Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 02:25 PM EDT

PDB ID	:	1Q7Y
Title	:	Crystal Structure of CCdAP-Puromycin bound at the Peptidyl transferase center of the 50S ribosomal subunit
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	3.20 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:

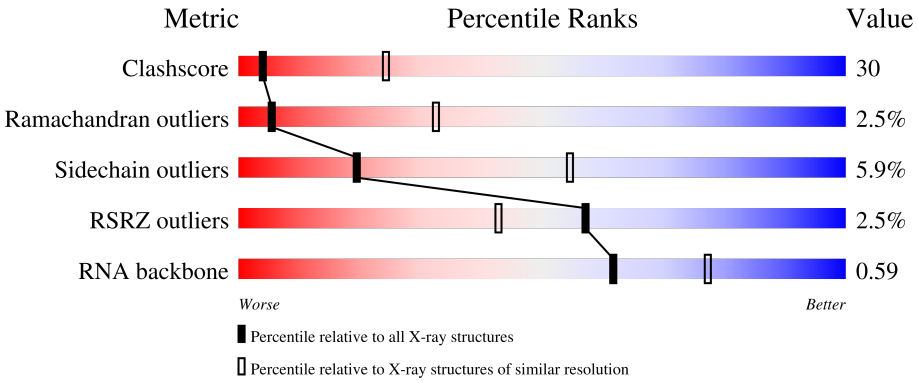
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2922	% 32% 45% 15% • 6%
2	B	122	3% 30% 48% 17% •
3	5	3	33% 67%
4	C	239	4% 46% 46% 6% •
5	D	337	42% 52% 6%

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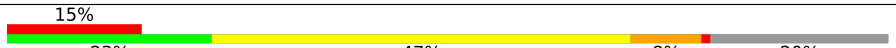
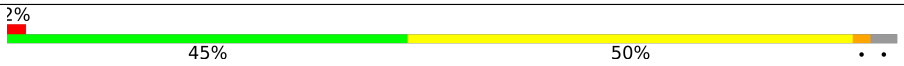
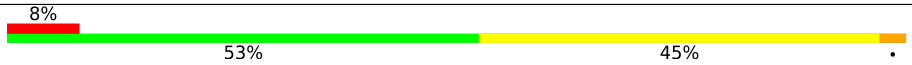
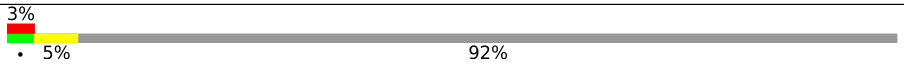
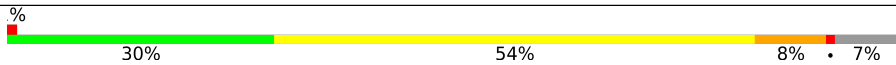
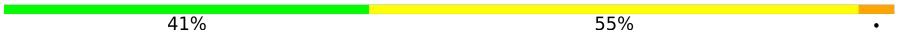
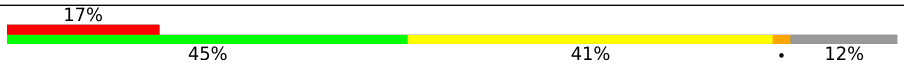
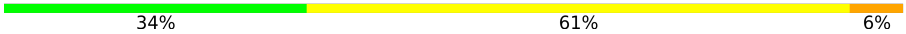
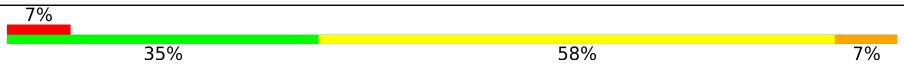
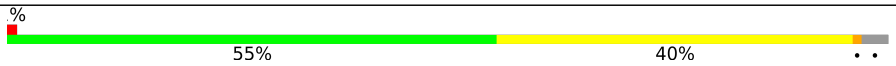
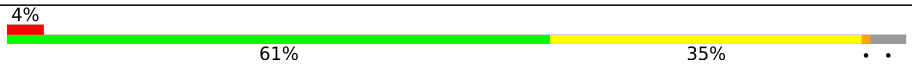
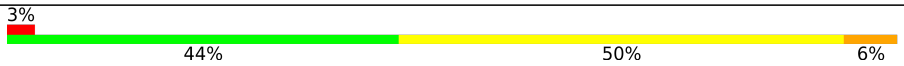
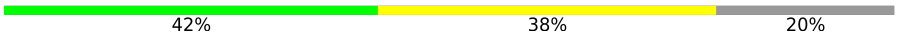
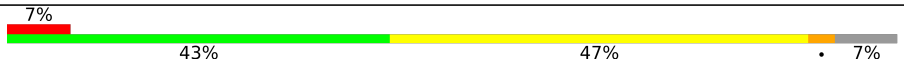
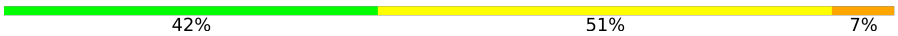
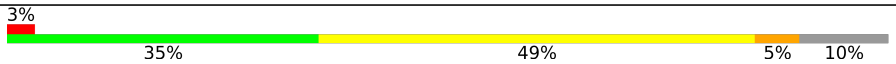
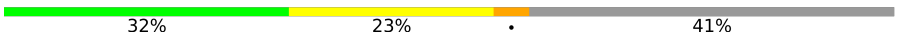
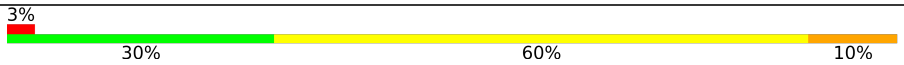
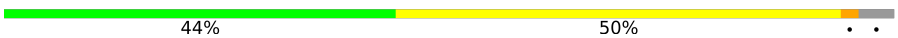
Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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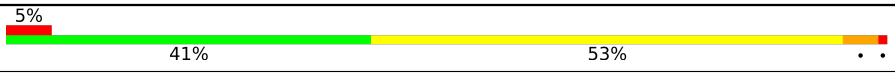
Mol	Chain	Length	Quality of chain
31	4	92	

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
34	NA	A	8303	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8370	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	A	8511	-	-	-	X
35	CL	O	8507	-	-	-	X
35	CL	P	8508	-	-	-	X
38	CD	4	8404	-	-	X	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 98616 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
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

- Molecule 3 is DNA/RNA hybrid called CCdA-P-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	3	58	28	11	17	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	109	Total Mg 109 109	0	0
32	B	1	Total Mg 1 1	0	0
32	5	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	1	Total Mg 1 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	72	Total Na 72 72	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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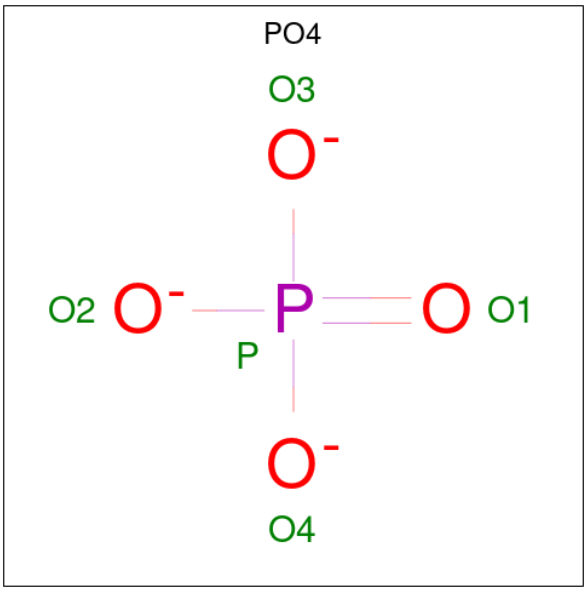
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0

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

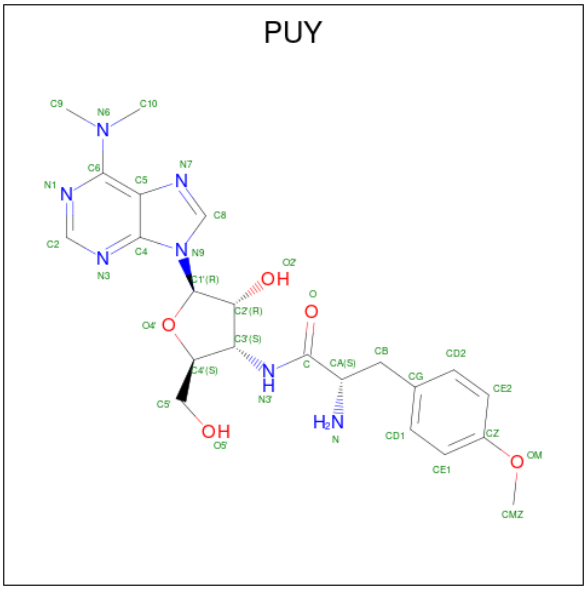
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	11	Total Cl 11 11	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	P	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0
35	Z	1	Total Cl 1 1	0	0
35	4	1	Total Cl 1 1	0	0

- Molecule 36 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total O P 3 2 1	0	0

- Molecule 37 is PUROMYCIN (three-letter code: PUY) (formula: $C_{22}H_{29}N_7O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	5	1	Total C N O 34 22 7 5	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	P	1	Total Cd 1 1	0	0
38	V	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	2	1	Total Cd 1 1	0	0
38	4	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	5861	Total O 5861 5861	0	0
39	B	154	Total O 154 154	0	0
39	5	6	Total O 6 6	0	0
39	C	123	Total O 123 123	0	0
39	D	149	Total O 149 149	0	0
39	E	178	Total O 178 178	0	0
39	F	50	Total O 50 50	0	0
39	G	46	Total O 46 46	0	0
39	H	27	Total O 27 27	0	0
39	I	20	Total O 20 20	0	0
39	J	75	Total O 75 75	0	0
39	K	56	Total O 56 56	0	0
39	L	60	Total O 60 60	0	0
39	M	90	Total O 90 90	0	0
39	N	128	Total O 128 128	0	0

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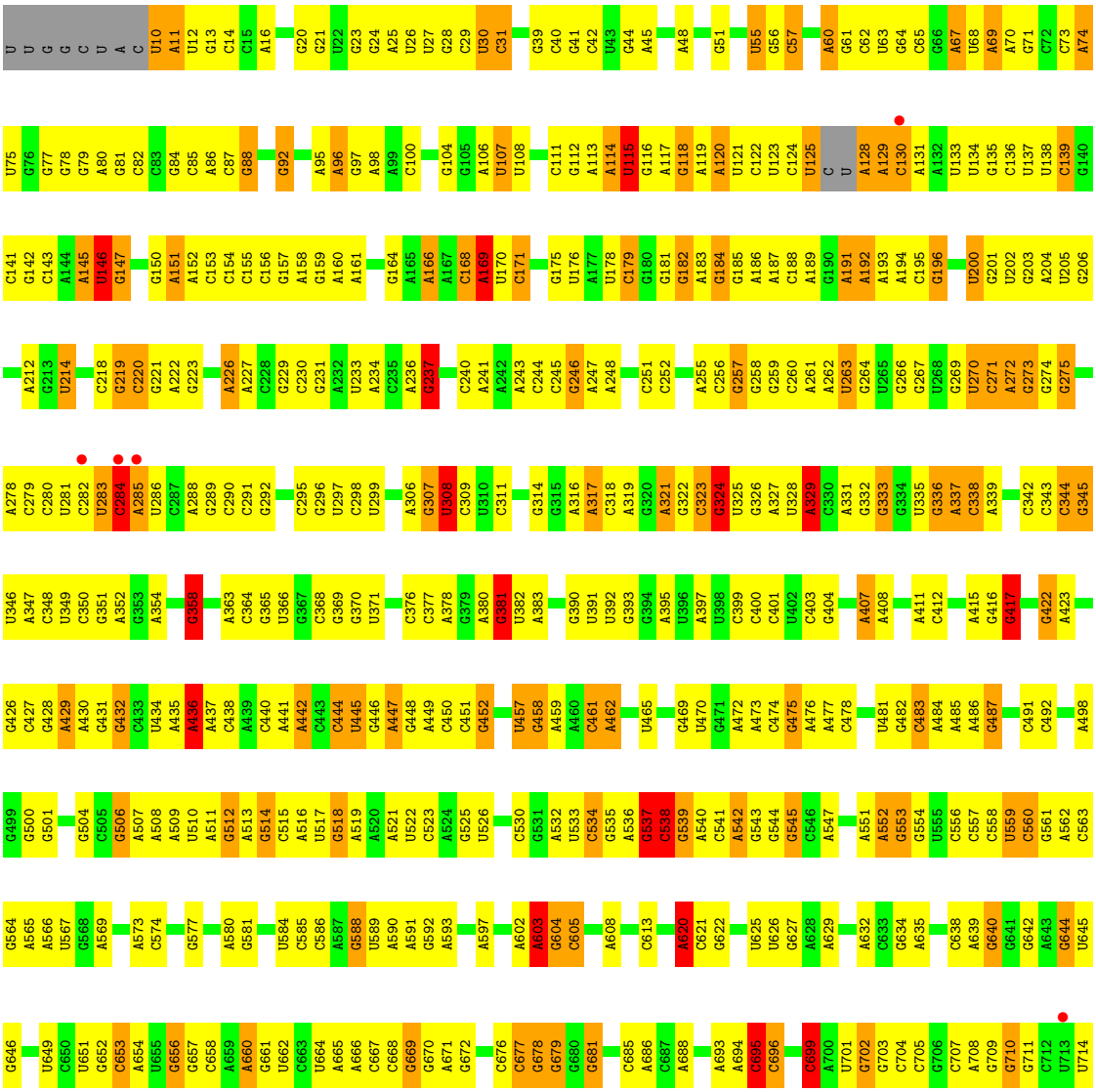
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	O	63	Total O 63 63	0	0
39	P	45	Total O 45 45	0	0
39	Q	62	Total O 62 62	0	0
39	R	53	Total O 53 53	0	0
39	S	86	Total O 86 86	0	0
39	T	36	Total O 36 36	0	0
39	U	42	Total O 42 42	0	0
39	V	30	Total O 30 30	0	0
39	W	15	Total O 15 15	0	0
39	X	73	Total O 73 73	0	0
39	Y	30	Total O 30 30	0	0
39	Z	99	Total O 99 99	0	0
39	1	36	Total O 36 36	0	0
39	2	63	Total O 63 63	0	0
39	3	42	Total O 42 42	0	0
39	4	73	Total O 73 73	0	0

