1:0:958:G:H2'	1:0:959:C:H6	1.84	0.43
1:0:1058:A:H2'	1:0:1060:C:H5''	2.00	0.43
1:0:1414:A:H2'	1:0:1415:G:O4'	2.18	0.43
1:0:2894:C:O2'	1:0:2895:C:H5'	2.18	0.43
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.48	0.43
4:B:189:ALA:O	4:B:192:ASP:HB2	2.19	0.43
8:F:102:GLY:O	8:F:103:GLU:C	2.61	0.43
24:V:12:THR:HG23	24:V:14:ALA:N	2.34	0.43
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	2.01	0.43
31:3:30:GLN:HE21	31:3:30:GLN:HB3	1.55	0.43
1:0:327:A:N3	5:C:206:ASN:ND2	2.62	0.43
1:0:407:A:O2'	1:0:408:A:H5'	2.19	0.43
1:0:424:C:H2'	1:0:425:U:H6	1.83	0.43
1:0:441:A:H1'	1:0:442:A:N7	2.33	0.43
1:0:559:U:H6	1:0:559:U:C5'	2.23	0.43
1:0:858:U:H2'	1:0:859:C:C6	2.53	0.43
1:0:1819:G:H2'	1:0:1820:G:C5'	2.49	0.43
1:0:1827:G:H2'	1:0:1828:G:C8	2.54	0.43
1:0:1878:G:O2'	1:0:1879:U:OP2	2.36	0.43
1:0:1999:C:H2'	1:0:2000:G:H8	1.83	0.43
1:0:2612:A:H4'	38:0:3680:HOH:O	2.19	0.43
2:9:29:C:C2'	2:9:30:C:H5'	2.45	0.43
2:9:92:G:C6	2:9:93:A:C6	3.06	0.43
3:A:94:LEU:N	3:A:94:LEU:CD2	2.80	0.43
3:A:136:ALA:N	3:A:148:LEU:O	2.52	0.43
3:A:231:LYS:O	3:A:232:ARG:HB3	2.19	0.43
4:B:166:VAL:O	4:B:174:ARG:HD2	2.19	0.43
4:B:182:VAL:O	4:B:183:GLU:C	2.61	0.43
11:I:96:SER:OG	11:I:99:GLN:HG3	2.18	0.43
13:K:22:ASP:HA	13:K:108:GLU:O	2.18	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.82	0.43
14:L:10:SER:O	14:L:11:ARG:HB3	2.18	0.43
14:L:12:THR:HG21	14:L:16:GLY:O	2.18	0.43
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.85	0.43
20:R:15:LYS:HE3	38:R:8873:HOH:O	2.18	0.43
26:X:78:GLU:CG	26:X:79:GLU:H	2.29	0.43
27:Y:119:GLN:O	27:Y:120:ARG:C	2.62	0.43
1:0:602:A:O2'	1:0:605:C:H4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1020:A:H5'	19:Q:38:LYS:HE3	2.00	0.43
1:0:1051:C:H2'	1:0:1052:G:O4'	2.19	0.43
1:0:1164:U:O4'	1:0:1166:A:H5'	2.19	0.43
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.46	0.43
1:0:1444:G:O2'	1:0:1445:G:H5'	2.18	0.43
1:0:1483:C:O2'	1:0:1484:G:H5'	2.18	0.43
1:0:1923:G:H1'	31:3:33:MET:HE2	2.01	0.43
1:0:2416:G:H2'	1:0:2417:C:C6	2.54	0.43
1:0:2785:C:H4'	1:0:2786:G:OP2	2.19	0.43
1:0:2852:A:H5''	38:0:5221:HOH:O	2.19	0.43
5:C:218:VAL:CG1	38:C:8621:HOH:O	2.67	0.43
10:H:60:LEU:O	10:H:65:LEU:HD21	2.19	0.43
13:K:22:ASP:C	13:K:22:ASP:OD1	2.62	0.43
14:L:34:GLY:C	14:L:36:ASP:H	2.27	0.43
14:L:104:ASP:HB3	38:L:8866:HOH:O	2.18	0.43
15:M:48:LYS:O	15:M:52:GLN:HG3	2.18	0.43
16:N:35:VAL:N	16:N:46:GLN:O	2.48	0.43
22:T:49:GLU:OE2	22:T:97:ARG:NH1	2.41	0.43
27:Y:145:LYS:O	27:Y:147:ARG:HG2	2.18	0.43
1:0:622:G:O2'	1:0:623:U:H5'	2.18	0.43
1:0:639:A:H2'	1:0:640:G:C8	2.53	0.43
1:0:644:G:H1'	38:0:6386:HOH:O	2.19	0.43
1:0:821:U:H2'	1:0:822:C:C6	2.54	0.43
1:0:1886:A:H5'	38:Z:8727:HOH:O	2.18	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.19	0.43
1:0:2361:A:H2'	1:0:2362:A:O4'	2.19	0.43
1:0:2414:A:C2	1:0:2415:A:C6	3.07	0.43
1:0:2511:A:H5'	1:0:2511:A:H8	1.83	0.43
1:0:2869:G:H2'	1:0:2870:C:H6	1.83	0.43
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.54	0.43
5:C:27:ARG:N	5:C:113:SER:OG	2.52	0.43
7:E:8:PRO:HB2	7:E:11:VAL:HG23	2.00	0.43
9:G:15:TRP:CE2	9:G:16:LYS:HG3	2.53	0.43
11:I:126:THR:C	38:I:7330:HOH:O	2.61	0.43
14:L:97:VAL:HG12	14:L:98:GLU:O	2.18	0.43
18:P:115:SER:O	18:P:118:GLN:HG3	2.19	0.43
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
1:0:250:C:O2'	1:0:251:C:H5'	2.18	0.42
1:0:635:A:H2'	1:0:636:G:H5''	2.01	0.42
1:0:934:C:H2'	1:0:935:G:C8	2.54	0.42
1:0:1188:A:C6	1:0:1189:A:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1511:U:O2'	1:0:1512:G:H5'	2.19	0.42
1:0:2768:A:O2'	1:0:2769:C:H5'	2.19	0.42
1:0:2773:G:H5'	38:0:7175:HOH:O	2.19	0.42
38:0:4062:HOH:O	4:B:27:ASN:HB2	2.19	0.42
38:0:5398:HOH:O	14:L:34:GLY:HA2	2.18	0.42
3:A:30:ARG:HE	3:A:30:ARG:HB3	1.49	0.42
6:D:20:LYS:HA	6:D:75:LEU:O	2.19	0.42
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.42
8:F:60:VAL:O	8:F:61:MET:C	2.62	0.42
10:H:46:TYR:HA	10:H:47:PRO:HD3	1.75	0.42
15:M:27:ARG:O	15:M:28:GLN:C	2.62	0.42
16:N:166:ALA:O	16:N:167:ASP:HB2	2.19	0.42
20:R:23:MET:HE3	20:R:28:SER:OG	2.19	0.42
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.54	0.42
28:Z:46:ARG:HH11	28:Z:59:TYR:HA	1.84	0.42
1:0:485:A:O2'	1:0:487:G:H5'	2.19	0.42
1:0:488:U:H2'	38:0:4001:HOH:O	2.19	0.42
1:0:707:C:C2	1:0:708:A:C8	3.07	0.42
1:0:1333:U:H2'	1:0:1334:C:H6	1.84	0.42
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
1:0:2036:C:C4'	13:K:44:LEU:HG	2.49	0.42
1:0:2590:U:H2'	1:0:2591:C:H5'	1.99	0.42
1:0:2781:U:H2'	1:0:2782:G:C5'	2.49	0.42
1:0:2896:A:H5''	38:0:6089:HOH:O	2.20	0.42
3:A:32:VAL:O	3:A:33:GLU:C	2.62	0.42
3:A:33:GLU:OE1	3:A:33:GLU:N	2.36	0.42
3:A:95:PRO:HA	3:A:153:ARG:HA	2.00	0.42
3:A:157:GLY:HA2	28:Z:79:VAL:HG11	2.01	0.42
3:A:228:ILE:O	3:A:229:ALA:C	2.61	0.42
4:B:51:VAL:HG22	4:B:53:LEU:HD12	2.01	0.42
6:D:41:LEU:C	6:D:44:ILE:HG22	2.44	0.42
6:D:52:THR:N	6:D:70:GLY:O	2.53	0.42
12:J:74:ARG:NH1	12:J:76:ASP:OD2	2.33	0.42
15:M:14:ASN:C	15:M:16:GLY:H	2.27	0.42
16:N:163:PHE:O	16:N:164:ASP:OD1	2.38	0.42
17:O:39:THR:HB	38:O:3360:HOH:O	2.18	0.42
18:P:92:GLU:HA	18:P:95:GLU:OE1	2.20	0.42
20:R:12:THR:HA	20:R:104:PHE:HE2	1.84	0.42
25:W:108:ARG:NH2	38:W:2359:HOH:O	2.51	0.42
25:W:122:ARG:HG3	25:W:122:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:677:C:P	38:C:8653:HOH:O	2.76	0.42
1:0:790:A:H1'	1:0:1710:A:H2'	2.01	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.18	0.42
1:0:890:C:O2'	29:1:50:TRP:O	2.35	0.42
1:0:1135:G:H5'	38:0:5917:HOH:O	2.19	0.42
1:0:1181:A:H2'	1:0:1182:C:C5'	2.49	0.42
1:0:1299:G:O6	14:L:6:ARG:HD3	2.19	0.42
1:0:1377:C:H5'	1:0:1377:C:C6	2.51	0.42
1:0:1498:G:O2'	1:0:1499:U:H5'	2.19	0.42
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.19	0.42
1:0:1718:G:O2'	1:0:1719:G:H5'	2.19	0.42
1:0:2028:U:H2'	1:0:2029:C:H6	1.85	0.42
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.42
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.19	0.42
1:0:2504:A:H4'	10:H:74:ARG:HH11	1.85	0.42
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.19	0.42
38:0:5652:HOH:O	22:T:68:ASP:HB2	2.19	0.42
2:9:3:A:N6	2:9:22:G:H1'	2.35	0.42
4:B:41:PHE:HB3	4:B:190:MET:HE3	2.00	0.42
4:B:75:GLU:C	4:B:77:PRO:HD3	2.45	0.42
4:B:238:ASN:ND2	4:B:240:GLY:N	2.49	0.42
5:C:131:PHE:CD2	5:C:131:PHE:N	2.87	0.42
8:F:79:GLN:HG2	38:F:2750:HOH:O	2.19	0.42
10:H:80:LEU:HD12	10:H:86:TYR:HD2	1.82	0.42
10:H:98:LEU:HD11	10:H:127:ALA:HB2	2.00	0.42
11:I:88:GLN:NE2	11:I:128:THR:HG22	2.34	0.42
12:J:39:VAL:HG13	12:J:106:GLY:O	2.19	0.42
15:M:5:TYR:O	15:M:7:TYR:N	2.53	0.42
16:N:48:VAL:HG12	16:N:49:THR:N	2.34	0.42
20:R:82:GLU:HG3	20:R:83:LYS:N	2.34	0.42
26:X:25:ARG:O	26:X:26:ALA:C	2.62	0.42
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	2.01	0.42
1:0:154:C:H3'	15:M:188:ARG:NH1	2.35	0.42
1:0:474:C:O3'	5:C:73:LEU:CD2	2.67	0.42
1:0:646:G:H5''	5:C:96:LYS:HD2	2.01	0.42
1:0:870:G:OP2	3:A:3:ARG:HD3	2.19	0.42
1:0:1765:G:O2'	1:0:1766:U:H5'	2.19	0.42
5:C:151:GLN:O	5:C:154:VAL:HB	2.19	0.42
8:F:21:GLU:O	8:F:24:ARG:HG3	2.19	0.42
10:H:142:ASN:O	10:H:144:GLU:N	2.52	0.42
19:Q:88:ALA:O	19:Q:90:HIS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:48:VAL:CG1	25:W:48:VAL:O	2.67	0.42
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.54	0.42
29:1:22:CYS:HA	38:1:2086:HOH:O	2.20	0.42
1:0:105:G:H1'	38:0:5156:HOH:O	2.19	0.42
1:0:282:C:H1'	1:0:368:C:H41	1.81	0.42
1:0:645:U:O2	1:0:761:A:H2	2.02	0.42
1:0:1590:A:H3'	38:0:6330:HOH:O	2.18	0.42
1:0:2070:G:H2'	1:0:2072:G:OP1	2.19	0.42
1:0:2346:C:H5'	6:D:54:ALA:HB2	2.00	0.42
1:0:2533:C:H6	1:0:2533:C:C5'	2.23	0.42
1:0:2598:U:O2	1:0:2600:A:H8	2.02	0.42
1:0:2825:C:H4'	1:0:2826:G:O5'	2.20	0.42
1:0:2899:A:H2'	1:0:2900:G:C8	2.54	0.42
2:9:39:U:H3'	2:9:40:C:C5'	2.49	0.42
3:A:43:VAL:HG21	3:A:59:GLU:OE2	2.19	0.42
3:A:191:GLY:C	3:A:193:ALA:H	2.27	0.42
4:B:254:GLN:HG2	4:B:255:GLY:N	2.33	0.42
6:D:172:VAL:CG1	6:D:173:GLU:N	2.82	0.42
14:L:27:ARG:HG3	14:L:27:ARG:HH11	1.84	0.42