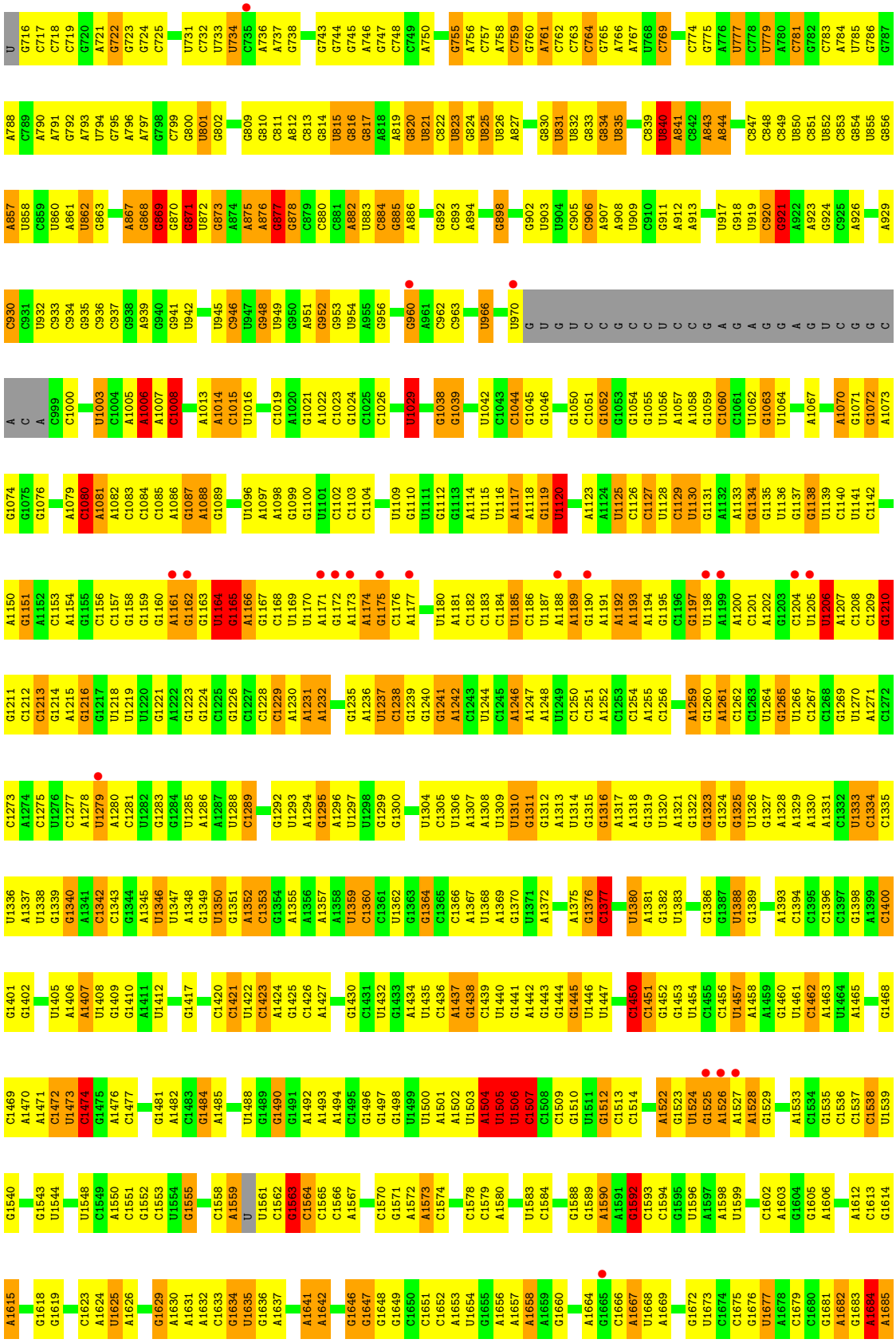
3 Residue-property plots (i)

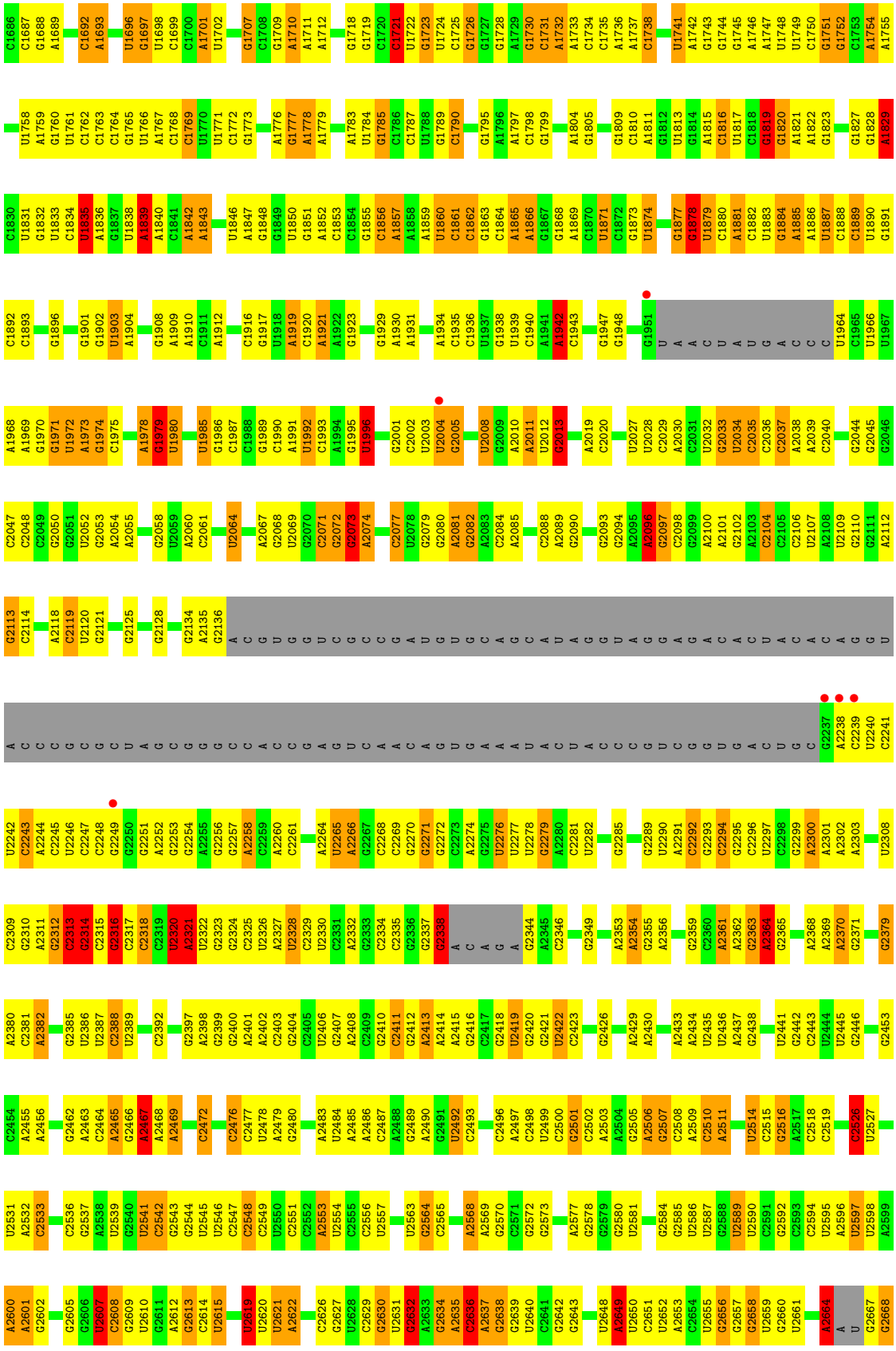
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

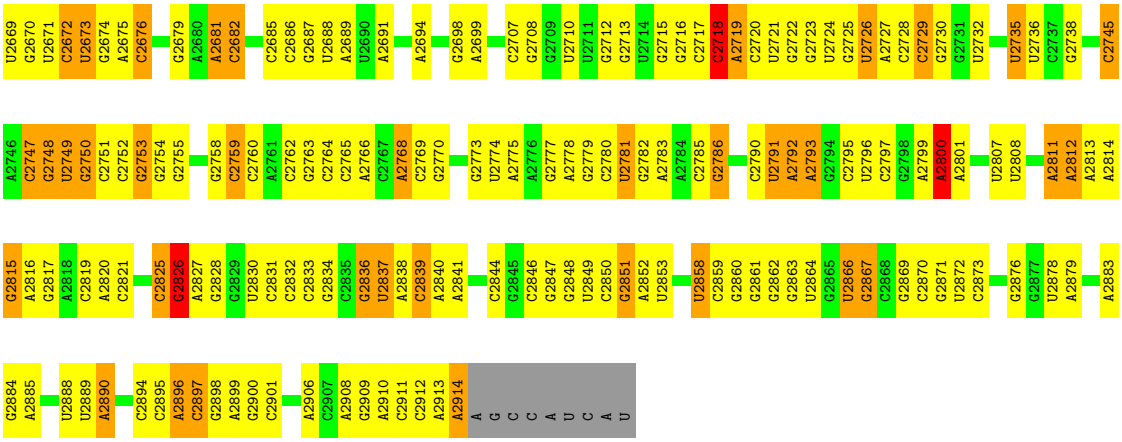
- Molecule 1: 23S ribosomal rna

Chain A:



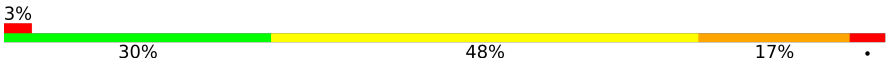


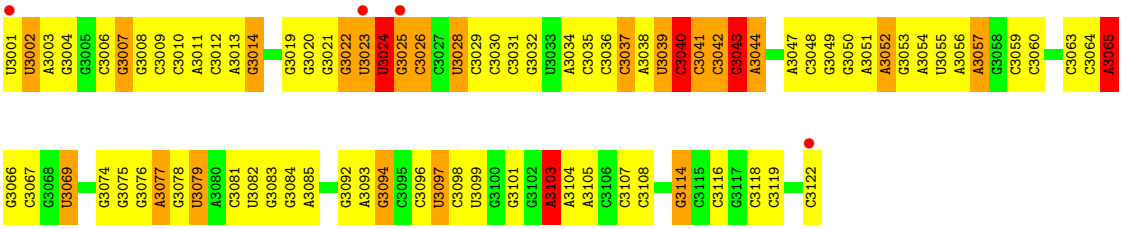




• Molecule 2: 5S ribosomal RNA

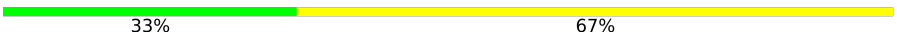
Chain B:





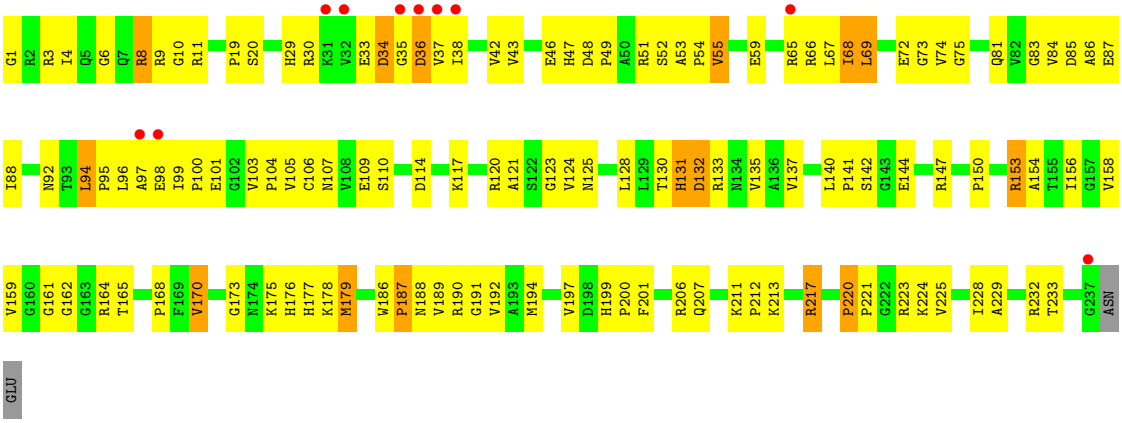
• Molecule 3: CCdA-P-Puromycin

Chain 5:



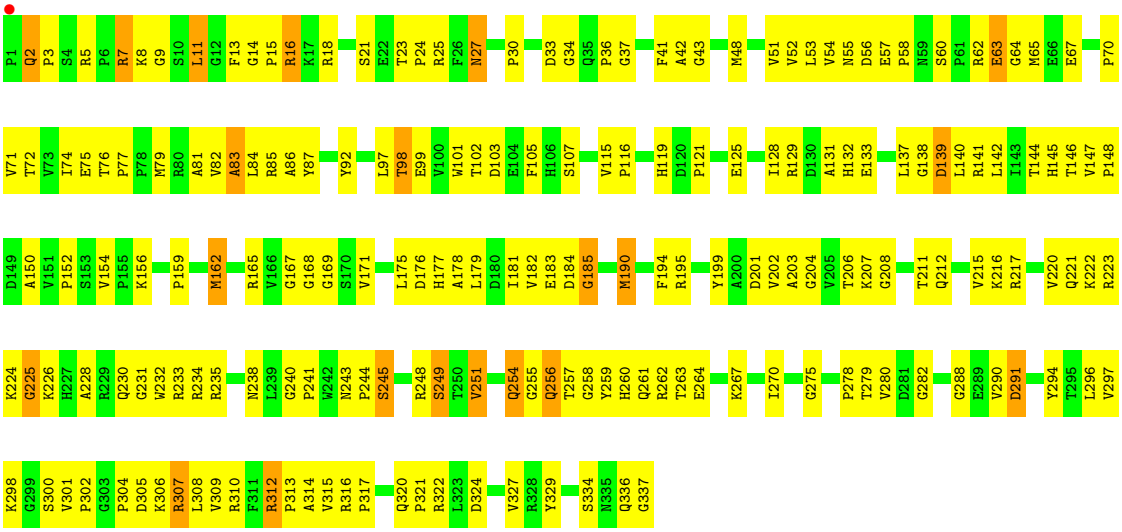
• Molecule 4: 50S ribosomal protein L2P

Chain C:



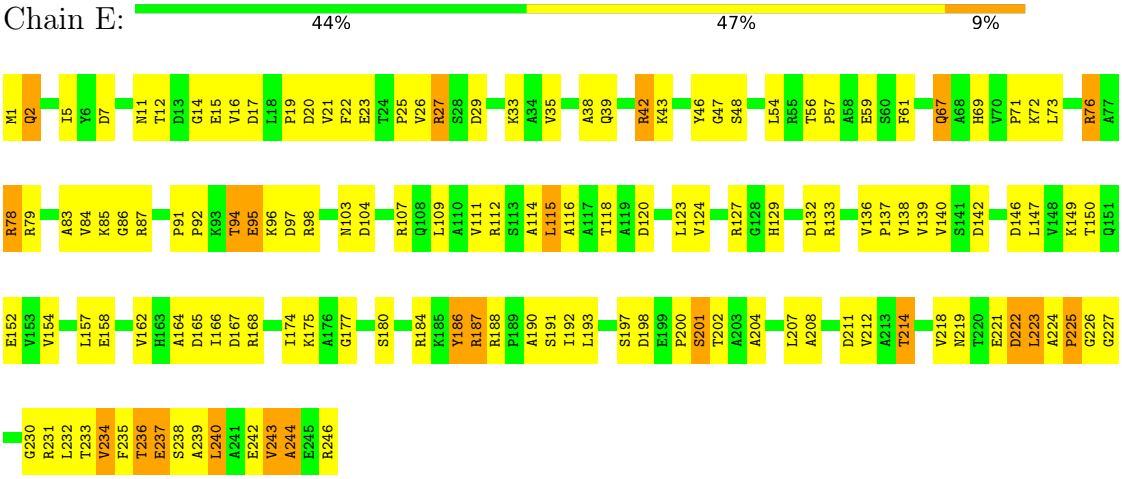
• Molecule 5: 50S ribosomal protein L3P

Chain D:



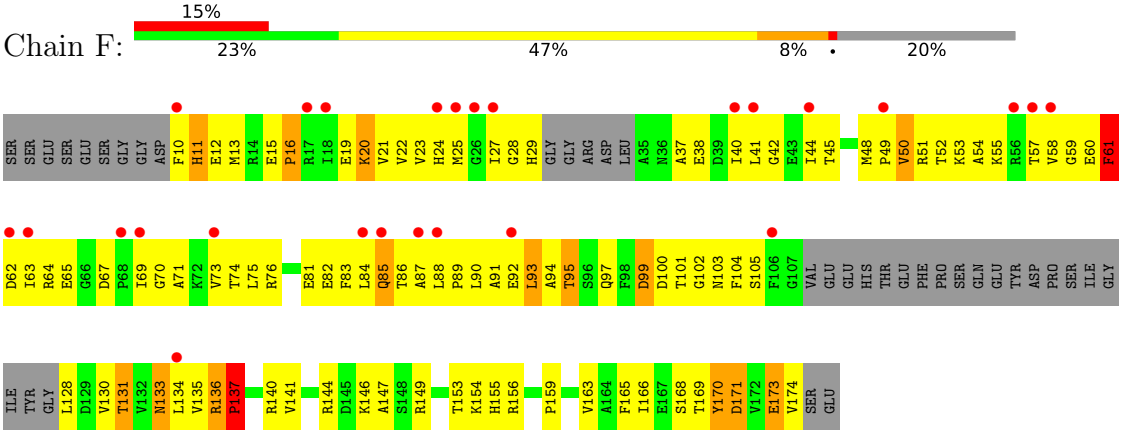
• Molecule 6: 50S ribosomal protein L4E

Chain E:



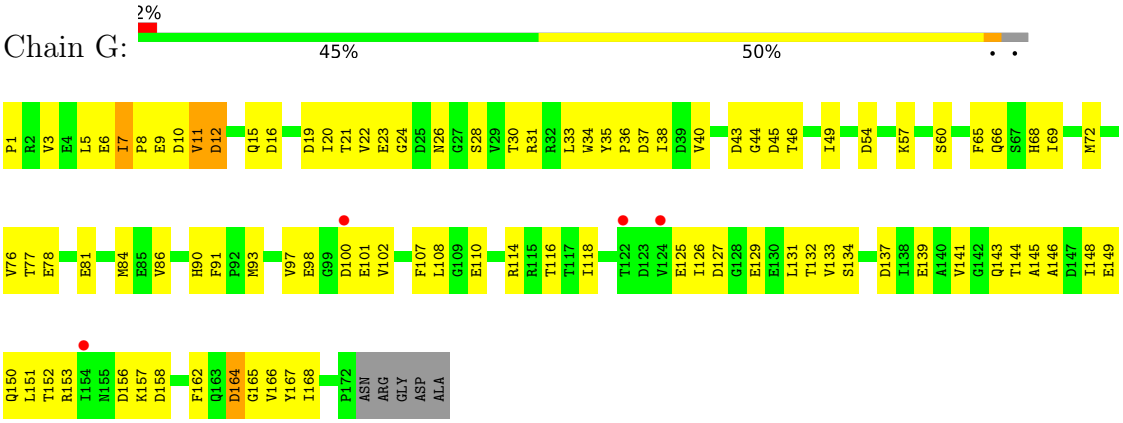
• Molecule 7: 50S ribosomal protein L5P

Chain F:



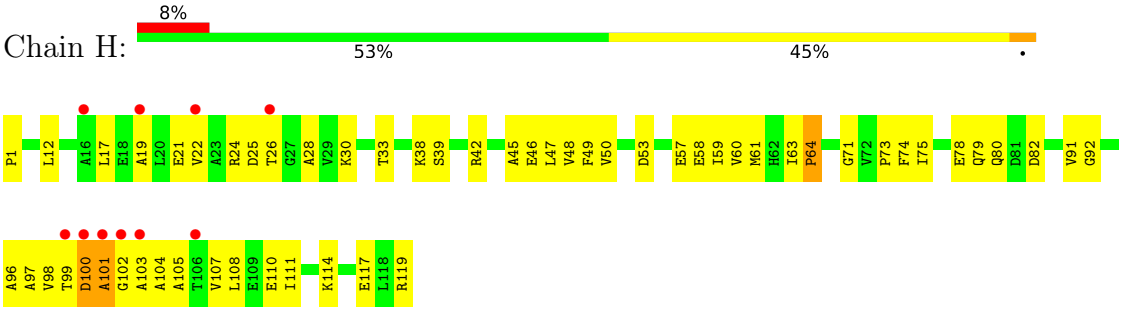
• Molecule 8: 50S ribosomal protein L6P

Chain G:



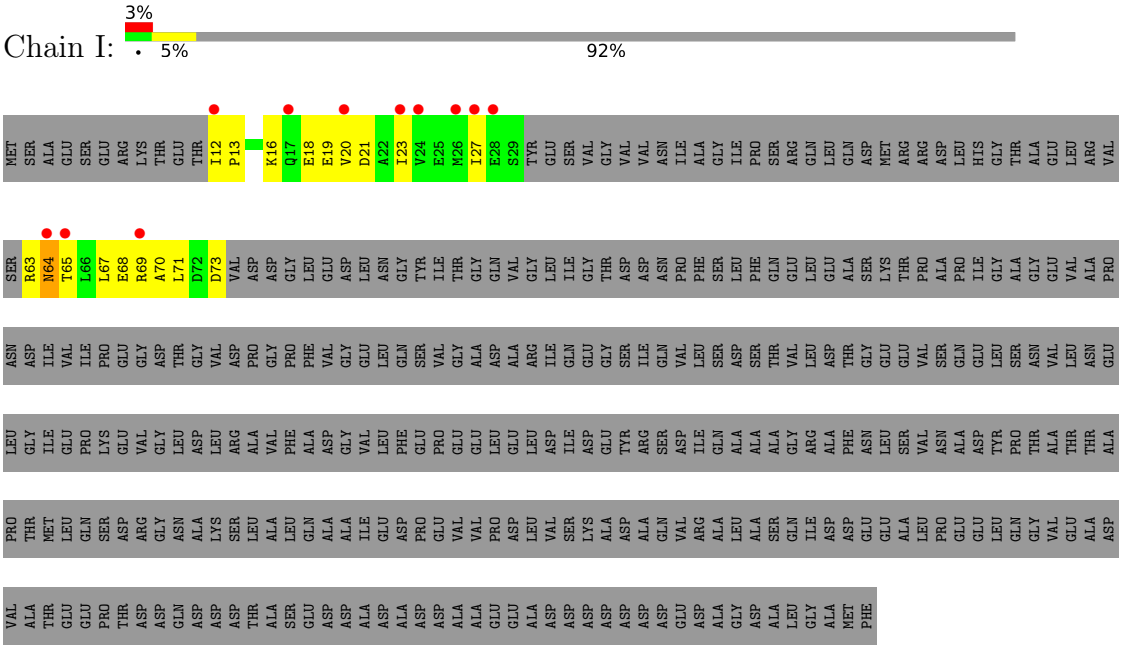
• Molecule 9: 50S ribosomal protein L7Ae