16:N:31:LYS:HB2	16:N:101:VAL:HG23	2.01	0.42
25:W:140:LYS:C	25:W:141:HIS:CD2	2.98	0.42
26:X:80:GLU:O	26:X:80:GLU:HG2	2.18	0.42
31:3:6:ARG:NH1	31:3:21:GLU:HB2	2.34	0.42
1:0:132:A:C6	1:0:133:U:C4	3.08	0.42
1:0:420:U:H2'	1:0:421:C:C6	2.54	0.42
1:0:911:G:H5'	1:0:932:U:OP1	2.20	0.42
1:0:1861:C:H4'	3:A:6:GLY:O	2.19	0.42
1:0:2071:C:H5'	38:0:9520:HOH:O	2.18	0.42
1:0:2344:G:H2'	1:0:2344:G:N3	2.34	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.20	0.42
1:0:2498:C:O2'	1:0:2499:U:H5'	2.19	0.42
1:0:2506:A:N6	1:0:2511:A:O2'	2.49	0.42
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.42
2:9:33:U:H2'	38:9:8645:HOH:O	2.18	0.42
2:9:61:C:H2'	2:9:62:A:H8	1.85	0.42
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.49	0.42
6:D:87:ALA:O	6:D:88:LEU:C	2.62	0.42
9:G:19:GLU:O	9:G:20:VAL:C	2.63	0.42
11:I:85:GLY:O	11:I:86:GLU:HG3	2.20	0.42
13:K:55:VAL:O	13:K:68:VAL:HA	2.20	0.42
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:119:VAL:O	20:R:119:VAL:HG12	2.19	0.42
21:S:6:LYS:HD3	38:S:8523:HOH:O	2.18	0.42
25:W:13:MET:HE2	25:W:18:GLN:N	2.34	0.42
1:O:282:C:O2'	1:O:283:U:C4'	2.68	0.42
1:O:834:G:H3'	1:O:835:U:H4'	2.02	0.42
1:O:1307:A:H2'	1:O:1308:A:C8	2.55	0.42
1:O:2371:G:H5'	38:O:5002:HOH:O	2.20	0.42
1:O:2780:C:H2'	1:O:2781:U:H6	1.82	0.42
2:9:1:U:C4'	2:9:3:A:OP1	2.68	0.42
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.44	0.42
4:B:7:ARG:HD3	4:B:9:GLY:O	2.20	0.42
4:B:162:MET:HE2	4:B:310:ARG:CD	2.47	0.42
5:C:144:PHE:CD1	5:C:147:LEU:HD12	2.54	0.42
6:D:21:VAL:HA	6:D:131:THR:O	2.20	0.42
6:D:40:ILE:O	6:D:44:ILE:HG22	2.19	0.42
8:F:4:VAL:HA	8:F:76:PHE:CZ	2.54	0.42
9:G:12:ILE:O	9:G:13:PRO:C	2.60	0.42
15:M:35:GLY:C	38:M:8836:HOH:O	2.63	0.42
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.02	0.42
16:N:151:ASP:CG	16:N:165:ALA:O	2.62	0.42
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.20	0.42
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.19	0.42
27:Y:196:VAL:CG1	27:Y:226:ILE:HD13	2.50	0.42
28:Z:73:THR:O	28:Z:76:GLY:N	2.51	0.42
1:O:11:A:H5'	1:O:12:U:OP2	2.19	0.42
1:O:553:G:C2'	1:O:554:G:H5'	2.50	0.42
1:O:709:G:O2'	17:O:25:VAL:CG1	2.68	0.42
1:O:1127:C:H2'	1:O:1128:U:H5'	2.02	0.42
1:O:1202:A:C2'	1:O:1203:G:H5'	2.49	0.42
1:O:1829:A:H5''	38:O:3075:HOH:O	2.19	0.42
1:O:2277:U:H2'	1:O:2278:U:O4'	2.20	0.42
3:A:206:ARG:HH12	3:A:208:HIS:CE1	2.37	0.42
4:B:224:LYS:HD3	4:B:224:LYS:HA	1.84	0.42
4:B:310:ARG:HB3	38:B:8948:HOH:O	2.18	0.42
14:L:51:PHE:H	14:L:51:PHE:HD2	1.68	0.42
16:N:22:GLN:HG2	16:N:26:LEU:HD22	2.01	0.42
21:S:15:MET:O	21:S:18:MET:N	2.53	0.42
23:U:35:LYS:NZ	38:U:6621:HOH:O	2.52	0.42
24:V:64:GLY:O	24:V:65:ASP:CB	2.66	0.42
25:W:118:LEU:HD12	25:W:153:MET:HE3	2.01	0.42
31:3:70:ARG:HB3	38:3:8873:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:228:C:C2'	1:0:229:G:H5'	2.49	0.42
1:0:496:G:H3'	38:0:7638:HOH:O	2.19	0.42
1:0:503:G:H2'	1:0:504:G:H8	1.85	0.42
1:0:508:A:H2'	1:0:509:A:H5''	2.00	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.42
1:0:2793:A:H2'	1:0:2794:G:H5'	2.02	0.42
2:9:42:C:H5'	2:9:43:G:OP2	2.20	0.42
2:9:42:C:O2	6:D:76:ARG:HD2	2.20	0.42
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.42
11:I:87:PRO:HB2	11:I:129:SER:C	2.45	0.42
19:Q:86:VAL:HG22	19:Q:87:THR:O	2.19	0.42
30:2:40:ARG:HG3	30:2:45:ASN:HB2	2.01	0.42
31:3:55:VAL:C	38:3:8849:HOH:O	2.62	0.42
1:0:314:G:N2	1:0:316:A:H3'	2.34	0.42
1:0:645:U:OP2	14:L:4:LYS:CE	2.68	0.42
1:0:663:C:H5''	5:C:103:ASN:ND2	2.35	0.42
1:0:722:G:H22	1:0:938:G:P	2.43	0.42
1:0:1746:A:O2'	1:0:1752:G:N7	2.51	0.42
1:0:1754:A:H2'	1:0:1755:A:O4'	2.19	0.42
1:0:2345:A:H3'	1:0:2346:C:C6	2.55	0.42
1:0:2472:C:H3'	38:0:3602:HOH:O	2.19	0.42
2:9:96:C:H2'	2:9:97:U:H6	1.85	0.42
3:A:29:HIS:HB2	3:A:153:ARG:HH12	1.85	0.42
4:B:84:LEU:HD23	4:B:142:LEU:HD23	2.01	0.42
5:C:127:ARG:HD2	5:C:229:PRO:O	2.19	0.42
5:C:192:ILE:HG22	5:C:193:LEU:N	2.35	0.42
5:C:219:ASN:CG	5:C:222:ASP:OD1	2.62	0.42
6:D:35:ALA:HB3	38:D:7502:HOH:O	2.20	0.42
18:P:119:TYR:C	18:P:121:ASP:N	2.78	0.42
21:S:23:LYS:HA	21:S:66:VAL:O	2.20	0.42
23:U:30:HIS:HB3	38:U:6215:HOH:O	2.19	0.42
23:U:52:THR:HG22	23:U:54:THR:HB	2.02	0.42
24:V:44:GLY:O	24:V:48:GLU:HG2	2.19	0.42
27:Y:170:SER:OG	27:Y:175:ARG:HG3	2.19	0.42
31:3:69:TYR:CB	31:3:78:HIS:CE1	3.02	0.42
1:0:154:C:O2'	1:0:155:C:H5'	2.20	0.41
1:0:166:A:N7	14:L:25:GLY:HA2	2.35	0.41
1:0:218:C:P	31:3:39:GLN:HE21	2.43	0.41
1:0:463:A:H5''	38:0:3814:HOH:O	2.20	0.41
1:0:494:C:H2'	1:0:496:G:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.41
1:0:1202:A:H2'	1:0:1203:G:H5'	2.02	0.41
1:0:1375:A:C2'	1:0:1376:G:H5'	2.50	0.41
1:0:1479:G:H2'	1:0:1480:A:C8	2.55	0.41
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.52	0.41
1:0:1594:C:C5	18:P:120:ARG:NH1	2.88	0.41
1:0:1603:A:H5'	1:0:1605:G:C4'	2.49	0.41
1:0:1891:G:H1'	1:0:1972:U:C2	2.55	0.41
1:0:2081:A:H2'	1:0:2082:G:O4'	2.20	0.41
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.41
1:0:2338:G:H1'	6:D:105:SER:HG	1.84	0.41
1:0:2350:G:O2'	1:0:2351:C:H5'	2.20	0.41
1:0:2404:G:H4'	19:Q:68:GLY:CA	2.50	0.41
1:0:2656:G:C2'	1:0:2657:G:H5'	2.50	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.55	0.41
2:9:69:U:OP1	16:N:4:PRO:HG3	2.20	0.41
3:A:157:GLY:HA2	28:Z:79:VAL:CG1	2.50	0.41
4:B:36:PRO:HA	4:B:167:GLY:O	2.20	0.41
4:B:55:ASN:HB3	4:B:64:GLY:H	1.85	0.41
4:B:62:ARG:CB	4:B:65:MET:HE3	2.49	0.41
4:B:140:LEU:HA	38:B:8874:HOH:O	2.19	0.41
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.82	0.41
5:C:234:VAL:HG13	5:C:234:VAL:O	2.20	0.41
7:E:22:VAL:O	7:E:76:VAL:HG11	2.20	0.41
7:E:31:ARG:NH1	38:E:5919:HOH:O	2.52	0.41
8:F:26:THR:CG2	8:F:102:GLY:C	2.93	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.41
12:J:77:GLY:O	12:J:80:LYS:N	2.53	0.41
16:N:81:ALA:O	16:N:82:TYR:C	2.62	0.41
27:Y:189:ASN:ND2	27:Y:192:ASP:N	2.68	0.41
30:2:48:ASP:O	30:2:49:GLU:CB	2.67	0.41
31:3:11:CYS:SG	31:3:14:CYS:HB2	2.60	0.41
1:0:39:G:H2'	1:0:40:C:O4'	2.21	0.41
1:0:51:G:O2'	1:0:52:A:H5'	2.21	0.41
1:0:155:C:OP1	15:M:189:SER:HB3	2.20	0.41
1:0:163:U:O3'	1:0:896:C:H4'	2.20	0.41
1:0:807:A:H2'	1:0:808:A:O4'	2.20	0.41
1:0:1514:C:O2'	1:0:1515:A:H5'	2.20	0.41
1:0:1942:A:H2'	1:0:1943:C:C6	2.55	0.41
1:0:2102:G:N2	1:0:2103:A:C6	2.88	0.41
1:0:2487:C:H5	38:0:4882:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2819:C:H2'	1:0:2820:A:C8	2.55	0.41
38:0:3595:HOH:O	3:A:236:GLY:HA3	2.19	0.41
38:0:4704:HOH:O	16:N:101:VAL:HG12	2.20	0.41
4:B:171:VAL:O	4:B:175:LEU:HB2	2.20	0.41
38:C:8566:HOH:O	22:T:2:LYS:CE	2.64	0.41
6:D:149:ARG:NH2	38:D:3066:HOH:O	2.53	0.41
8:F:26:THR:HB	8:F:102:GLY:O	2.20	0.41
11:I:134:ILE:HG22	11:I:135:GLU:N	2.35	0.41
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.20	0.41
14:L:105:TYR:CD1	14:L:105:TYR:C	2.98	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.45	0.41
17:O:33:LEU:HA	17:O:40:HIS:NE2	2.36	0.41
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.50	0.41
24:V:12:THR:HG23	24:V:14:ALA:H	1.85	0.41
25:W:21:LEU:HD22	25:W:26:ILE:HD11	2.02	0.41
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.55	0.41
31:3:7:PHE:CD1	31:3:7:PHE:C	2.98	0.41
31:3:34:LYS:HD2	31:3:34:LYS:N	2.35	0.41
1:0:29:C:O2'	1:0:30:U:H5'	2.20	0.41
1:0:297:U:H2'	1:0:298:C:H6	1.85	0.41
1:0:514:G:O6	30:2:35:ARG:NH2	2.52	0.41
1:0:1311:G:C2	1:0:1312:G:C8	3.07	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1790:C:H2'	1:0:1791:U:H6	1.84	0.41
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.20	0.41
1:0:2032:U:O2'	1:0:2033:G:H5''	2.21	0.41
1:0:2036:C:C1'	13:K:44:LEU:HG	2.51	0.41
1:0:2103:A:N3	1:0:2103:A:H2'	2.34	0.41
1:0:2353:A:H1'	19:Q:21:ARG:HH12	1.84	0.41
1:0:2656:G:O2'	1:0:2657:G:H5'	2.20	0.41
38:0:4913:HOH:O	15:M:14:ASN:HB3	2.19	0.41
38:0:9546:HOH:O	25:W:119:HIS:HE1	2.02	0.41
38:0:9790:HOH:O	13:K:39:GLY:HA3	2.20	0.41
3:A:232:ARG:NH2	3:A:236:GLY:O	2.50	0.41
8:F:49:PHE:CD1	8:F:49:PHE:N	2.88	0.41