Chain H:



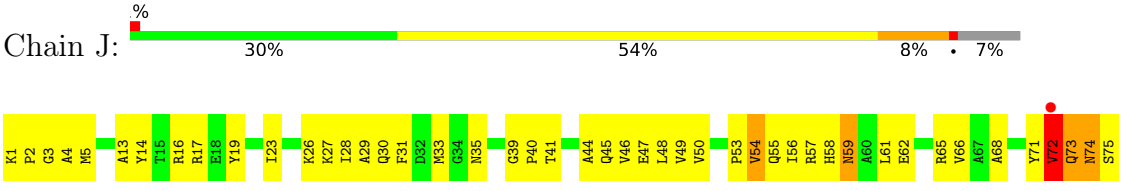
• Molecule 10: Acidic ribosomal protein P0 homolog

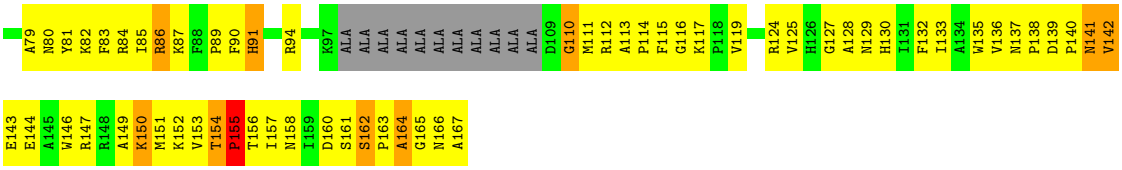
Chain I:



• Molecule 11: L10 Ribosomal Protein

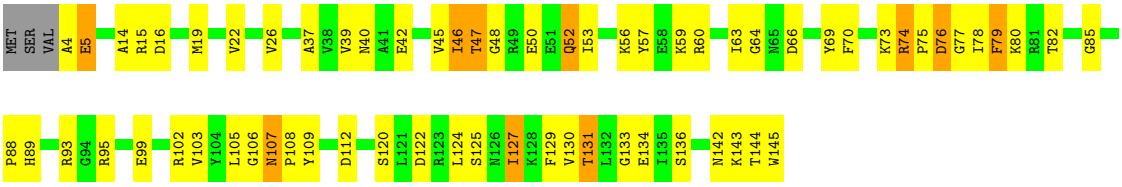
Chain J:





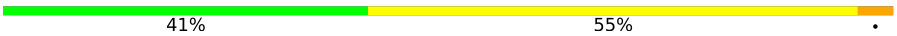
• Molecule 12: 50S ribosomal protein L13P

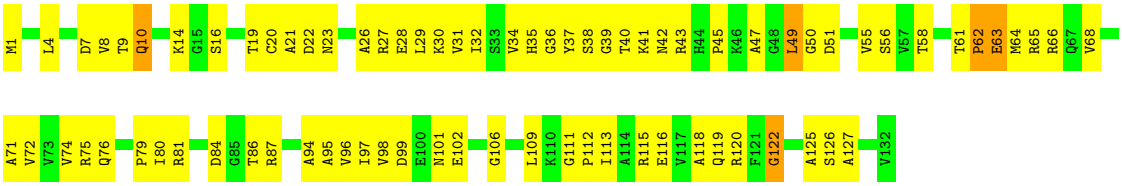
Chain K:



• Molecule 13: 50S ribosomal protein L14P

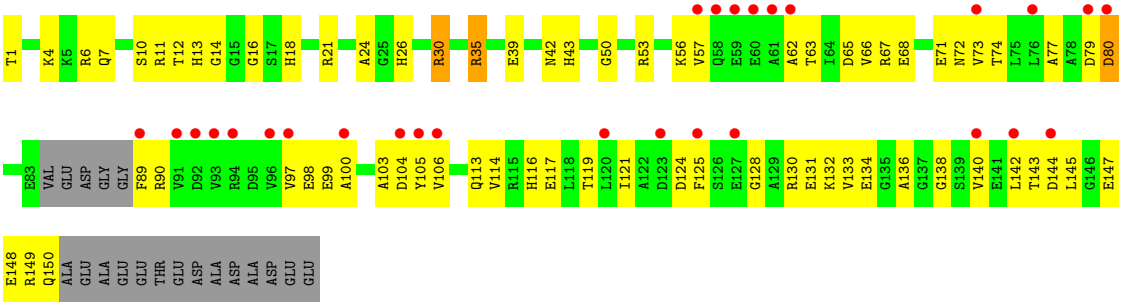
Chain L:





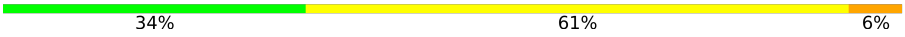
• Molecule 14: 50S ribosomal protein L15P

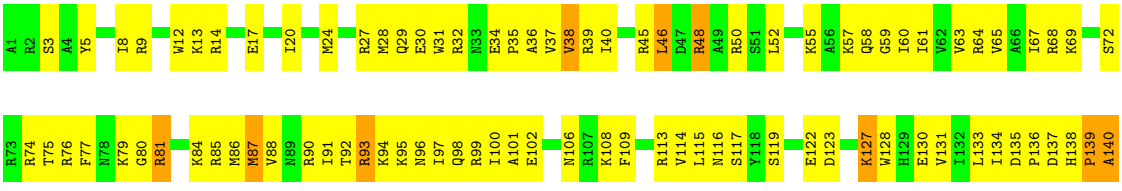
Chain M:

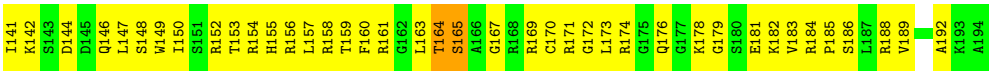


• Molecule 15: L15 Ribosomal Protein

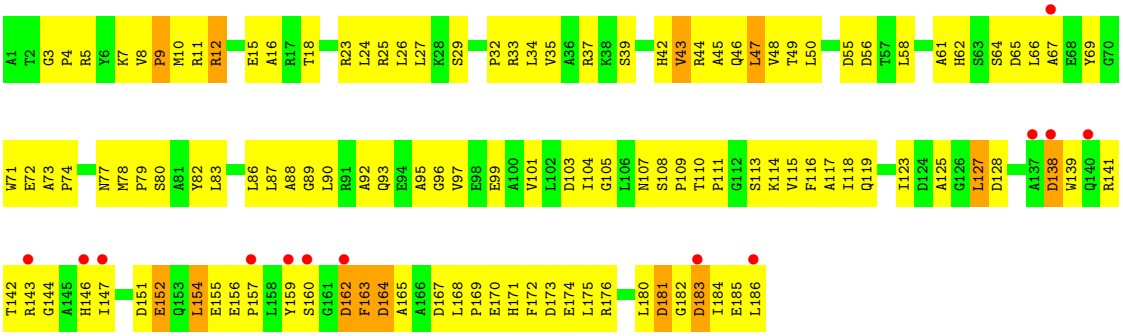
Chain N:



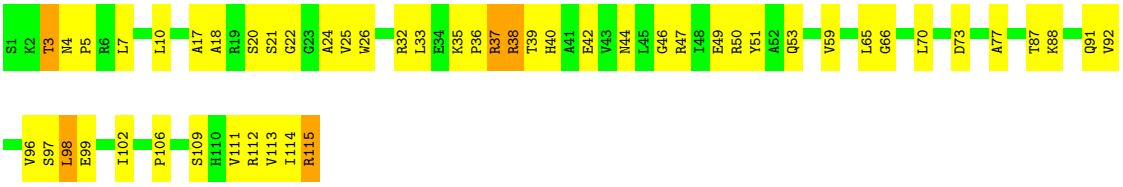




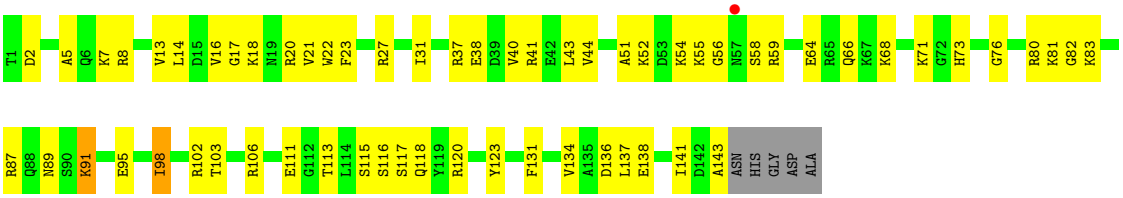
• Molecule 16: 50S ribosomal protein L18P



• Molecule 17: 50S ribosomal protein L18e



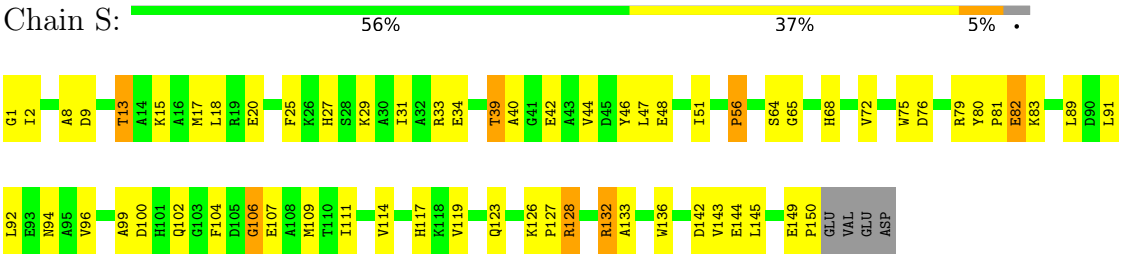
• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e

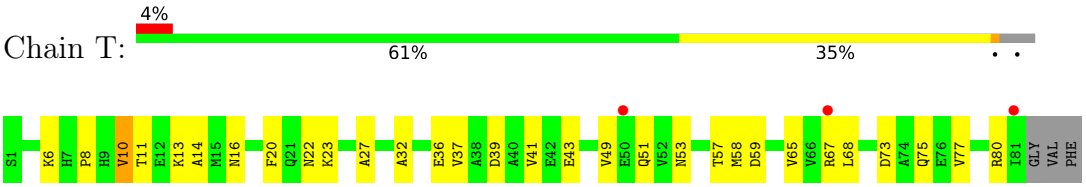
• Molecule 20: 50S ribosomal protein L22P

Chain S:



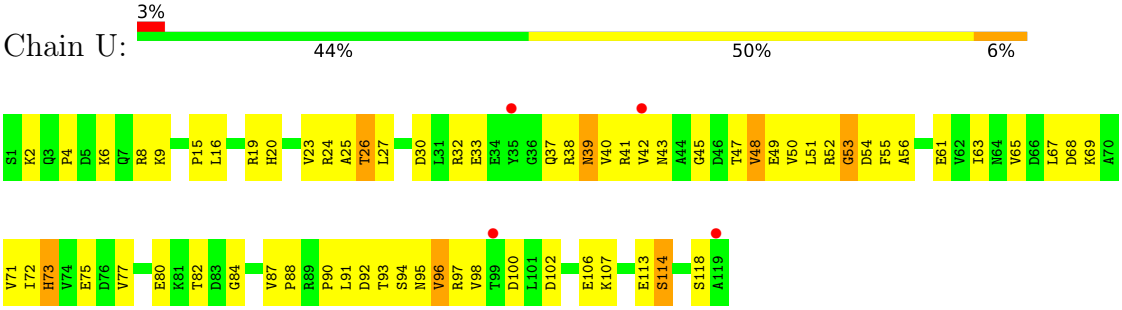
• Molecule 21: 50S ribosomal protein L23P