10:H:69:ARG:CZ	38:H:8566:HOH:O	2.67	0.41
13:K:99:ASP:OD1	13:K:101:ASN:N	2.53	0.41
14:L:40:PHE:CD1	14:L:40:PHE:C	2.98	0.41
17:O:63:LYS:NZ	38:O:2363:HOH:O	2.53	0.41
20:R:59:PHE:O	20:R:63:ASN:HB3	2.20	0.41
20:R:75:TRP:CG	20:R:76:ASP:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:102:ASP:O	22:T:103:LEU:HD23	2.20	0.41
25:W:80:ASP:O	25:W:81:ASP:C	2.62	0.41
1:0:152:A:H2'	1:0:153:C:C6	2.55	0.41
1:0:329:A:OP2	5:C:206:ASN:HB2	2.20	0.41
1:0:1515:A:H2'	1:0:1516:U:C6	2.54	0.41
1:0:1634:G:H2'	1:0:1635:U:H6	1.81	0.41
1:0:1790:C:H2'	1:0:1791:U:C6	2.54	0.41
1:0:1804:A:H2'	1:0:1805:G:C8	2.55	0.41
1:0:1874:U:H2'	3:A:120:ARG:HG3	2.03	0.41
1:0:1921:A:O2'	1:0:1922:A:H5'	2.20	0.41
1:0:2438:G:H2'	1:0:2439:C:O4'	2.20	0.41
1:0:2446:G:H1'	38:0:4236:HOH:O	2.20	0.41
1:0:2509:A:OP2	1:0:2510:C:H5	2.04	0.41
1:0:2596:A:O2'	13:K:32:ILE:HG22	2.20	0.41
2:9:31:C:H2'	2:9:32:G:O4'	2.21	0.41
6:D:153:THR:C	6:D:155:HIS:H	2.28	0.41
6:D:170:TYR:N	6:D:170:TYR:HD1	2.18	0.41
13:K:75:ARG:HH11	13:K:112:PRO:HD2	1.85	0.41
15:M:7:TYR:O	15:M:8:ILE:C	2.63	0.41
16:N:143:ARG:NH2	16:N:169:PRO:HB2	2.35	0.41
27:Y:127:GLN:O	27:Y:128:PHE:C	2.64	0.41
27:Y:189:ASN:ND2	27:Y:191:ASP:N	2.67	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.48	0.41
1:0:74:G:H1	1:0:103:C:H42	1.67	0.41
1:0:919:U:H5	38:0:6989:HOH:O	2.04	0.41
1:0:1164:U:OP1	11:I:70:THR:N	2.51	0.41
1:0:1268:C:H2'	1:0:1269:G:C8	2.55	0.41
1:0:1601:G:H1'	38:0:9889:HOH:O	2.20	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.64	0.41
1:0:1947:G:N2	1:0:1966:U:C2	2.88	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
1:0:2385:G:H2'	1:0:2386:U:C6	2.56	0.41
1:0:2432:C:O2'	1:0:2433:A:H5'	2.21	0.41
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.41
1:0:2570:G:H8	38:0:4907:HOH:O	2.03	0.41
2:9:42:C:O2	6:D:76:ARG:NH1	2.54	0.41
2:9:94:G:O2'	2:9:95:C:H5'	2.21	0.41
3:A:20:SER:C	3:A:22:ARG:H	2.26	0.41
6:D:81:GLU:O	6:D:83:PHE:N	2.53	0.41
7:E:99:GLY:N	38:E:4191:HOH:O	2.53	0.41
7:E:102:VAL:HG13	7:E:116:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.55	0.41
10:H:61:ARG:HG3	10:H:61:ARG:HH11	1.85	0.41
13:K:1:MET:HE1	38:K:6646:HOH:O	2.19	0.41
13:K:106:GLY:HA3	38:K:5264:HOH:O	2.20	0.41
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.66	0.41
16:N:124:ASP:C	16:N:126:GLY:H	2.29	0.41
20:R:119:VAL:HG12	38:R:8820:HOH:O	2.20	0.41
27:Y:144:ARG:NH1	38:Y:8879:HOH:O	2.54	0.41
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.48	0.41
31:3:40:ARG:HD2	38:3:8848:HOH:O	2.19	0.41
1:0:21:G:H5''	20:R:2:ILE:HA	1.98	0.41
1:0:145:A:H4'	15:M:137:ASN:ND2	2.35	0.41
1:0:275:G:C2	1:0:376:C:N3	2.88	0.41
1:0:332:G:H4'	22:T:2:LYS:O	2.20	0.41
1:0:473:A:H1'	38:0:6370:HOH:O	2.20	0.41
1:0:832:U:H2'	1:0:833:G:H8	1.85	0.41
1:0:1063:G:H5''	38:0:9851:HOH:O	2.20	0.41
1:0:1262:C:H4'	25:W:30:ASN:HB2	2.01	0.41
1:0:1588:G:C5	1:0:1589:G:C6	3.08	0.41
1:0:1766:U:O4'	1:0:1779:A:N6	2.53	0.41
1:0:2588:OMG:H3'	1:0:2589:U:H5''	2.02	0.41
38:0:4297:HOH:O	27:Y:208:LYS:HD2	2.21	0.41
2:9:59:C:O5'	2:9:59:C:H6	2.04	0.41
3:A:42:VAL:HG21	3:A:74:VAL:CG1	2.51	0.41
3:A:75:GLY:HA2	28:Z:64:PHE:HA	2.03	0.41
4:B:246:ARG:HH11	4:B:246:ARG:HG3	1.85	0.41
4:B:315:VAL:HG23	4:B:316:ARG:HG2	2.02	0.41
6:D:81:GLU:O	6:D:85:GLN:HG3	2.20	0.41
7:E:21:THR:HA	7:E:30:THR:HA	2.02	0.41
10:H:36:MET:HE1	10:H:88:MET:HE3	2.02	0.41
10:H:122:LYS:HB2	10:H:122:LYS:HE3	1.85	0.41
12:J:52:GLN:O	12:J:53:ILE:C	2.63	0.41
13:K:125:ALA:C	13:K:127:ALA:N	2.78	0.41
20:R:61:GLN:HE21	20:R:61:GLN:HB2	1.61	0.41
20:R:80:TYR:O	20:R:82:GLU:N	2.53	0.41
23:U:6:CYS:HB2	23:U:32:CYS:HB3	2.03	0.41
24:V:20:LEU:HD12	24:V:20:LEU:HA	1.92	0.41
28:Z:80:ARG:O	28:Z:81:ARG:C	2.63	0.41
1:0:56:G:C8	1:0:59:A:C8	3.09	0.41
1:0:87:C:C2	30:2:30:ASP:OD2	2.73	0.41
1:0:121:U:OP2	30:2:10:ARG:NH2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:247:A:H2'	38:0:3922:HOH:O	2.21	0.41
1:0:281:U:O2'	1:0:282:C:H5'	2.20	0.41
1:0:302:A:O2'	1:0:303:C:H5'	2.20	0.41
1:0:646:G:H2'	1:0:647:U:C6	2.56	0.41
1:0:834:G:H4'	1:0:835:U:OP2	2.21	0.41
1:0:1071:G:H4'	27:Y:154:ARG:NH2	2.36	0.41
1:0:1298:U:H2'	1:0:1299:G:C8	2.55	0.41
1:0:1593:C:OP1	18:P:117:SER:HB3	2.21	0.41
1:0:2132:C:H1'	15:M:124:GLY:HA3	2.03	0.41
1:0:2249:G:N2	1:0:2251:G:H3'	2.36	0.41
1:0:2316:G:H4'	38:0:6082:HOH:O	2.20	0.41
38:0:7484:HOH:O	31:3:42:ARG:HD3	2.20	0.41
2:9:88:G:N2	2:9:89:C:C2	2.88	0.41
4:B:35:GLN:O	4:B:36:PRO:C	2.64	0.41
4:B:203:ALA:HA	4:B:262:ARG:O	2.21	0.41
4:B:277:GLU:N	4:B:278:PRO:CD	2.83	0.41
5:C:27:ARG:NH1	5:C:29:ASP:OD2	2.53	0.41
6:D:27:ILE:HG22	6:D:28:GLY:N	2.35	0.41
7:E:118:ILE:CG2	7:E:122:THR:HB	2.50	0.41
10:H:57:THR:N	10:H:132:ALA:HB2	2.35	0.41
15:M:5:TYR:C	15:M:7:TYR:N	2.78	0.41
16:N:184:ILE:O	16:N:184:ILE:HG23	2.21	0.41
19:Q:72:LYS:HG2	19:Q:85:ILE:CD1	2.50	0.41
20:R:149:GLU:HA	20:R:150:PRO:HD3	1.92	0.41
24:V:23:LEU:O	24:V:24:LYS:C	2.63	0.41
25:W:59:GLN:NE2	25:W:97:ALA:CB	2.83	0.41
27:Y:97:LEU:O	27:Y:98:GLN:HG2	2.20	0.41
27:Y:205:ILE:O	27:Y:206:ALA:C	2.63	0.41
28:Z:61:ASP:O	28:Z:62:TYR:C	2.63	0.41
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.56	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
1:0:939:A:N1	1:0:1027:G:O2'	2.53	0.41
1:0:941:G:O2'	1:0:942:U:H5'	2.20	0.41
1:0:1023:C:H2'	1:0:1024:G:O4'	2.20	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.56	0.41
1:0:1987:C:H2'	1:0:1988:C:C6	2.56	0.41
1:0:2002:C:H2'	1:0:2003:U:C5'	2.51	0.41
1:0:2251:G:H2'	1:0:2252:A:H8	1.80	0.41
1:0:2708:G:N2	13:K:1:MET:O	2.48	0.41
2:9:78:G:O2'	2:9:79:U:OP2	2.39	0.41
2:9:114:G:H2'	2:9:115:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.56	0.41
4:B:109:LEU:CG	4:B:113:LEU:HD12	2.51	0.41
5:C:57:PRO:HD2	5:C:73:LEU:HD22	2.02	0.41
7:E:102:VAL:HG11	7:E:148:ILE:HG12	2.02	0.41
12:J:14:ALA:HB1	12:J:44:ALA:HB2	2.02	0.41
12:J:52:GLN:CG	12:J:53:ILE:N	2.80	0.41
13:K:2:GLU:O	13:K:3:ALA:C	2.63	0.41
13:K:81:ARG:HD3	13:K:87:ARG:NH2	2.35	0.41
17:O:26:TRP:N	38:O:3062:HOH:O	2.54	0.41
18:P:109:ARG:NH1	18:P:119:TYR:CE2	2.89	0.41
18:P:119:TYR:C	18:P:121:ASP:H	2.29	0.41
18:P:141:ILE:O	18:P:143:ALA:N	2.49	0.41
20:R:61:GLN:CD	38:R:8836:HOH:O	2.63	0.41
26:X:15:ARG:HH11	26:X:15:ARG:HB3	1.86	0.41
1:0:446:G:OP2	22:T:6:LYS:NZ	2.52	0.41
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.41
1:0:776:A:H1'	1:0:779:U:O4	2.21	0.41
1:0:1215:A:O3'	1:0:1216:G:C4'	2.68	0.41
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.41
1:0:1500:U:P	18:P:41:ARG:NH2	2.93	0.41
1:0:1506:U:H6	1:0:1506:U:H5'	1.85	0.41
1:0:1787:C:C4'	1:0:2883:A:O4'	2.69	0.41
1:0:1942:A:H3'	38:0:7321:HOH:O	2.20	0.41
1:0:2443:C:H5'	14:L:57:VAL:HG21	2.02	0.41
1:0:2596:A:H3'	38:0:3827:HOH:O	2.21	0.41
1:0:2809:G:H2'	1:0:2810:G:O4'	2.21	0.41
2:9:31:C:H1'	38:9:8592:HOH:O	2.21	0.41
3:A:43:VAL:HG21	3:A:59:GLU:CG	2.49	0.41
3:A:153:ARG:HD3	38:A:8825:HOH:O	2.21	0.41
5:C:16:VAL:HG12	5:C:17:ASP:H	1.84	0.41
5:C:68:ALA:O	5:C:70:VAL:N	2.54	0.41
6:D:60:GLU:HG3	6:D:62:ASP:HB2	2.03	0.41
6:D:80:ALA:O	6:D:83:PHE:HB3	2.21	0.41
7:E:132:THR:HG23	7:E:132:THR:O	2.21	0.41
7:E:146:ALA:O	7:E:147:ASP:C	2.62	0.41
8:F:61:MET:HB3	15:M:19:GLN:OE1	2.21	0.41
12:J:95:ARG:O	12:J:99:GLU:HB2	2.20	0.41
15:M:46:LEU:HD22	15:M:50:ARG:CD	2.50	0.41
16:N:44:ARG:HG3	16:N:45:ALA:N	2.36	0.41
16:N:67:ALA:HA	16:N:71:TRP:CB	2.49	0.41
19:Q:16:ASN:HD22	19:Q:16:ASN:HA	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:9:ASP:HA	20:R:10:PRO:HD2	1.91	0.41
25:W:26:ILE:HG22	38:W:5420:HOH:O	2.21	0.41
25:W:52:VAL:CG2	25:W:53:ALA:N	2.84	0.41
26:X:20:GLU:OE1	26:X:21:PRO:HD2	2.21	0.41
26:X:22:ASN:C	26:X:24:LYS:H	2.28	0.41
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.63	0.41
31:3:91:GLN:O	31:3:92:GLU:HB2	2.20	0.41
1:0:35:U:H5'	5:C:47:GLY:O	2.21	0.41
1:0:62:C:C4	1:0:63:U:C4	3.09	0.41
1:0:416:G:H5''	38:0:7392:HOH:O	2.20	0.41
1:0:894:A:C2	5:C:87:ARG:NH2	2.88	0.41
1:0:1262:C:H1'	25:W:120:PRO:HG3	2.03	0.41
1:0:1472:C:H6	1:0:1472:C:O5'	2.03	0.41