Chain T:



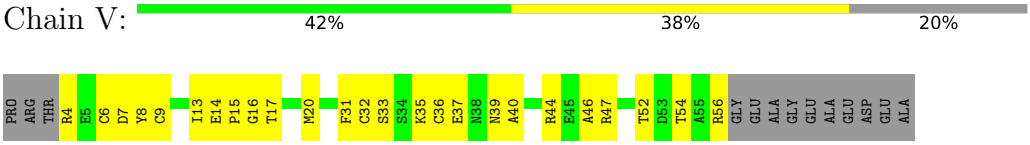
• Molecule 22: 50S ribosomal protein L24P

Chain U:



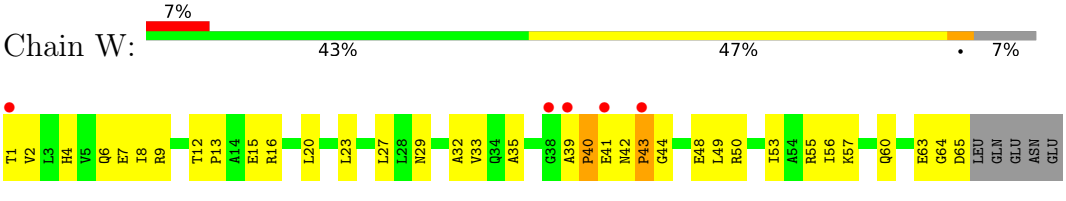
• Molecule 23: 50S ribosomal protein L24E

Chain V:



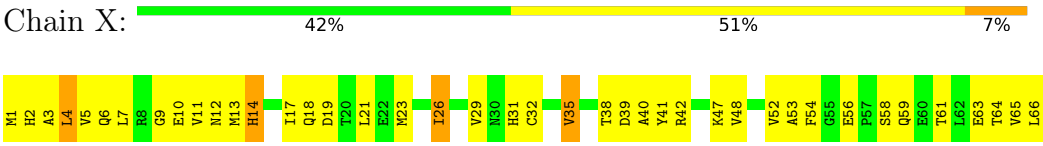
• Molecule 24: 50S ribosomal protein L29P

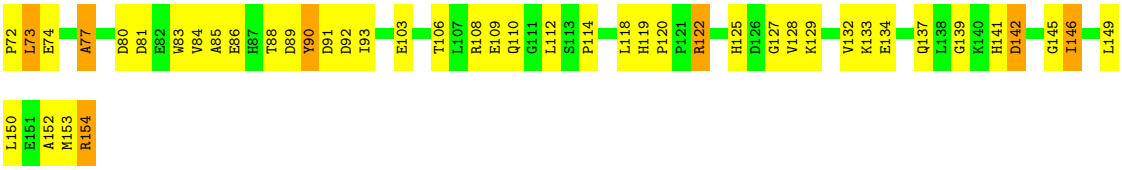
Chain W:



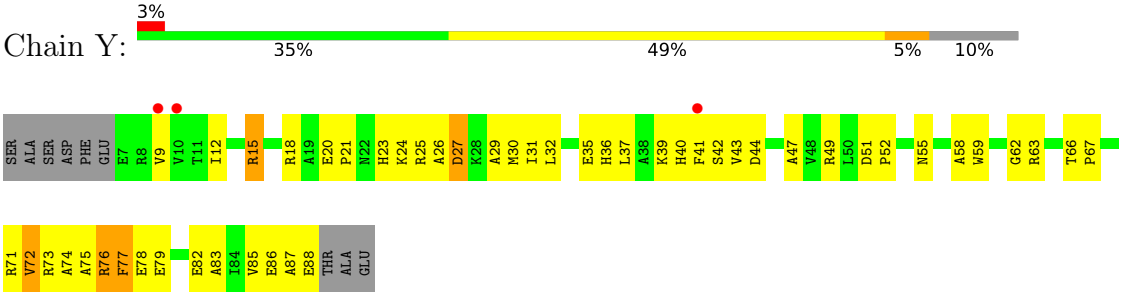
• Molecule 25: 50S ribosomal protein L30P

Chain X:

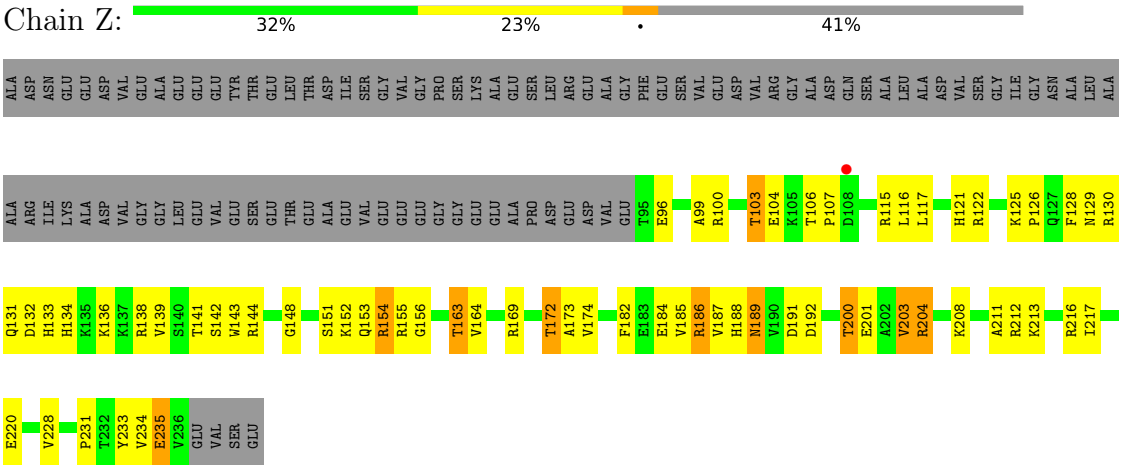




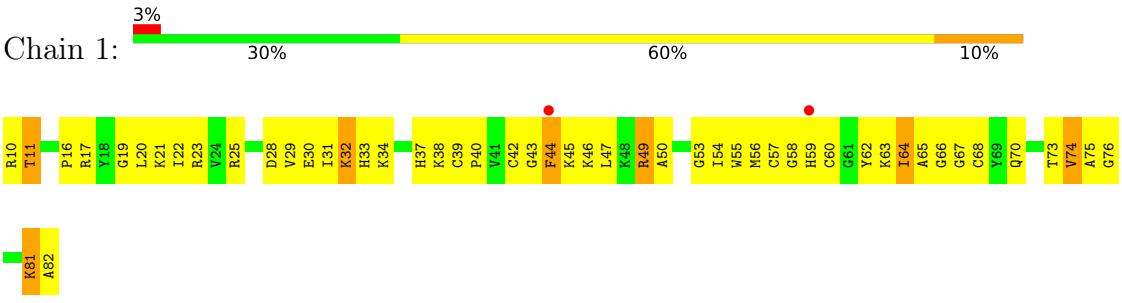
• Molecule 26: 50S ribosomal protein L31e



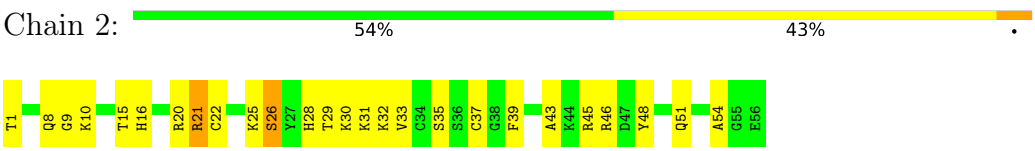
• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: L37Ae 50S ribosomal protein

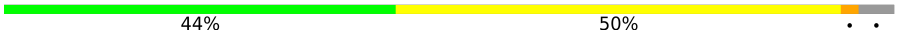


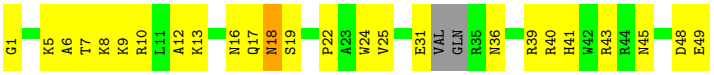
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e

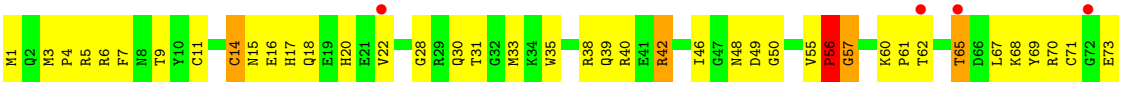
Chain 3:

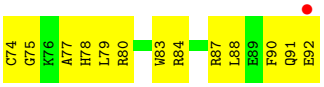




• Molecule 31: 50S ribosomal protein L44E

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 49.89 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.1 (19.99-3.20) 88.4 (49.89-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.59 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.280 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	98616	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, CL, PO4, PUY, CD, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.03	52/66076 (0.1%)	0.96	138/103052 (0.1%)
2	B	0.91	0/2905	0.95	10/4528 (0.2%)
3	5	1.87	0/64	1.14	0/97
4	C	0.76	0/1787	0.95	1/2409 (0.0%)
5	D	0.73	0/2689	0.96	1/3652 (0.0%)
6	E	0.77	0/1883	0.97	1/2551 (0.0%)
7	F	0.63	0/1111	0.79	0/1498
8	G	0.71	0/1382	0.85	1/1880 (0.1%)
9	H	0.69	0/896	0.85	0/1219
10	I	0.99	0/241	0.91	0/324
11	J	0.79	0/1246	1.05	4/1686 (0.2%)
12	K	0.76	0/1135	0.89	0/1530
13	L	0.80	1/1003 (0.1%)	1.00	0/1351
14	M	0.75	0/1126	1.00	1/1504 (0.1%)
15	N	0.89	0/1633	1.04	2/2180 (0.1%)
16	O	0.70	0/1473	0.94	0/1999
17	P	0.78	0/873	0.97	2/1181 (0.2%)
18	Q	0.74	0/1143	0.91	0/1521
19	R	0.77	0/748	1.00	2/1005 (0.2%)
20	S	0.81	0/1172	0.99	1/1578 (0.1%)
21	T	0.79	0/648	0.94	0/875
22	U	0.76	0/957	0.95	0/1289
23	V	0.74	0/417	0.88	0/562
24	W	0.66	0/502	0.81	0/675
25	X	0.75	1/1218 (0.1%)	0.94	0/1655
26	Y	0.74	0/664	0.94	0/895
27	Z	0.74	0/1146	0.93	0/1536
28	1	0.79	0/575	0.98	0/763
29	2	0.87	0/437	1.08	0/578
30	3	0.70	0/398	0.86	0/527
31	4	0.81	1/771 (0.1%)	0.97	1/1024 (0.1%)
All	All	0.95	55/98319 (0.1%)	0.96	165/147124 (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	A	1	386
2	B	1	12
5	D	0	2
6	E	0	1
25	X	0	1
29	2	0	1
All	All	2	403

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2638	G	P-OP2	12.82	1.70	1.49
1	A	2636	C	C3'-O3'	11.93	1.58	1.42
1	A	2619	U	C3'-O3'	10.66	1.57	1.42
1	A	2620	U	C5'-C4'	-10.62	1.38	1.51
1	A	2619	U	C2'-O2'	-10.44	1.28	1.41
1	A	2620	U	C4'-C3'	-10.34	1.41	1.53
1	A	2637	A	P-OP2	9.12	1.64	1.49
1	A	2620	U	C4'-O4'	-8.95	1.33	1.45
1	A	2634	G	C4'-C3'	-8.51	1.43	1.53
1	A	2620	U	O3'-P	-7.89	1.51	1.61
1	A	2619	U	C4'-O4'	-7.71	1.35	1.45
1	A	2636	C	O3'-P	7.43	1.70	1.61
1	A	2636	C	C4'-O4'	-7.34	1.36	1.45
1	A	2619	U	C2'-C1'	-7.33	1.45	1.53
1	A	2634	G	O3'-P	-7.28	1.52	1.61
1	A	2637	A	C5-C6	7.17	1.47	1.41
1	A	2620	U	C3'-O3'	6.89	1.51	1.42
1	A	2636	C	P-O5'	-6.88	1.52	1.59
1	A	2636	C	P-OP2	6.57	1.60	1.49
1	A	2635	A	O3'-P	6.56	1.69	1.61
1	A	2638	G	C5'-C4'	6.41	1.59	1.51
1	A	2637	A	N9-C4	6.38	1.41	1.37
1	A	2246	U	N1-C2	6.31	1.44	1.38
1	A	2637	A	C5-C4	6.25	1.43	1.38
1	A	2637	A	O3'-P	6.24	1.68	1.61
1	A	2637	A	P-O5'	-6.21	1.53	1.59
1	A	2637	A	C6-N1	6.20	1.39	1.35
1	A	2635	A	C4'-O4'	5.90	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2637	A	N1-C2	5.89	1.39	1.34
1	A	2620	U	O5'-C5'	-5.79	1.33	1.42
1	A	1014	A	C2-N3	-5.74	1.28	1.33
1	A	1835	U	N3-C4	-5.57	1.33	1.38
31	4	14	CYS	CB-SG	-5.48	1.72	1.81
1	A	620	A	C5-C6	-5.42	1.36	1.41
1	A	329	A	C5-C6	5.37	1.45	1.41
1	A	2637	A	C5'-C4'	-5.32	1.45	1.51
1	A	2812	A	C5-C6	-5.31	1.36	1.41
1	A	2637	A	C2-N3	5.28	1.38	1.33
1	A	1231	A	C2-N3	-5.27	1.28	1.33
1	A	2622	A	O3'-P	5.22	1.67	1.61
1	A	2620	U	C4-C5	5.19	1.48	1.43
1	A	2585	G	C5-C6	-5.18	1.37	1.42
1	A	2370	A	N9-C4	-5.17	1.34	1.37
1	A	2636	C	N1-C2	-5.16	1.34	1.40
1	A	2632	G	C5-C6	-5.13	1.37	1.42
1	A	2620	U	C2'-C1'	-5.12	1.47	1.53
1	A	2635	A	P-O5'	5.12	1.64	1.59
1	A	2556	C	C2-O2	-5.10	1.19	1.24
1	A	271	C	C2-O2	5.10	1.29	1.24
1	A	465	U	N1-C2	5.09	1.43	1.38
1	A	2635	A	C3'-C2'	5.08	1.58	1.52
13	L	63	GLU	CB-CG	5.08	1.61	1.52
1	A	2637	A	C6-N6	5.04	1.38	1.33
1	A	841	A	C5-C6	-5.02	1.36	1.41
25	X	86	GLU	CG-CD	5.00	1.59	1.51