1:0:1772:C:H5'	1:0:1773:G:C5	2.55	0.41
1:0:2712:G:OP1	13:K:43:ARG:NH1	2.51	0.41
3:A:42:VAL:HG12	3:A:76:VAL:HA	2.02	0.41
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.36	0.41
4:B:294:TYR:CD1	4:B:294:TYR:C	2.99	0.41
5:C:233:THR:CG2	5:C:234:VAL:H	2.11	0.41
5:C:235:PHE:C	38:C:8645:HOH:O	2.63	0.41
6:D:60:GLU:O	6:D:61:PHE:C	2.63	0.41
7:E:11:VAL:CG1	7:E:12:ASP:N	2.82	0.41
7:E:32:ARG:C	7:E:33:LEU:HD23	2.45	0.41
7:E:143:GLN:O	7:E:147:ASP:N	2.39	0.41
12:J:70:PHE:O	12:J:81:ARG:NH2	2.52	0.41
15:M:112:LEU:HD23	15:M:135:ASP:HA	2.02	0.41
18:P:8:ARG:HG3	38:P:191:HOH:O	2.19	0.41
18:P:16:VAL:HG12	18:P:17:GLY:N	2.36	0.41
22:T:55:PHE:HB2	38:T:6384:HOH:O	2.21	0.41
25:W:142:ASP:CB	25:W:145:GLY:H	2.22	0.41
1:0:63:U:H2'	1:0:64:G:O4'	2.21	0.40
1:0:92:G:H2'	1:0:93:C:H6	1.86	0.40
1:0:229:G:O2'	1:0:230:C:H5'	2.21	0.40
1:0:727:G:H3'	1:0:728:C:H6	1.86	0.40
1:0:1119:G:N2	1:0:1246:A:H2	2.15	0.40
1:0:1181:A:N1	1:0:1192:A:O2'	2.53	0.40
1:0:1562:C:N4	38:0:5857:HOH:O	2.54	0.40
1:0:2404:G:C5'	19:Q:68:GLY:HA3	2.51	0.40
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.40
2:9:52:A:H2'	2:9:53:G:O4'	2.21	0.40
2:9:63:C:O2'	2:9:64:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:109:LEU:CD1	4:B:113:LEU:HD12	2.52	0.40
4:B:280:VAL:CG1	4:B:334:SER:HA	2.51	0.40
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.37	0.40
6:D:134:LEU:CD1	6:D:166:ILE:HD11	2.42	0.40
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.52	0.40
6:D:166:ILE:HD12	38:D:6326:HOH:O	2.22	0.40
8:F:36:THR:HG23	8:F:97:ALA:HB2	2.02	0.40
13:K:6:ALA:HB3	13:K:116:GLU:HG2	2.02	0.40
14:L:142:LEU:HG	14:L:146:GLY:HA3	2.02	0.40
15:M:17:ASP:O	15:M:21:ALA:HB2	2.21	0.40
16:N:38:LYS:HB2	16:N:38:LYS:HE3	1.83	0.40
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.21	0.40
17:O:37:ARG:O	17:O:40:HIS:HB2	2.21	0.40
25:W:31:HIS:C	38:W:5420:HOH:O	2.64	0.40
25:W:73:LEU:O	25:W:74:GLU:HG2	2.21	0.40
1:0:47:G:N3	1:0:114:A:C2	2.90	0.40
1:0:753:U:H3'	38:0:5515:HOH:O	2.21	0.40
1:0:765:G:O3'	5:C:69:HIS:HB3	2.20	0.40
1:0:800:G:H4'	38:0:7031:HOH:O	2.20	0.40
1:0:1052:G:N3	1:0:1052:G:H2'	2.36	0.40
1:0:2820:A:H4'	4:B:99:GLU:HB2	2.04	0.40
38:0:9671:HOH:O	27:Y:163:THR:HG23	2.21	0.40
3:A:214:SER:HA	3:A:227:ASP:O	2.21	0.40
4:B:27:ASN:HD22	4:B:27:ASN:N	2.12	0.40
4:B:36:PRO:HB3	4:B:174:ARG:HB3	2.03	0.40
5:C:25:PRO:HD2	38:C:8626:HOH:O	2.20	0.40
5:C:57:PRO:O	5:C:58:ALA:C	2.63	0.40
10:H:91:ARG:HH11	10:H:138:THR:CB	2.35	0.40
10:H:169:GLU:C	38:H:8530:HOH:O	2.64	0.40
12:J:127:ILE:O	12:J:127:ILE:HG12	2.20	0.40
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.02	0.40
25:W:21:LEU:HD23	25:W:21:LEU:HA	1.87	0.40
25:W:59:GLN:HE22	25:W:97:ALA:HB3	1.86	0.40
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.55	0.40
1:0:525:G:H2'	1:0:526:U:O4'	2.21	0.40
1:0:670:G:H2'	1:0:671:A:C8	2.56	0.40
1:0:814:G:H4'	38:0:3127:HOH:O	2.20	0.40
1:0:1198:U:H1'	1:0:1201:C:H5	1.86	0.40
1:0:1245:C:O5'	1:0:1245:C:H6	2.04	0.40
1:0:1473:U:C1'	29:1:42:SER:HB2	2.52	0.40
1:0:1513:C:O2'	1:0:1514:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1548:U:O2'	1:0:1549:C:H5'	2.21	0.40
1:0:1829:A:C2'	1:0:1830:C:H5'	2.50	0.40
1:0:1894:C:C2	1:0:1939:U:C4	3.09	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.22	0.40
1:0:2710:U:H1'	38:0:7592:HOH:O	2.21	0.40
1:0:2739:A:C5	1:0:2740:G:N7	2.89	0.40
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.86	0.40
2:9:29:C:H5''	6:D:140:ARG:HD3	2.03	0.40
2:9:61:C:H2'	2:9:62:A:C8	2.56	0.40
3:A:101:GLU:O	3:A:103:VAL:HG23	2.21	0.40
5:C:107:ARG:HB3	5:C:107:ARG:CZ	2.51	0.40
6:D:94:ALA:CB	6:D:97:GLN:HE21	2.34	0.40
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.51	0.40
7:E:157:LYS:NZ	38:E:2401:HOH:O	2.52	0.40
12:J:74:ARG:CB	12:J:74:ARG:NH1	2.75	0.40
13:K:79:PRO:HG3	13:K:89:LYS:HD3	2.03	0.40
13:K:109:LEU:HD13	13:K:113:ILE:HD11	2.04	0.40
17:O:32:ARG:NE	38:O:3360:HOH:O	2.53	0.40
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.84	0.40
20:R:119:VAL:CG2	20:R:142:ASP:HB2	2.51	0.40
21:S:45:TYR:CD1	21:S:45:TYR:N	2.89	0.40
27:Y:197:ASP:C	27:Y:199:ASP:H	2.29	0.40
1:0:301:C:O2'	1:0:302:A:H5'	2.21	0.40
1:0:318:U:O2'	1:0:338:C:H2'	2.21	0.40
1:0:567:U:O2'	1:0:568:G:H5'	2.21	0.40
1:0:736:A:H2'	1:0:737:A:O4'	2.22	0.40
1:0:1157:C:H2'	1:0:1158:G:C8	2.54	0.40
1:0:1168:C:H5	38:0:7467:HOH:O	2.03	0.40
1:0:1197:G:H1'	1:0:1203:G:N1	2.36	0.40
1:0:1432:U:H5'	38:0:9193:HOH:O	2.20	0.40
1:0:1562:C:O2	1:0:1562:C:C2'	2.70	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.22	0.40
1:0:1890:U:H4'	1:0:2010:A:C6	2.57	0.40
2:9:92:G:H2'	2:9:93:A:H8	1.79	0.40
3:A:132:ASP:OD1	3:A:133:ARG:N	2.51	0.40
4:B:268:ARG:NE	38:B:8904:HOH:O	2.51	0.40
7:E:166:VAL:HB	38:E:6341:HOH:O	2.22	0.40
11:I:128:THR:N	38:I:5371:HOH:O	2.54	0.40
14:L:89:PHE:N	14:L:117:GLU:O	2.55	0.40
20:R:31:ILE:O	20:R:32:ALA:C	2.64	0.40
21:S:67:ARG:HH11	21:S:67:ARG:CB	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:81:LYS:HG3	22:T:87:VAL:HG13	2.03	0.40
1:0:595:U:O2'	1:0:596:C:H5'	2.22	0.40
1:0:1118:A:N6	1:0:1244:U:H3	2.01	0.40
1:0:1933:G:O2'	1:0:1934:A:H5'	2.22	0.40
1:0:2299:G:O6	19:Q:1:PRO:HA	2.21	0.40
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.54	0.40
1:0:2671:U:C2'	1:0:2672:C:O5'	2.70	0.40
1:0:2698:G:H2'	1:0:2699:A:C8	2.56	0.40
1:0:2720:C:O2	13:K:87:ARG:NH2	2.52	0.40
2:9:6:C:O2'	16:N:33:ARG:NH2	2.54	0.40
3:A:105:VAL:HG12	3:A:106:CYS:N	2.37	0.40
3:A:135:VAL:HG22	3:A:136:ALA:N	2.36	0.40
3:A:167:LYS:HG3	28:Z:29:ILE:HD12	2.03	0.40
4:B:36:PRO:HG3	4:B:169:GLY:H	1.86	0.40
4:B:68:THR:HG21	23:U:16:GLY:HA3	2.04	0.40
4:B:221:GLN:HE22	13:K:42:ASN:ND2	2.19	0.40
4:B:241:PRO:HD2	38:B:8955:HOH:O	2.21	0.40
4:B:310:ARG:HD2	38:B:8883:HOH:O	2.22	0.40
5:C:37:ALA:HB2	38:C:8578:HOH:O	2.21	0.40
5:C:79:ARG:O	5:C:87:ARG:HG2	2.21	0.40
6:D:35:ALA:HB1	38:D:6716:HOH:O	2.22	0.40
10:H:25:GLY:O	10:H:27:PRO:HD3	2.22	0.40
11:I:114:TYR:N	11:I:114:TYR:HD1	2.20	0.40
16:N:152:GLU:C	16:N:154:LEU:N	2.78	0.40
17:O:15:LYS:O	17:O:16:SER:C	2.64	0.40
19:Q:30:VAL:O	19:Q:31:GLU:C	2.64	0.40
20:R:79:ARG:C	20:R:81:PRO:HD3	2.46	0.40
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.21	0.40
27:Y:149:GLN:HE21	27:Y:149:GLN:HB3	1.76	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	235/240 (98%)	192 (82%)	34 (14%)	9 (4%)	2	15
4	B	335/338 (99%)	289 (86%)	38 (11%)	8 (2%)	4	24
5	C	244/246 (99%)	213 (87%)	24 (10%)	7 (3%)	3	20
6	D	134/177 (76%)	89 (66%)	35 (26%)	10 (8%)	1	4
7	E	170/178 (96%)	157 (92%)	13 (8%)	0	100	100
8	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	1	7
9	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	2	14
10	H	156/177 (88%)	140 (90%)	14 (9%)	2 (1%)	9	38
11	I	68/162 (42%)	45 (66%)	22 (32%)	1 (2%)	8	35
12	J	140/145 (97%)	124 (89%)	11 (8%)	5 (4%)	2	16
13	K	130/132 (98%)	114 (88%)	15 (12%)	1 (1%)	16	50
14	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	9	36
15	M	192/195 (98%)	172 (90%)	18 (9%)	2 (1%)	12	45
16	N	184/187 (98%)	151 (82%)	26 (14%)	7 (4%)	2	15
17	O	113/116 (97%)	100 (88%)	11 (10%)	2 (2%)	6	31
18	P	141/149 (95%)	128 (91%)	11 (8%)	2 (1%)	9	36
19	Q	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	11	43
20	R	148/155 (96%)	133 (90%)	13 (9%)	2 (1%)	9	36
21	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
22	T	117/120 (98%)	102 (87%)	14 (12%)	1 (1%)	14	48
23	U	51/66 (77%)	44 (86%)	5 (10%)	2 (4%)	2	14
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	3	18
25	W	152/154 (99%)	141 (93%)	9 (6%)	2 (1%)	9	38
26	X	80/92 (87%)	67 (84%)	9 (11%)	4 (5%)	1	10
27	Y	140/241 (58%)	125 (89%)	13 (9%)	2 (1%)	9	36
28	Z	71/83 (86%)	57 (80%)	11 (16%)	3 (4%)	2	13
29	1	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
30	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
31	3	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
All	All	3705/4437 (84%)	3196 (86%)	424 (11%)	85 (2%)	5	25

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
3	A	36	ASP
3	A	132	ASP
4	B	139	ASP
5	C	234	VAL
6	D	16	PRO
6	D	137	PRO
8	F	44	SER
8	F	101	ALA
10	H	143	VAL
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	81	ARG
3	A	37	VAL
4	B	34	GLY
4	B	184	ASP
4	B	206	THR
5	C	8	LEU
6	D	27	ILE
6	D	90	LEU
6	D	164	ALA
6	D	173	GLU
8	F	61	MET
8	F	104	ALA
12	J	7	ASP
15	M	6	SER
16	N	133	ASP
17	O	20	SER
18	P	116	SER
18	P	117	SER
22	T	53	GLY
26	X	87	ALA
27	Y	198	GLY
3	A	35	GLY
3	A	229	ALA
5	C	15	GLU
6	D	171	ASP
12	J	89	HIS
13	K	126	SER
14	L	21	ARG
15	M	18	GLY

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Mol	Chain	Res	Type
16	N	139	TRP
16	N	164	ASP
17	O	21	SER
19	Q	89	ALA
20	R	20	GLU
23	U	46	ALA
24	V	43	PRO
25	W	77	ALA
28	Z	59	TYR
3	A	69	LEU
4	B	2	GLN
4	B	306	LYS
5	C	13	ASP
5	C	58	ALA
5	C	79	ARG
6	D	56	ARG
8	F	64	PRO
9	G	72	ASP
10	H	19	ARG
11	I	109	PRO
12	J	15	ARG
25	W	49	ASN
26	X	77	PHE
27	Y	173	ALA
28	Z	20	ARG
3	A	119	ALA
4	B	182	VAL
5	C	181	ALA
6	D	82	GLU
6	D	168	SER
12	J	5	GLU
26	X	78	GLU
8	F	71	GLY
12	J	78	ILE
16	N	2	THR
23	U	7	ASP
26	X	70	ILE
4	B	181	ILE
8	F	108	VAL
24	V	40	PRO
3	A	211	LYS
20	R	81	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	167 (93%)	12 (7%)	15	46
4	B	282/283 (100%)	262 (93%)	20 (7%)	13	43
5	C	193/193 (100%)	180 (93%)	13 (7%)	15	46
6	D	117/148 (79%)	112 (96%)	5 (4%)	26	60
7	E	152/156 (97%)	142 (93%)	10 (7%)	15	46
8	F	93/94 (99%)	90 (97%)	3 (3%)	34	67
9	G	27/283 (10%)	25 (93%)	2 (7%)	13	42
10	H	134/145 (92%)	130 (97%)	4 (3%)	36	69
11	I	58/130 (45%)	57 (98%)	1 (2%)	53	78
12	J	118/121 (98%)	112 (95%)	6 (5%)	21	55
13	K	106/106 (100%)	103 (97%)	3 (3%)	38	70
14	L	113/127 (89%)	108 (96%)	5 (4%)	25	60
15	M	158/159 (99%)	154 (98%)	4 (2%)	42	72
16	N	149/150 (99%)	142 (95%)	7 (5%)	23	58
17	O	93/94 (99%)	88 (95%)	5 (5%)	20	53
18	P	113/117 (97%)	107 (95%)	6 (5%)	20	54
19	Q	79/80 (99%)	74 (94%)	5 (6%)	16	48
20	R	117/122 (96%)	112 (96%)	5 (4%)	26	60
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	80
22	T	105/106 (99%)	99 (94%)	6 (6%)	18	52
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	62
25	W	130/130 (100%)	124 (95%)	6 (5%)	24	58
26	X	66/74 (89%)	60 (91%)	6 (9%)	9	33
27	Y	120/196 (61%)	114 (95%)	6 (5%)	22	56
28	Z	60/68 (88%)	59 (98%)	1 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	75 (95%)	4 (5%)	21	55
All	All	3095/3619 (86%)	2947 (95%)	148 (5%)	23	57