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	U	OP1-P-O3'	-19.52	62.25	105.20
1	A	1164	U	OP2-P-O3'	-16.77	68.31	105.20
1	A	1165	G	O5'-P-OP1	-15.53	91.72	105.70
1	A	1563	G	C2'-C3'-O3'	10.27	132.10	109.50
1	A	1942	A	C5'-C4'-C3'	9.66	131.46	116.00
2	B	3024	U	C2'-C3'-O3'	9.52	130.45	109.50
1	A	2914	A	C2'-C3'-O3'	9.41	130.21	109.50
1	A	2316	G	C5'-C4'-C3'	-8.68	102.11	116.00
1	A	2635	A	O5'-P-OP1	7.78	120.03	110.70
1	A	1707	G	N9-C1'-C2'	-7.74	103.48	112.00
1	A	2636	C	OP2-P-O3'	7.73	122.21	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2338	G	C2'-C3'-O3'	7.67	126.38	109.50
1	A	2664	A	N9-C1'-C2'	7.61	123.89	114.00
1	A	871	G	C5'-C4'-O4'	-7.57	100.02	109.10
1	A	1165	G	O5'-P-OP2	-7.55	98.90	105.70
1	A	1979	G	C2'-C3'-O3'	7.52	126.05	109.50
4	C	187	PRO	N-CA-C	7.50	131.59	112.10
1	A	1504	A	N9-C1'-C2'	7.48	123.73	114.00
1	A	2313	C	C5'-C4'-O4'	7.44	118.03	109.10
1	A	1971	G	O4'-C1'-N9	7.28	114.03	108.20
1	A	128	A	O5'-C5'-C4'	7.23	125.43	111.70
1	A	921	G	N9-C1'-C2'	7.22	123.39	114.00
1	A	146	U	N1-C1'-C2'	7.22	123.38	114.00
1	A	2636	C	O3'-P-O5'	-7.21	90.31	104.00
1	A	1504	A	C5'-C4'-O4'	7.20	117.74	109.10
1	A	1165	G	OP1-P-OP2	7.00	130.10	119.60
2	B	3039	U	N1-C1'-C2'	6.93	123.01	114.00
1	A	656	G	N9-C1'-C2'	-6.91	104.40	112.00
1	A	2318	C	N1-C1'-C2'	-6.85	104.47	112.00
1	A	603	A	N9-C1'-C2'	6.78	122.81	114.00
1	A	2636	C	C1'-O4'-C4'	-6.68	104.55	109.90
1	A	2526	C	N1-C1'-C2'	6.66	122.66	114.00
1	A	2667	G	O5'-C5'-C4'	6.49	124.03	111.70
1	A	206	G	C5'-C4'-C3'	-6.47	105.65	116.00
1	A	1504	A	C1'-O4'-C4'	-6.46	104.73	109.90
1	A	2615	U	N1-C1'-C2'	6.44	122.37	114.00
1	A	710	G	N9-C1'-C2'	-6.43	104.93	112.00
11	J	74	ASN	N-CA-C	-6.38	93.78	111.00
1	A	2836	G	N9-C1'-C2'	-6.35	105.01	112.00
1	A	407	A	O4'-C4'-C3'	-6.30	97.70	104.00
1	A	1120	U	C5'-C4'-C3'	-6.28	105.95	116.00
1	A	1473	U	O5'-P-OP1	-6.28	100.05	105.70
1	A	2419	U	N1-C1'-C2'	6.28	122.17	114.00
1	A	1819	G	C5'-C4'-C3'	6.26	126.02	116.00
1	A	1819	G	C4'-C3'-C2'	-6.26	96.34	102.60
1	A	2096	A	N9-C1'-C2'	6.26	122.14	114.00
1	A	1641	A	N9-C1'-C2'	-6.25	105.12	112.00
1	A	324	G	N9-C1'-C2'	-6.21	105.17	112.00
1	A	1942	A	C4'-C3'-C2'	-6.21	96.39	102.60
1	A	2071	C	N1-C1'-C2'	6.20	122.06	114.00
1	A	537	G	N9-C1'-C2'	6.18	122.04	114.00
17	P	37	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	1275	C	N1-C1'-C2'	-6.12	105.27	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1334	C	OP2-P-O3'	6.12	118.67	105.20
1	A	530	C	N1-C1'-C2'	-6.07	105.33	112.00
15	N	139	PRO	N-CA-C	-6.06	96.34	112.10
1	A	237	G	C5'-C4'-O4'	6.06	116.37	109.10
1	A	1862	C	O5'-P-OP2	-6.02	100.28	105.70
1	A	1721	C	N1-C1'-C2'	6.00	121.81	114.00
1	A	1738	C	O4'-C4'-C3'	-5.98	98.02	104.00
19	R	17	LYS	N-CA-C	-5.98	94.85	111.00
1	A	2620	U	O4'-C1'-N1	5.96	112.97	108.20
1	A	504	G	N9-C1'-C2'	-5.95	105.46	112.00
1	A	1359	U	N1-C1'-C2'	5.93	121.70	114.00
1	A	2312	G	N9-C1'-C2'	-5.93	105.48	112.00
1	A	1884	G	OP2-P-O3'	5.91	118.19	105.20
19	R	69	ASP	CB-CG-OD1	5.89	123.61	118.30
1	A	2635	A	OP1-P-O3'	5.88	118.12	105.20
1	A	381	G	N9-C1'-C2'	5.87	121.63	114.00
11	J	110	GLY	N-CA-C	-5.86	98.44	113.10
1	A	1210	G	N9-C1'-C2'	-5.84	105.57	112.00
1	A	2726	U	N1-C1'-C2'	5.84	121.60	114.00
1	A	323	C	N1-C1'-C2'	-5.81	105.61	112.00
1	A	1861	C	O4'-C4'-C3'	-5.79	98.21	104.00
1	A	1206	U	N1-C1'-C2'	-5.77	105.66	112.00
1	A	2637	A	O5'-P-OP1	5.76	117.61	110.70
1	A	1615	A	C5'-C4'-C3'	5.75	125.21	116.00
1	A	1618	G	N9-C1'-C2'	-5.75	105.67	112.00
1	A	457	U	C1'-O4'-C4'	-5.75	105.30	109.90
1	A	1559	A	C2'-C3'-O3'	5.73	122.86	113.70
1	A	1877	G	N9-C1'-C2'	5.70	121.41	114.00
1	A	755	G	O4'-C4'-C3'	-5.68	98.32	104.00
1	A	1450	C	N1-C1'-C2'	-5.67	105.76	112.00
1	A	2364	A	N9-C1'-C2'	-5.67	105.76	112.00
5	D	84	LEU	CA-CB-CG	5.67	128.33	115.30
2	B	3103	A	C4'-C3'-C2'	-5.64	96.96	102.60
1	A	1189	A	N9-C1'-C2'	5.58	121.25	114.00
1	A	2363	G	O4'-C4'-C3'	-5.55	98.45	104.00
1	A	2675	A	N9-C1'-C2'	5.55	121.21	114.00
11	J	141	ASN	N-CA-C	-5.54	96.04	111.00
1	A	2313	C	C4'-C3'-C2'	-5.53	97.07	102.60
2	B	3037	C	N1-C1'-C2'	-5.52	105.93	112.00
1	A	1492	A	C5'-C4'-C3'	-5.52	107.17	116.00
1	A	2635	A	C5'-C4'-O4'	5.51	115.72	109.10
1	A	2718	C	C5'-C4'-O4'	-5.51	102.49	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	G	O4'-C4'-C3'	-5.51	98.49	104.00
1	A	2077	C	N1-C1'-C2'	5.51	121.16	114.00
1	A	2853	U	N1-C1'-C2'	-5.50	105.95	112.00
1	A	2314	G	OP1-P-O3'	5.49	117.27	105.20
2	B	3019	G	N9-C1'-C2'	-5.49	105.97	112.00
1	A	1592	G	N9-C1'-C2'	5.48	121.12	114.00
1	A	270	U	N1-C1'-C2'	5.47	121.11	114.00
1	A	2098	C	N1-C1'-C2'	-5.47	105.98	112.00
1	A	699	C	C1'-O4'-C4'	-5.45	105.54	109.90
15	N	127	LYS	N-CA-C	-5.45	96.29	111.00
1	A	920	C	O4'-C4'-C3'	-5.43	98.57	104.00
1	A	226	A	OP2-P-O3'	5.42	117.13	105.20
1	A	1283	G	N9-C1'-C2'	-5.42	106.04	112.00
1	A	1839	A	N9-C1'-C2'	5.41	121.03	114.00
1	A	2313	C	C1'-O4'-C4'	-5.40	105.58	109.90
1	A	1450	C	C4'-C3'-O3'	5.40	123.81	113.00
1	A	1684	A	C5'-C4'-C3'	-5.39	107.37	116.00
1	A	1232	A	O4'-C1'-C2'	-5.38	100.42	105.80
1	A	1602	C	N1-C1'-C2'	-5.36	106.10	112.00
1	A	358	G	N9-C1'-C2'	5.36	120.97	114.00
14	M	43	HIS	N-CA-C	-5.33	96.60	111.00
2	B	3040	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	A	877	G	OP1-P-O3'	5.33	116.92	105.20
1	A	129	A	C2'-C3'-O3'	5.32	122.21	113.70
1	A	2294	C	C5'-C4'-C3'	-5.31	107.50	116.00
20	S	128	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	876	A	O4'-C4'-C3'	-5.30	98.70	104.00
1	A	2328	U	N1-C1'-C2'	-5.29	106.18	112.00
1	A	1738	C	C5'-C4'-C3'	5.28	124.45	116.00
2	B	3024	U	C4'-C3'-O3'	5.28	123.56	113.00
1	A	475	G	N9-C1'-C2'	-5.27	106.20	112.00
31	4	5	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	1878	G	O4'-C1'-N9	5.26	112.41	108.20
1	A	2637	A	OP1-P-O3'	5.23	116.71	105.20
1	A	1885	A	N9-C1'-C2'	-5.23	106.24	112.00
1	A	96	A	N9-C1'-C2'	5.22	120.78	114.00
1	A	1386	G	N9-C1'-C2'	-5.21	106.27	112.00
2	B	3103	A	C5'-C4'-O4'	5.20	115.34	109.10
1	A	1697	G	OP2-P-O3'	5.19	116.61	105.20
2	B	3103	A	C1'-O4'-C4'	-5.19	105.75	109.90
1	A	1388	U	N1-C1'-C2'	-5.18	106.31	112.00
1	A	1044	C	OP2-P-O3'	5.17	116.57	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	11	VAL	N-CA-C	5.17	124.94	111.00
1	A	1512	G	O4'-C4'-C3'	-5.16	98.84	104.00
1	A	1261	A	N9-C1'-C2'	5.16	120.71	114.00
1	A	189	A	C5'-C4'-O4'	-5.14	102.93	109.10
1	A	1651	C	N1-C1'-C2'	5.14	120.68	114.00
1	A	284	C	N1-C1'-C2'	5.13	120.67	114.00
1	A	2668	G	O4'-C4'-C3'	-5.13	98.87	104.00
2	B	3103	A	O4'-C4'-C3'	-5.10	98.90	104.00
1	A	2300	A	N9-C1'-C2'	5.10	120.63	114.00
1	A	2620	U	C5'-C4'-C3'	-5.10	107.85	116.00
1	A	2620	U	C1'-O4'-C4'	5.09	113.98	109.90
1	A	118	G	C4'-C3'-C2'	-5.09	97.51	102.60
17	P	66	GLY	N-CA-C	5.09	125.83	113.10
1	A	1942	A	C1'-O4'-C4'	-5.09	105.83	109.90
1	A	1080	C	C4'-C3'-C2'	-5.07	97.53	102.60
1	A	695	C	OP2-P-O3'	5.07	116.35	105.20
1	A	476	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	A	1438	G	N9-C1'-C2'	5.06	120.58	114.00
1	A	307	G	OP2-P-O3'	5.06	116.33	105.20
6	E	157	LEU	CA-CB-CG	-5.05	103.68	115.30
1	A	2607	U	N1-C1'-C2'	5.04	120.55	114.00
1	A	605	C	O4'-C4'-C3'	-5.03	98.97	104.00
11	J	155	PRO	N-CA-C	5.02	125.16	112.10
1	A	436	A	N9-C1'-C2'	5.02	120.53	114.00
1	A	1942	A	C5'-C4'-O4'	5.01	115.11	109.10
1	A	2539	U	O5'-P-OP1	-5.01	101.19	105.70
1	A	2826	G	N9-C1'-C2'	5.01	120.51	114.00
1	A	2467	A	C1'-O4'-C4'	-5.00	105.90	109.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (403) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	48	TYR	Sidechain
1	A	1003	U	Sidechain
1	A	1005	A	Sidechain
1	A	1006	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1008	C	Sidechain
1	A	1013	A	Sidechain
1	A	1026	C	Sidechain
1	A	1029	U	Sidechain
1	A	1038	G	Sidechain
1	A	1039	G	Sidechain
1	A	1052	G	Sidechain
1	A	1054	G	Sidechain
1	A	1062	U	Sidechain
1	A	1063	G	Sidechain
1	A	1064	U	Sidechain
1	A	107	U	Sidechain
1	A	1070	A	Sidechain
1	A	1076	G	Sidechain
1	A	1100	G	Sidechain
1	A	1117	A	Sidechain
1	A	1125	U	Sidechain
1	A	1127	C	Sidechain
1	A	1129	C	Sidechain
1	A	1134	G	Sidechain
1	A	115	U	Sidechain
1	A	117	A	Sidechain
1	A	1197	G	Sidechain
1	A	1206	U	Sidechain
1	A	1210	G	Sidechain
1	A	1213	C	Sidechain
1	A	122	C	Sidechain
1	A	1229	C	Sidechain
1	A	1230	A	Sidechain
1	A	1240	G	Sidechain
1	A	1241	G	Sidechain
1	A	125	U	Sidechain
1	A	1259	A	Sidechain
1	A	1265	G	Sidechain
1	A	1267	C	Sidechain
1	A	1288	U	Sidechain
1	A	1295	G	Sidechain
1	A	1309	U	Sidechain
1	A	1310	U	Sidechain
1	A	1311	G	Sidechain
1	A	1316	G	Sidechain
1	A	1320	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1323	G	Sidechain
1	A	1325	G	Sidechain
1	A	1326	U	Sidechain
1	A	1333	U	Sidechain
1	A	1340	G	Sidechain
1	A	1346	U	Sidechain
1	A	1347	U	Sidechain
1	A	1348	A	Sidechain
1	A	1349	G	Sidechain
1	A	1350	U	Sidechain
1	A	1351	G	Sidechain
1	A	1357	A	Sidechain
1	A	1360	C	Sidechain
1	A	1364	G	Sidechain
1	A	1376	G	Sidechain
1	A	1377	C	Sidechain
1	A	1380	U	Sidechain
1	A	1388	U	Sidechain
1	A	1398	G	Sidechain
1	A	1400	C	Sidechain
1	A	1410	G	Sidechain
1	A	1412	U	Sidechain
1	A	1417	G	Sidechain
1	A	1421	C	Sidechain
1	A	1423	C	Sidechain
1	A	1430	G	Sidechain
1	A	1432	U	Sidechain
1	A	1437	A	Sidechain
1	A	1443	G	Sidechain
1	A	1444	G	Sidechain
1	A	1445	G	Sidechain
1	A	145	A	Sidechain
1	A	1454	U	Sidechain
1	A	1458	A	Sidechain
1	A	146	U	Sidechain
1	A	1462	C	Sidechain
1	A	147	G	Sidechain
1	A	1472	C	Sidechain
1	A	1474	C	Sidechain
1	A	1484	G	Sidechain
1	A	1490	G	Sidechain
1	A	1505	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1506	U	Sidechain
1	A	1507	C	Sidechain
1	A	1514	C	Sidechain
1	A	1522	A	Sidechain
1	A	1533	A	Sidechain
1	A	1537	C	Sidechain
1	A	1538	C	Sidechain
1	A	1548	U	Sidechain
1	A	1551	C	Sidechain
1	A	1555	G	Sidechain
1	A	1561	U	Sidechain
1	A	1572	A	Sidechain
1	A	1573	A	Sidechain
1	A	1579	C	Sidechain
1	A	1588	G	Sidechain
1	A	1590	A	Sidechain
1	A	1599	U	Sidechain
1	A	16	A	Sidechain
1	A	1629	G	Sidechain
1	A	1635	U	Sidechain
1	A	1642	A	Sidechain
1	A	1646	G	Sidechain
1	A	1647	G	Sidechain
1	A	1658	A	Sidechain
1	A	166	A	Sidechain
1	A	1660	G	Sidechain
1	A	1673	U	Sidechain
1	A	1677	U	Sidechain
1	A	168	C	Sidechain
1	A	1681	G	Sidechain
1	A	169	A	Sidechain
1	A	1693	A	Sidechain
1	A	1696	U	Sidechain
1	A	1699	C	Sidechain
1	A	171	C	Sidechain
1	A	1710	A	Sidechain
1	A	1721	C	Sidechain
1	A	1726	G	Sidechain
1	A	1730	G	Sidechain
1	A	1744	G	Sidechain
1	A	1749	U	Sidechain
1	A	1751	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1754	A	Sidechain
1	A	176	U	Sidechain
1	A	1769	C	Sidechain
1	A	1777	G	Sidechain
1	A	1785	G	Sidechain
1	A	179	C	Sidechain
1	A	1790	C	Sidechain
1	A	1809	G	Sidechain
1	A	1816	C	Sidechain
1	A	1819	G	Sidechain
1	A	182	G	Sidechain
1	A	1829	A	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	184	G	Sidechain
1	A	1842	A	Sidechain
1	A	1843	A	Sidechain
1	A	1850	U	Sidechain
1	A	1857	A	Sidechain
1	A	1860	U	Sidechain
1	A	1865	A	Sidechain
1	A	1866	A	Sidechain
1	A	1871	U	Sidechain
1	A	1874	U	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1881	A	Sidechain
1	A	1883	U	Sidechain
1	A	1887	U	Sidechain
1	A	1889	C	Sidechain
1	A	1903	U	Sidechain
1	A	1912	A	Sidechain
1	A	1921	A	Sidechain
1	A	196	G	Sidechain
1	A	1970	G	Sidechain
1	A	1972	U	Sidechain
1	A	1975	C	Sidechain
1	A	1978	A	Sidechain
1	A	1985	U	Sidechain
1	A	1992	U	Sidechain
1	A	1995	G	Sidechain
1	A	1996	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2013	G	Sidechain
1	A	2020	C	Sidechain
1	A	2028	U	Sidechain
1	A	2035	C	Sidechain
1	A	2037	C	Sidechain
1	A	2052	U	Sidechain
1	A	2069	U	Sidechain
1	A	2073	G	Sidechain
1	A	2077	C	Sidechain
1	A	2081	A	Sidechain
1	A	2082	G	Sidechain
1	A	2093	G	Sidechain
1	A	2104	C	Sidechain
1	A	2113	G	Sidechain
1	A	2119	C	Sidechain
1	A	2134	G	Sidechain
1	A	214	U	Sidechain
1	A	220	C	Sidechain
1	A	2258	A	Sidechain
1	A	2260	A	Sidechain
1	A	2264	A	Sidechain
1	A	2265	U	Sidechain
1	A	2266	A	Sidechain
1	A	2268	C	Sidechain
1	A	2276	U	Sidechain
1	A	2279	G	Sidechain
1	A	2292	C	Sidechain
1	A	2293	G	Sidechain
1	A	2294	C	Sidechain
1	A	2300	A	Sidechain
1	A	2308	U	Sidechain
1	A	2313	C	Sidechain
1	A	2314	G	Sidechain
1	A	2320	U	Sidechain
1	A	2321	A	Sidechain
1	A	2337	G	Sidechain
1	A	2338	G	Sidechain
1	A	2364	A	Sidechain
1	A	2382	A	Sidechain
1	A	2388	C	Sidechain
1	A	2411	C	Sidechain
1	A	2413	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2423	C	Sidechain
1	A	2429	A	Sidechain
1	A	2442	G	Sidechain
1	A	246	G	Sidechain
1	A	2463	A	Sidechain
1	A	2472	C	Sidechain
1	A	2476	C	Sidechain
1	A	248	A	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2501	G	Sidechain
1	A	2506	A	Sidechain
1	A	2510	C	Sidechain
1	A	2514	U	Sidechain
1	A	2516	G	Sidechain
1	A	2542	C	Sidechain
1	A	2548	C	Sidechain
1	A	2551	C	Sidechain
1	A	2564	G	Sidechain
1	A	2568	A	Sidechain
1	A	257	G	Sidechain
1	A	2597	U	Sidechain
1	A	2600	A	Sidechain
1	A	2607	U	Sidechain
1	A	261	A	Sidechain
1	A	2619	U	Sidechain
1	A	2621	U	Sidechain
1	A	263	U	Sidechain
1	A	2630	G	Sidechain
1	A	2632	G	Sidechain
1	A	2636	C	Sidechain
1	A	264	G	Sidechain
1	A	2640	U	Sidechain
1	A	2649	A	Sidechain
1	A	2656	G	Sidechain
1	A	2658	G	Sidechain
1	A	2672	C	Sidechain
1	A	2673	U	Sidechain
1	A	2676	C	Sidechain
1	A	2710	U	Sidechain
1	A	2720	C	Sidechain
1	A	2722	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2729	C	Sidechain
1	A	2735	U	Sidechain
1	A	2745	C	Sidechain
1	A	275	G	Sidechain
1	A	2753	G	Sidechain
1	A	2759	C	Sidechain
1	A	2774	U	Sidechain
1	A	2781	U	Sidechain
1	A	2793	A	Sidechain
1	A	2800	A	Sidechain
1	A	2807	U	Sidechain
1	A	2811	A	Sidechain
1	A	2815	G	Sidechain
1	A	2826	G	Sidechain
1	A	2837	U	Sidechain
1	A	2839	C	Sidechain
1	A	2840	A	Sidechain
1	A	2851	G	Sidechain
1	A	2858	U	Sidechain
1	A	2866	U	Sidechain
1	A	2867	G	Sidechain
1	A	2873	C	Sidechain
1	A	2888	U	Sidechain
1	A	2897	C	Sidechain
1	A	30	U	Sidechain
1	A	308	U	Sidechain
1	A	311	C	Sidechain
1	A	321	A	Sidechain
1	A	324	G	Sidechain
1	A	329	A	Sidechain
1	A	333	G	Sidechain
1	A	344	C	Sidechain
1	A	404	G	Sidechain
1	A	412	C	Sidechain
1	A	416	G	Sidechain
1	A	417	G	Sidechain
1	A	422	G	Sidechain
1	A	429	A	Sidechain
1	A	432	G	Sidechain
1	A	434	U	Sidechain
1	A	436	A	Sidechain
1	A	437	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	438	C	Sidechain
1	A	44	G	Sidechain
1	A	442	A	Sidechain
1	A	444	C	Sidechain
1	A	445	U	Sidechain
1	A	446	G	Sidechain
1	A	447	A	Sidechain
1	A	452	G	Sidechain
1	A	458	G	Sidechain
1	A	462	A	Sidechain
1	A	470	U	Sidechain
1	A	481	U	Sidechain
1	A	482	G	Sidechain
1	A	483	C	Sidechain
1	A	506	G	Sidechain
1	A	507	A	Sidechain
1	A	512	G	Sidechain
1	A	518	G	Sidechain
1	A	534	C	Sidechain
1	A	535	G	Sidechain
1	A	537	G	Sidechain
1	A	538	C	Sidechain
1	A	55	U	Sidechain
1	A	552	A	Sidechain
1	A	554	G	Sidechain
1	A	560	C	Sidechain
1	A	57	C	Sidechain
1	A	608	A	Sidechain
1	A	640	G	Sidechain
1	A	649	U	Sidechain
1	A	651	U	Sidechain
1	A	653	C	Sidechain
1	A	669	G	Sidechain
1	A	677	C	Sidechain
1	A	678	G	Sidechain
1	A	679	G	Sidechain
1	A	695	C	Sidechain
1	A	696	C	Sidechain
1	A	702	G	Sidechain
1	A	722	G	Sidechain
1	A	723	G	Sidechain
1	A	734	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	74	A	Sidechain
1	A	743	G	Sidechain
1	A	75	U	Sidechain
1	A	750	A	Sidechain
1	A	761	A	Sidechain
1	A	764	C	Sidechain
1	A	769	C	Sidechain
1	A	779	U	Sidechain
1	A	781	C	Sidechain
1	A	788	A	Sidechain
1	A	791	A	Sidechain
1	A	801	U	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	817	G	Sidechain
1	A	820	G	Sidechain
1	A	823	U	Sidechain
1	A	825	U	Sidechain
1	A	827	A	Sidechain
1	A	831	U	Sidechain
1	A	840	U	Sidechain
1	A	843	A	Sidechain
1	A	844	A	Sidechain
1	A	852	U	Sidechain
1	A	855	U	Sidechain
1	A	857	A	Sidechain
1	A	86	A	Sidechain
1	A	862	U	Sidechain
1	A	867	A	Sidechain
1	A	868	G	Sidechain
1	A	869	G	Sidechain
1	A	871	G	Sidechain
1	A	873	G	Sidechain
1	A	892	G	Sidechain
1	A	893	C	Sidechain
1	A	898	G	Sidechain
1	A	902	G	Sidechain
1	A	906	C	Sidechain
1	A	913	A	Sidechain
1	A	919	U	Sidechain
1	A	92	G	Sidechain
1	A	930	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	946	C	Sidechain
1	A	948	G	Sidechain
1	A	952	G	Sidechain
1	A	954	U	Sidechain
1	A	966	U	Sidechain
2	B	3024	U	Sidechain
2	B	3028	U	Sidechain
2	B	3042	C	Sidechain
2	B	3043	G	Sidechain
2	B	3060	C	Sidechain
2	B	3065	A	Sidechain
2	B	3067	C	Sidechain
2	B	3069	U	Sidechain
2	B	3079	U	Sidechain
2	B	3097	U	Sidechain
2	B	3099	U	Sidechain
2	B	3116	C	Sidechain
5	D	199	TYR	Sidechain
5	D	259	TYR	Sidechain
6	E	186	TYR	Sidechain
25	X	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29801	2017	0
2	B	2600	0	1326	128	0
3	5	58	0	34	2	0
4	C	1754	0	1763	155	0
5	D	2624	0	2533	238	0
6	E	1858	0	1816	194	0
7	F	1094	0	1085	172	0
8	G	1357	0	1266	103	0
9	H	885	0	854	74	0
10	I	240	0	231	33	0
11	J	1215	0	1215	194	0
12	K	1119	0	1098	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	993	0	1027	88	0
14	M	1114	0	1072	85	0
15	N	1605	0	1676	207	0
16	O	1444	0	1401	182	0
17	P	864	0	873	65	0
18	Q	1133	0	1127	74	0
19	R	734	0	728	62	0
20	S	1149	0	1122	87	0
21	T	641	0	605	27	0
22	U	949	0	923	87	0
23	V	410	0	364	44	0
24	W	499	0	511	40	0
25	X	1195	0	1137	120	0
26	Y	654	0	653	64	0
27	Z	1130	0	1133	81	0
28	1	563	0	599	76	0
29	2	430	0	427	38	0
30	3	393	0	406	34	0
31	4	755	0	730	64	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	72	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	1	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	0	0
35	A	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	1	0	0	1	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	1	0
35	P	1	0	0	1	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	3	0	0	1	0
37	5	34	0	28	0	0
38	1	1	0	0	0	0
38	2	1	0	0	0	0
38	4	1	0	0	2	0
38	P	1	0	0	0	0
38	V	1	0	0	0	0
39	1	36	0	0	15	0
39	2	63	0	0	13	0
39	3	42	0	0	7	0
39	4	73	0	0	17	0
39	5	6	0	0	0	0
39	A	5861	0	0	566	2
39	B	154	0	0	27	0
39	C	123	0	0	34	0
39	D	149	0	0	35	0
39	E	178	0	0	56	0
39	F	50	0	0	34	0
39	G	46	0	0	17	0
39	H	27	0	0	14	0
39	I	20	0	0	5	0
39	J	75	0	0	34	0
39	K	56	0	0	10	0
39	L	60	0	0	20	0
39	M	90	0	0	27	0
39	N	128	0	0	35	0
39	O	63	0	0	41	0
39	P	45	0	0	21	0
39	Q	62	0	0	11	0
39	R	53	0	0	10	0
39	S	86	0	0	15	0
39	T	36	0	0	6	0
39	U	42	0	0	14	0
39	V	30	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	W	15	0	0	5	1
39	X	73	0	0	20	0
39	Y	30	0	0	11	0
39	Z	99	0	0	19	0
All	All	98616	0	59564	4529	2