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	64	ASP
3	A	66	ARG
3	A	69	LEU
3	A	85	SER
3	A	94	LEU
3	A	153	ARG
3	A	175	LYS
3	A	179	MET
3	A	206	ARG
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	36	PRO
4	B	49	THR
4	B	97	LEU
4	B	139	ASP
4	B	140	LEU
4	B	162	MET
4	B	175	LEU
4	B	190	MET
4	B	195	ARG
4	B	234	ARG
4	B	251	VAL
4	B	254	GLN
4	B	264	GLU
4	B	277	GLU
4	B	304	PRO
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN

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Mol	Chain	Res	Type
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	187	ARG
5	C	214	THR
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	136	ARG
6	D	137	PRO
6	D	149	ARG
6	D	170	TYR
7	E	7	ILE
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
7	E	108	LEU
7	E	115	ARG
7	E	116	THR
7	E	126	ILE
7	E	133	VAL
7	E	154	ILE
8	F	46	GLU
8	F	65	GLU
8	F	78	GLU
9	G	64	ASN
9	G	72	ASP
10	H	33	GLN
10	H	87	LYS
10	H	157	TYR
10	H	170	ARG
11	I	135	GLU
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	93	ARG
12	J	130	VAL

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Mol	Chain	Res	Type
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	35	ARG
14	L	51	PHE
14	L	99	GLU
14	L	117	GLU
14	L	140	VAL
15	M	23	LEU
15	M	93	ARG
15	M	99	ARG
15	M	130	GLU
16	N	17	ARG
16	N	26	LEU
16	N	49	THR
16	N	50	LEU
16	N	53	ASN
16	N	93	GLN
16	N	138	ASP
17	O	3	THR
17	O	34	GLU
17	O	97	SER
17	O	98	LEU
17	O	102	ILE
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	94	TRP
18	P	98	ILE
18	P	116	SER
19	Q	11	ARG
19	Q	16	ASN
19	Q	30	VAL
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	61	GLN
20	R	82	GLU
20	R	143	VAL
21	S	10	VAL

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Mol	Chain	Res	Type
22	T	19	ARG
22	T	26	THR
22	T	39	ASN
22	T	86	GLU
22	T	96	VAL
22	T	112	LEU
24	V	43	PRO
24	V	65	ASP
25	W	26	ILE
25	W	60	GLU
25	W	73	LEU
25	W	88	THR
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	44	ASP
26	X	49	ARG
26	X	79	GLU
26	X	82	GLU
26	X	84	ILE
27	Y	95	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	231	PRO
27	Y	235	GLU
28	Z	41	ASN
31	3	3	MET
31	3	14	CYS
31	3	30	GLN
31	3	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	29	HIS
3	A	47	HIS
3	A	92	ASN
3	A	176	HIS
3	A	199	HIS
3	A	218	ASN
4	B	27	ASN

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Mol	Chain	Res	Type
4	B	106	HIS
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	67	GLN
5	C	129	HIS
5	C	163	HIS
5	C	178	GLN
6	D	85	GLN
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	66	GLN
7	E	119	HIS
7	E	143	GLN
8	F	80	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	131	GLN
11	I	88	GLN
11	I	108	HIS
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
14	L	58	GLN
15	M	14	ASN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN

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Mol	Chain	Res	Type
15	M	142	GLN
15	M	170	ASN
16	N	22	GLN
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	27	GLN
19	Q	40	HIS
19	Q	94	GLN
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	7	HIS
21	S	53	ASN
21	S	55	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
24	V	4	HIS
24	V	60	GLN
25	W	2	HIS
25	W	14	HIS
25	W	27	HIS
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	98	GLN
27	Y	133	HIS
27	Y	149	GLN

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Mol	Chain	Res	Type
27	Y	153	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	18	GLN
31	3	30	GLN
31	3	39	GLN
31	3	48	ASN
31	3	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	248 (9%)	28 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	264 (9%)	29 (1%)

All (264) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
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	185	G
1	0	186	A

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Mol	Chain	Res	Type
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	219	G
1	0	236	A
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	317	A
1	0	319	A
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	581	G
1	0	588	G
1	0	603	A
1	0	604	G
1	0	605	C
1	0	620	A

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Mol	Chain	Res	Type
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
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

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Mol	Chain	Res	Type
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U

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Mol	Chain	Res	Type
1	0	1626	A
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	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
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	1968	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G

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Mol	Chain	Res	Type
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2526	C
1	0	2527	U
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	2607	U
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2664	A

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Mol	Chain	Res	Type
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
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	7	G
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (29) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	318	U
1	0	603	A
1	0	604	G
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1165	G
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2718	C
1	0	2761	A
1	0	2791	U
2	9	65	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	OMU	0	2587	1	19,22,23	0.25	0	25,31,34	0.40	0
1	OMG	0	2588	1	23,26,27	0.31	0	32,38,41	0.32	0
1	UR3	0	2619	1	19,22,23	0.45	0	26,32,35	0.67	1 (3%)
1	PSU	0	2621	1	18,21,22	1.58	2 (11%)	21,30,33	1.33	3 (14%)
1	1MA	0	628	1	21,25,26	0.72	1 (4%)	30,37,40	0.76	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	OMU	0	2587	1	-	0/9/27/28	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
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.00	1.43	1.36
1	0	2621	PSU	C6-C5	3.48	1.39	1.35
1	0	628	1MA	C6-N6	2.42	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-N1-C2	-3.11	119.81	122.69
1	0	2621	PSU	O2-C2-N1	3.05	125.93	122.79
1	0	2621	PSU	C6-C5-C4	2.94	120.16	118.17
1	0	628	1MA	N1-C2-N3	2.90	129.44	126.00
1	0	2619	UR3	C4-N3-C2	2.62	126.69	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0
1	0	2621	PSU	1	0
1	0	628	1MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 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	CLY	0	9000	-	26,28,28	1.90	9 (34%)	31,40,40	1.27	3 (9%)

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	CLY	0	9000	-	-	4/21/53/53	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	CLY	C14-N2	4.32	1.53	1.47
32	0	9000	CLY	O5-C4	3.52	1.49	1.44
32	0	9000	CLY	C15-N2	3.36	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	CLY	C10-N1	2.89	1.40	1.34
32	0	9000	CLY	C11-N2	2.37	1.52	1.46
32	0	9000	CLY	C6-S1	2.34	1.84	1.79
32	0	9000	CLY	C3-C2	2.30	1.58	1.52
32	0	9000	CLY	C12-C11	-2.23	1.49	1.53
32	0	9000	CLY	C7-N1	2.02	1.49	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	CLY	C11-C10-N1	-3.91	107.96	116.52
32	0	9000	CLY	O8-C10-N1	2.83	128.03	122.96
32	0	9000	CLY	C12-C13-C16	-2.46	111.86	114.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

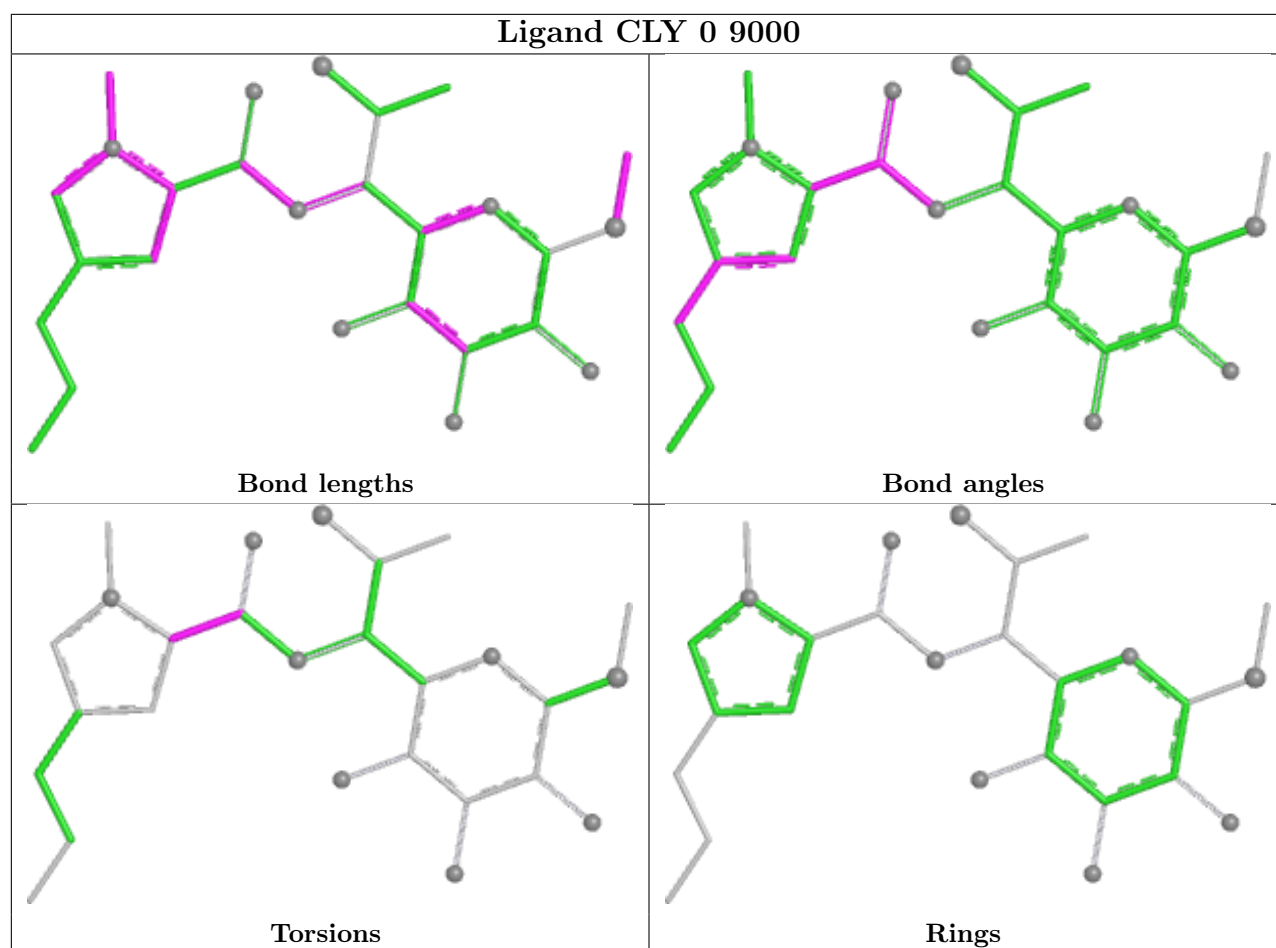
Mol	Chain	Res	Type	Atoms
32	0	9000	CLY	O8-C10-C11-C12
32	0	9000	CLY	N1-C10-C11-C12
32	0	9000	CLY	O8-C10-C11-N2
32	0	9000	CLY	N1-C10-C11-N2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	CLY	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-0.73	9 (0%) 90 79	23, 50, 94, 155	0
2	9	122/122 (100%)	-0.38	2 (1%) 70 47	37, 69, 94, 157	0
3	A	237/240 (98%)	-0.32	3 (1%) 75 53	31, 58, 94, 112	0
4	B	337/338 (99%)	-0.35	1 (0%) 90 79	30, 59, 85, 94	0
5	C	246/246 (100%)	-0.47	0 100 100	26, 48, 72, 82	0
6	D	140/177 (79%)	0.45	5 (3%) 46 26	63, 104, 125, 135	0
7	E	172/178 (96%)	-0.06	0 100 100	50, 72, 95, 99	0
8	F	119/120 (99%)	-0.11	0 100 100	51, 75, 98, 116	0
9	G	29/348 (8%)	0.34	0 100 100	77, 93, 105, 107	0
10	H	160/177 (90%)	-0.26	2 (1%) 75 53	43, 63, 96, 110	0
11	I	70/162 (43%)	0.88	5 (7%) 22 11	109, 125, 143, 145	0
12	J	142/145 (97%)	-0.39	1 (0%) 84 66	38, 54, 76, 92	0
13	K	132/132 (100%)	-0.36	0 100 100	37, 56, 77, 87	0
14	L	145/165 (87%)	-0.10	3 (2%) 63 40	28, 70, 108, 122	0
15	M	194/195 (99%)	-0.51	0 100 100	33, 47, 63, 70	0
16	N	186/187 (99%)	-0.09	0 100 100	45, 69, 114, 121	0
17	O	115/116 (99%)	-0.34	0 100 100	43, 58, 74, 78	0
18	P	143/149 (95%)	-0.29	0 100 100	41, 60, 75, 81	0
19	Q	95/96 (98%)	-0.56	0 100 100	36, 49, 65, 81	0
20	R	150/155 (96%)	-0.64	0 100 100	32, 47, 67, 79	0
21	S	81/85 (95%)	-0.38	0 100 100	45, 64, 82, 88	0
22	T	119/120 (99%)	-0.32	1 (0%) 82 64	40, 59, 86, 102	0
23	U	53/66 (80%)	-0.23	0 100 100	49, 62, 78, 88	0
24	V	65/71 (91%)	0.13	2 (3%) 51 30	59, 78, 115, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.57	0 100 100	32, 49, 68, 82	0
26	X	82/92 (89%)	-0.20	2 (2%) 59 36	48, 62, 86, 100	0
27	Y	142/241 (58%)	-0.54	0 100 100	31, 48, 69, 90	0
28	Z	73/83 (87%)	0.34	3 (4%) 41 23	72, 83, 98, 107	0
29	1	56/57 (98%)	-0.82	0 100 100	27, 35, 41, 49	0
30	2	46/50 (92%)	-0.04	0 100 100	35, 66, 94, 108	0
31	3	92/92 (100%)	-0.12	0 100 100	53, 72, 82, 90	0
All	All	6646/7481 (88%)	-0.46	39 (0%) 85 69	23, 56, 102, 157	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	1	U	4.7
24	V	1	THR	4.4
11	I	128	THR	4.2
26	X	88	GLU	3.6
11	I	71	ALA	3.0
6	D	10	PHE	3.0
6	D	107	GLY	2.9
10	H	171	GLY	2.8
1	0	1176	C	2.7
10	H	174	LEU	2.7
2	9	2	U	2.6
1	0	2103	A	2.6
3	A	36	ASP	2.6
14	L	60	GLU	2.6
11	I	112	LEU	2.6
24	V	2	VAL	2.6
28	Z	22	SER	2.6
3	A	237	GLY	2.6
28	Z	82	SER	2.5
14	L	99	GLU	2.5
11	I	88	GLN	2.4
14	L	82	ALA	2.4
1	0	10	U	2.4
11	I	85	GLY	2.3
3	A	37	VAL	2.3
12	J	4	ALA	2.2
28	Z	11	SER	2.2
1	0	138	U	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	1173	A	2.2
1	0	1171	A	2.1
1	0	1175	G	2.1
4	B	1	PRO	2.1
6	D	86	THR	2.1
26	X	87	ALA	2.1
1	0	1192	A	2.1
22	T	118	SER	2.0
6	D	63	ILE	2.0
1	0	960	G	2.0
6	D	174	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
1	1MA	0	628	23/24	0.98	0.06	29,32,34,35	0
1	OMU	0	2587	21/22	0.98	0.06	37,39,41,44	0
1	OMG	0	2588	24/25	0.98	0.06	37,40,41,44	0
1	UR3	0	2619	21/22	0.98	0.06	39,43,46,50	0
1	PSU	0	2621	20/21	0.98	0.05	28,31,37,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
35	NA	0	8529	1/1	0.58	0.24	79,79,79,79	0
33	MG	0	8050	1/1	0.79	0.14	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8584	1/1	0.81	0.13	63,63,63,63	0
32	CLY	0	9000	27/27	0.82	0.19	50,56,61,61	0
33	MG	0	8092	1/1	0.82	0.22	89,89,89,89	0
35	NA	0	8582	1/1	0.83	0.20	66,66,66,66	0
35	NA	0	8508	1/1	0.84	0.18	59,59,59,59	0
33	MG	0	8090	1/1	0.84	0.12	74,74,74,74	0
35	NA	R	8586	1/1	0.84	0.21	63,63,63,63	0
35	NA	9	8551	1/1	0.86	0.18	46,46,46,46	0
33	MG	0	8082	1/1	0.86	0.17	70,70,70,70	0
35	NA	0	8506	1/1	0.87	0.22	40,40,40,40	0
35	NA	9	8583	1/1	0.87	0.16	70,70,70,70	0
35	NA	0	8577	1/1	0.87	0.16	65,65,65,65	0
35	NA	0	8571	1/1	0.88	0.25	52,52,52,52	0
35	NA	S	8512	1/1	0.88	0.06	32,32,32,32	0
35	NA	B	8561	1/1	0.89	0.20	70,70,70,70	0
35	NA	0	8572	1/1	0.89	0.28	66,66,66,66	0
33	MG	0	8011	1/1	0.89	0.13	8,8,8,8	0
35	NA	0	8585	1/1	0.90	0.21	52,52,52,52	0
33	MG	0	8045	1/1	0.90	0.09	54,54,54,54	0
35	NA	0	8518	1/1	0.90	0.07	28,28,28,28	0
35	NA	0	8569	1/1	0.91	0.30	86,86,86,86	0
33	MG	0	8087	1/1	0.91	0.13	51,51,51,51	0
33	MG	0	8067	1/1	0.91	0.08	60,60,60,60	0
35	NA	0	8573	1/1	0.91	0.08	61,61,61,61	0
35	NA	0	8513	1/1	0.91	0.05	52,52,52,52	0
33	MG	0	8049	1/1	0.91	0.19	79,79,79,79	0
35	NA	0	8522	1/1	0.91	0.28	61,61,61,61	0
35	NA	0	8524	1/1	0.91	0.14	44,44,44,44	0
35	NA	0	8525	1/1	0.91	0.10	54,54,54,54	0
33	MG	T	8073	1/1	0.91	0.07	59,59,59,59	0
35	NA	0	8534	1/1	0.91	0.12	49,49,49,49	0
35	NA	0	8555	1/1	0.91	0.15	81,81,81,81	0
35	NA	0	8566	1/1	0.91	0.05	48,48,48,48	0
33	MG	0	8104	1/1	0.92	0.07	56,56,56,56	0
35	NA	0	8528	1/1	0.92	0.08	56,56,56,56	0
35	NA	0	8560	1/1	0.92	0.17	63,63,63,63	0
35	NA	0	8563	1/1	0.92	0.13	46,46,46,46	0
35	NA	C	8504	1/1	0.92	0.06	29,29,29,29	0
35	NA	0	8511	1/1	0.92	0.22	58,58,58,58	0
35	NA	0	8533	1/1	0.92	0.10	44,44,44,44	0
36	CL	0	8816	1/1	0.92	0.12	74,74,74,74	0
36	CL	B	8819	1/1	0.92	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	8526	1/1	0.93	0.20	57,57,57,57	0
35	NA	0	8562	1/1	0.93	0.22	66,66,66,66	0
33	MG	0	8113	1/1	0.93	0.06	69,69,69,69	0
35	NA	0	8540	1/1	0.93	0.12	49,49,49,49	0
35	NA	0	8568	1/1	0.93	0.11	84,84,84,84	0
35	NA	0	8552	1/1	0.93	0.13	49,49,49,49	0
33	MG	0	8070	1/1	0.93	0.08	52,52,52,52	0
36	CL	J	8802	1/1	0.93	0.07	83,83,83,83	0
33	MG	0	8046	1/1	0.94	0.06	43,43,43,43	0
35	NA	0	8523	1/1	0.94	0.09	42,42,42,42	0
35	NA	0	8556	1/1	0.94	0.18	49,49,49,49	0
35	NA	0	8557	1/1	0.94	0.08	45,45,45,45	0
35	NA	0	8558	1/1	0.94	0.25	70,70,70,70	0
35	NA	0	8531	1/1	0.94	0.23	77,77,77,77	0
35	NA	0	8502	1/1	0.94	0.09	45,45,45,45	0
36	CL	0	8822	1/1	0.94	0.11	92,92,92,92	0
33	MG	0	8075	1/1	0.94	0.09	73,73,73,73	0
35	NA	0	8507	1/1	0.94	0.10	65,65,65,65	0
36	CL	J	8821	1/1	0.94	0.06	61,61,61,61	0
36	CL	L	8810	1/1	0.94	0.11	74,74,74,74	0
36	CL	3	8804	1/1	0.94	0.07	76,76,76,76	0
34	K	0	8401	1/1	0.95	0.30	99,99,99,99	0
35	NA	0	8501	1/1	0.95	0.12	31,31,31,31	0
35	NA	0	8539	1/1	0.95	0.06	21,21,21,21	0
35	NA	0	8567	1/1	0.95	0.08	54,54,54,54	0
33	MG	0	8103	1/1	0.95	0.08	68,68,68,68	0
35	NA	L	8580	1/1	0.95	0.21	63,63,63,63	0
35	NA	Q	8548	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	8503	1/1	0.95	0.37	68,68,68,68	0
35	NA	0	8554	1/1	0.95	0.10	44,44,44,44	0
33	MG	0	8053	1/1	0.95	0.06	37,37,37,37	0
33	MG	0	8111	1/1	0.95	0.07	38,38,38,38	0
36	CL	A	8809	1/1	0.95	0.11	84,84,84,84	0
35	NA	0	8574	1/1	0.95	0.17	62,62,62,62	0
36	CL	J	8801	1/1	0.95	0.07	80,80,80,80	0
35	NA	0	8575	1/1	0.95	0.15	67,67,67,67	0
33	MG	0	8076	1/1	0.95	0.07	79,79,79,79	0
33	MG	B	8055	1/1	0.95	0.06	45,45,45,45	0
36	CL	O	8808	1/1	0.95	0.11	90,90,90,90	0
33	MG	0	8096	1/1	0.95	0.07	47,47,47,47	0
35	NA	0	8505	1/1	0.96	0.12	35,35,35,35	0
35	NA	0	8527	1/1	0.96	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8559	1/1	0.96	0.14	61,61,61,61	0
33	MG	0	8094	1/1	0.96	0.14	66,66,66,66	0
33	MG	0	8115	1/1	0.96	0.04	58,58,58,58	0
35	NA	J	8546	1/1	0.96	0.05	52,52,52,52	0
33	MG	9	8095	1/1	0.96	0.06	54,54,54,54	0
35	NA	0	8532	1/1	0.96	0.03	53,53,53,53	0
33	MG	0	8041	1/1	0.96	0.07	56,56,56,56	0
33	MG	K	8069	1/1	0.96	0.05	59,59,59,59	0
35	NA	T	8543	1/1	0.96	0.11	31,31,31,31	0
36	CL	0	8815	1/1	0.96	0.09	92,92,92,92	0
35	NA	0	8535	1/1	0.96	0.10	42,42,42,42	0
36	CL	0	8817	1/1	0.96	0.06	68,68,68,68	0
35	NA	0	8516	1/1	0.96	0.16	39,39,39,39	0
33	MG	0	8101	1/1	0.96	0.09	56,56,56,56	0
35	NA	0	8541	1/1	0.96	0.06	50,50,50,50	0
35	NA	0	8549	1/1	0.96	0.11	50,50,50,50	0
33	MG	0	8081	1/1	0.96	0.05	56,56,56,56	0
33	MG	0	8042	1/1	0.96	0.04	36,36,36,36	0
35	NA	0	8581	1/1	0.96	0.07	70,70,70,70	0
33	MG	0	8105	1/1	0.96	0.06	64,64,64,64	0
36	CL	Y	8820	1/1	0.96	0.06	42,42,42,42	0
33	MG	0	8093	1/1	0.96	0.04	45,45,45,45	0
35	NA	A	8545	1/1	0.97	0.07	41,41,41,41	0
35	NA	0	8565	1/1	0.97	0.10	50,50,50,50	0
35	NA	0	8536	1/1	0.97	0.04	61,61,61,61	0
33	MG	0	8062	1/1	0.97	0.07	62,62,62,62	0
33	MG	0	8102	1/1	0.97	0.04	77,77,77,77	0
33	MG	0	8064	1/1	0.97	0.13	33,33,33,33	0
35	NA	0	8570	1/1	0.97	0.22	55,55,55,55	0
33	MG	0	8066	1/1	0.97	0.06	87,87,87,87	0
33	MG	0	8024	1/1	0.97	0.04	33,33,33,33	0
36	CL	0	8811	1/1	0.97	0.07	63,63,63,63	0
36	CL	0	8813	1/1	0.97	0.07	54,54,54,54	0
35	NA	0	8553	1/1	0.97	0.06	37,37,37,37	0
35	NA	0	8510	1/1	0.97	0.08	41,41,41,41	0
33	MG	0	8057	1/1	0.97	0.08	50,50,50,50	0
35	NA	0	8576	1/1	0.97	0.08	48,48,48,48	0
34	K	0	8402	1/1	0.97	0.12	73,73,73,73	0
35	NA	0	8578	1/1	0.97	0.13	52,52,52,52	0
35	NA	0	8579	1/1	0.97	0.07	39,39,39,39	0
35	NA	0	8530	1/1	0.97	0.06	41,41,41,41	0
35	NA	0	8515	1/1	0.97	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8098	1/1	0.97	0.11	45,45,45,45	0
36	CL	M	8818	1/1	0.97	0.05	50,50,50,50	0
36	CL	N	8807	1/1	0.97	0.07	58,58,58,58	0
35	NA	0	8517	1/1	0.97	0.07	48,48,48,48	0
33	MG	0	8114	1/1	0.97	0.03	52,52,52,52	0
35	NA	0	8520	1/1	0.97	0.06	29,29,29,29	0
35	NA	0	8564	1/1	0.98	0.05	48,48,48,48	0
35	NA	H	8509	1/1	0.98	0.05	40,40,40,40	0
33	MG	0	8112	1/1	0.98	0.04	50,50,50,50	0
33	MG	0	8091	1/1	0.98	0.09	53,53,53,53	0
35	NA	M	8547	1/1	0.98	0.05	33,33,33,33	0
33	MG	0	8018	1/1	0.98	0.04	55,55,55,55	0
35	NA	R	8537	1/1	0.98	0.04	50,50,50,50	0
35	NA	0	8514	1/1	0.98	0.06	28,28,28,28	0
33	MG	0	8012	1/1	0.98	0.04	43,43,43,43	0
35	NA	0	8538	1/1	0.98	0.05	54,54,54,54	0
36	CL	0	8803	1/1	0.98	0.08	75,75,75,75	0
33	MG	0	8052	1/1	0.98	0.04	51,51,51,51	0
36	CL	0	8812	1/1	0.98	0.09	51,51,51,51	0
33	MG	0	8043	1/1	0.98	0.06	43,43,43,43	0
33	MG	0	8097	1/1	0.98	0.04	39,39,39,39	0
35	NA	0	8544	1/1	0.98	0.04	24,24,24,24	0
33	MG	0	8044	1/1	0.98	0.05	35,35,35,35	0
35	NA	0	8550	1/1	0.98	0.09	52,52,52,52	0
35	NA	0	8521	1/1	0.98	0.09	53,53,53,53	0
33	MG	Y	8108	1/1	0.98	0.04	40,40,40,40	0
33	MG	0	8100	1/1	0.98	0.04	80,80,80,80	0
33	MG	0	8059	1/1	0.98	0.04	44,44,44,44	0
33	MG	0	8060	1/1	0.98	0.05	50,50,50,50	0
33	MG	0	8085	1/1	0.98	0.04	67,67,67,67	0
33	MG	0	8035	1/1	0.98	0.04	48,48,48,48	0
33	MG	0	8088	1/1	0.98	0.04	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.08	80,80,80,80	0
36	CL	R	8806	1/1	0.98	0.05	46,46,46,46	0
33	MG	0	8110	1/1	0.98	0.04	47,47,47,47	0
33	MG	0	8039	1/1	0.98	0.07	49,49,49,49	0
37	CD	O	8705	1/1	0.98	0.05	87,87,87,87	0
35	NA	0	8542	1/1	0.99	0.02	39,39,39,39	0
33	MG	0	8051	1/1	0.99	0.03	67,67,67,67	0
33	MG	0	8032	1/1	0.99	0.07	41,41,41,41	0
33	MG	0	8033	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8056	1/1	0.99	0.02	55,55,55,55	0

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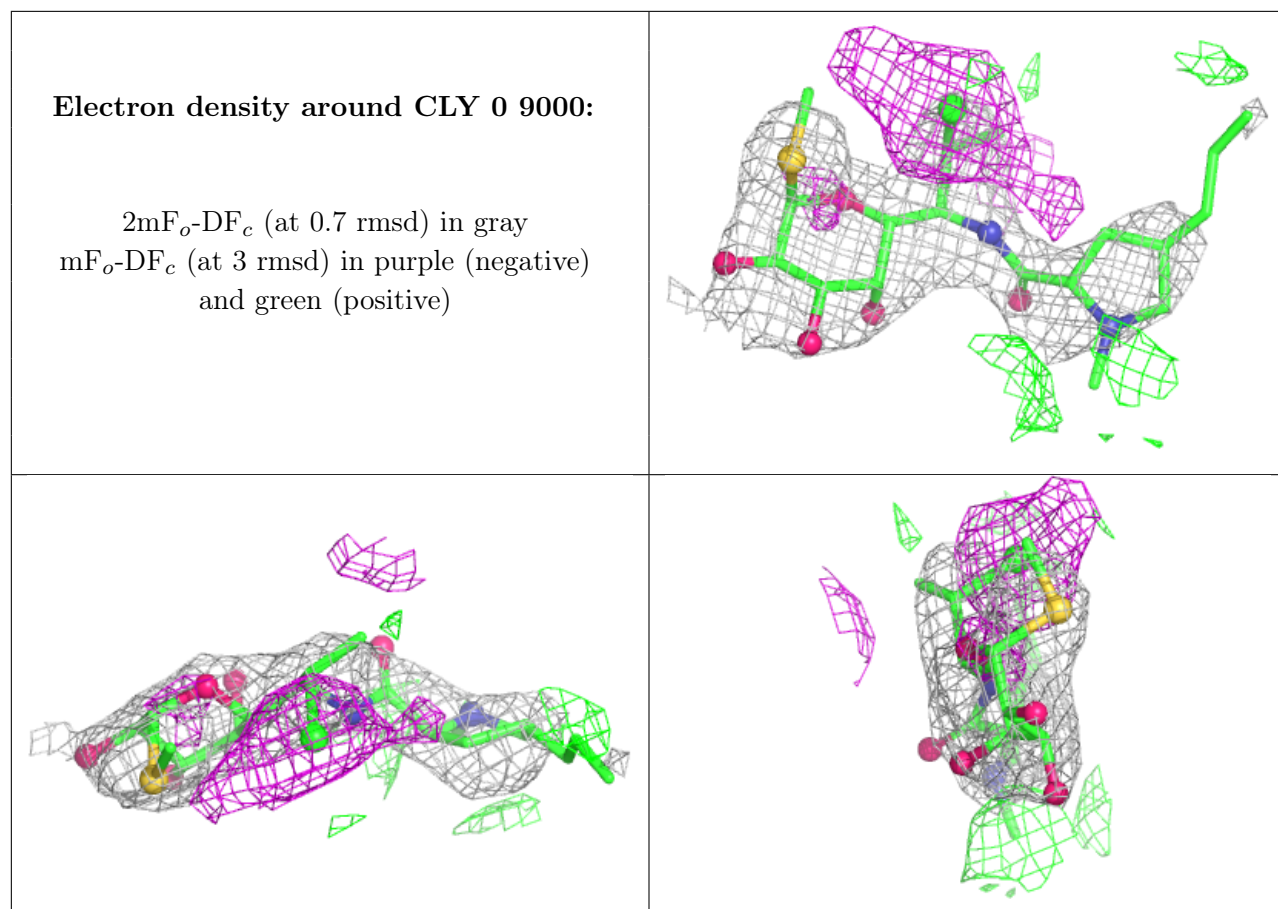
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8007	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8036	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8037	1/1	0.99	0.03	46,46,46,46	0
33	MG	0	8061	1/1	0.99	0.02	40,40,40,40	0
33	MG	0	8099	1/1	0.99	0.04	64,64,64,64	0
33	MG	0	8014	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8063	1/1	0.99	0.04	70,70,70,70	0
33	MG	0	8040	1/1	0.99	0.04	72,72,72,72	0
33	MG	0	8065	1/1	0.99	0.05	41,41,41,41	0
33	MG	0	8015	1/1	0.99	0.02	43,43,43,43	0
36	CL	0	8805	1/1	0.99	0.04	61,61,61,61	0
33	MG	0	8016	1/1	0.99	0.02	33,33,33,33	0
33	MG	0	8068	1/1	0.99	0.02	68,68,68,68	0
33	MG	0	8109	1/1	0.99	0.06	30,30,30,30	0
36	CL	0	8814	1/1	0.99	0.05	64,64,64,64	0
33	MG	0	8008	1/1	0.99	0.03	41,41,41,41	0
33	MG	0	8071	1/1	0.99	0.04	80,80,80,80	0
33	MG	0	8072	1/1	0.99	0.04	46,46,46,46	0
33	MG	0	8074	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8021	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8022	1/1	0.99	0.03	48,48,48,48	0
33	MG	0	8116	1/1	0.99	0.05	23,23,23,23	0
33	MG	0	8006	1/1	0.99	0.03	37,37,37,37	0
33	MG	0	8047	1/1	0.99	0.08	74,74,74,74	0
33	MG	0	8083	1/1	0.99	0.02	45,45,45,45	0
33	MG	0	8084	1/1	0.99	0.07	55,55,55,55	0
33	MG	0	8048	1/1	0.99	0.07	60,60,60,60	0
33	MG	3	8078	1/1	0.99	0.10	55,55,55,55	0
33	MG	0	8086	1/1	0.99	0.05	46,46,46,46	0
33	MG	0	8027	1/1	0.99	0.03	48,48,48,48	0
33	MG	0	8031	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8089	1/1	0.99	0.03	58,58,58,58	0
37	CD	3	8704	1/1	0.99	0.03	88,88,88,88	0
33	MG	0	8080	1/1	1.00	0.03	50,50,50,50	0
33	MG	0	8106	1/1	1.00	0.01	34,34,34,34	0
33	MG	0	8034	1/1	1.00	0.02	36,36,36,36	0
33	MG	0	8054	1/1	1.00	0.02	43,43,43,43	0
33	MG	0	8017	1/1	1.00	0.07	26,26,26,26	0
33	MG	0	8009	1/1	1.00	0.05	38,38,38,38	0
33	MG	0	8058	1/1	1.00	0.03	40,40,40,40	0
33	MG	0	8019	1/1	1.00	0.06	27,27,27,27	0
33	MG	0	8038	1/1	1.00	0.01	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8519	1/1	1.00	0.04	33,33,33,33	0
33	MG	0	8020	1/1	1.00	0.02	31,31,31,31	0
33	MG	0	8010	1/1	1.00	0.03	41,41,41,41	0
33	MG	0	8004	1/1	1.00	0.03	43,43,43,43	0
33	MG	0	8023	1/1	1.00	0.03	40,40,40,40	0
33	MG	0	8005	1/1	1.00	0.01	35,35,35,35	0
33	MG	0	8025	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8026	1/1	1.00	0.02	27,27,27,27	0
33	MG	0	8013	1/1	1.00	0.03	45,45,45,45	0
33	MG	0	8028	1/1	1.00	0.02	44,44,44,44	0
33	MG	0	8029	1/1	1.00	0.03	38,38,38,38	0
33	MG	0	8030	1/1	1.00	0.03	31,31,31,31	0
33	MG	0	8001	1/1	1.00	0.03	35,35,35,35	0
33	MG	0	8002	1/1	1.00	0.04	41,41,41,41	0
33	MG	0	8003	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8077	1/1	1.00	0.03	39,39,39,39	0
37	CD	U	8701	1/1	1.00	0.03	65,65,65,65	0
37	CD	Z	8703	1/1	1.00	0.04	97,97,97,97	0
37	CD	1	8702	1/1	1.00	0.03	64,64,64,64	0
33	MG	0	8079	1/1	1.00	0.03	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.