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 30.

All (4529) 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:A:871:G:H5'	1:A:871:G:C8	1.74	1.23
30:3:39:ARG:HG2	39:3:3143:HOH:O	1.36	1.22
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.55	1.19
1:A:1702:U:H5"	39:A:6685:HOH:O	1.35	1.19
1:A:871:G:H5'	1:A:871:G:H8	1.02	1.18
14:M:68:GLU:HA	39:M:8419:HOH:O	1.42	1.17
2:B:3023:U:H3'	39:B:8485:HOH:O	1.47	1.14
7:F:25:MET:HE2	7:F:41:LEU:HG	1.23	1.14
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.15	1.13
1:A:711:G:H1'	39:A:6562:HOH:O	1.47	1.12
1:A:1160:G:H5'	1:A:1161:A:H5'	1.14	1.12
15:N:164:THR:HG22	15:N:167:GLY:H	1.04	1.11
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.31	1.10
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.29	1.10
6:E:236:THR:HG22	6:E:239:ALA:H	1.00	1.10
1:A:1835:U:H5	1:A:1840:A:N7	1.50	1.10
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.66	1.09
6:E:180:SER:HB2	39:E:8453:HOH:O	1.51	1.09
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.17	1.08
1:A:542:A:H5'	1:A:542:A:H8	1.17	1.08
1:A:1667:A:H5'	1:A:1667:A:H8	1.18	1.08
16:O:144:GLY:O	16:O:147:ILE:HG22	1.54	1.08
39:A:6918:HOH:O	5:D:211:THR:HG21	1.54	1.07
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.94	1.07
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.27	1.07
5:D:140:LEU:HA	39:D:8584:HOH:O	1.52	1.07
2:B:3006:C:H5"	16:O:37:ARG:HH12	0.98	1.06
1:A:156:C:H5"	15:N:171:ARG:HD3	1.32	1.06
9:H:46:GLU:O	9:H:73:PRO:HD2	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.37	1.05
39:A:9068:HOH:O	5:D:267:LYS:HD3	1.56	1.05
8:G:107:PHE:CE2	8:G:108:LEU:HD13	1.91	1.05
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.57	1.05
15:N:164:THR:HG22	15:N:167:GLY:N	1.72	1.04
28:1:10:ARG:HA	39:1:3188:HOH:O	1.56	1.04
11:J:161:SER:HB3	39:J:8362:HOH:O	1.58	1.03
23:V:14:GLU:OE1	23:V:15:PRO:HD2	1.56	1.03
39:A:4340:HOH:O	15:N:14:ARG:HG2	1.58	1.02
15:N:94:LYS:HE3	39:N:8581:HOH:O	1.59	1.02
19:R:23:THR:HA	39:R:4792:HOH:O	1.57	1.01
1:A:962:C:H1'	16:O:5:ARG:NH1	1.74	1.01
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.24	1.01
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.72	1.01
1:A:1134:G:H4'	11:J:151:MET:HE1	1.42	1.01
1:A:1679:C:H5'	39:A:8833:HOH:O	1.60	1.00
9:H:107:VAL:HG23	39:H:6617:HOH:O	1.60	1.00
2:B:3056:A:H2'	2:B:3057:A:H5"	1.42	1.00
11:J:2:PRO:HB2	39:J:8365:HOH:O	1.59	1.00
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.43	1.00
1:A:856:G:H2'	39:A:4902:HOH:O	1.59	1.00
1:A:1127:C:H2'	1:A:1128:U:H5'	1.43	1.00
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.43	0.99
6:E:76:ARG:HD2	39:E:8441:HOH:O	1.61	0.99
39:A:3217:HOH:O	15:N:157:LEU:HD11	1.62	0.99
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.40	0.99
14:M:67:ARG:O	14:M:71:GLU:HG3	1.61	0.99
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.42	0.98
18:Q:115:SER:H	18:Q:118:GLN:HE21	0.99	0.98
2:B:3107:C:H5	39:B:8439:HOH:O	1.47	0.97
13:L:10:GLN:HE21	13:L:10:GLN:H	1.07	0.97
11:J:142:VAL:HG13	39:J:8380:HOH:O	1.62	0.97
27:Z:185:VAL:HA	39:Z:8565:HOH:O	1.62	0.97
1:A:1482:A:H1'	39:A:8923:HOH:O	1.64	0.97
12:K:131:THR:HG22	12:K:134:GLU:H	1.26	0.97
5:D:190:MET:HE2	5:D:194:PHE:CD1	1.98	0.97
1:A:2830:U:H3'	39:A:4706:HOH:O	1.63	0.97
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.45	0.96
7:F:174:VAL:HG11	39:F:2195:HOH:O	1.65	0.96
14:M:143:THR:HG21	39:M:8412:HOH:O	1.65	0.96
39:A:5133:HOH:O	4:C:192:VAL:HB	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:62:ARG:HA	5:D:65:MET:CE	1.95	0.96
15:N:64:ARG:HD2	39:N:8584:HOH:O	1.63	0.96
11:J:165:GLY:HA3	39:J:8396:HOH:O	1.63	0.96
15:N:35:PRO:CG	15:N:38:VAL:HG23	1.95	0.96
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.28	0.96
5:D:62:ARG:HA	5:D:65:MET:HE2	1.45	0.96
1:A:870:G:H2'	1:A:871:G:H5"	1.47	0.96
39:A:8965:HOH:O	20:S:83:LYS:HD3	1.66	0.96
6:E:61:PHE:HB3	39:E:8452:HOH:O	1.63	0.95
2:B:3035:C:H5"	39:B:8458:HOH:O	1.65	0.95
13:L:10:GLN:H	13:L:10:GLN:NE2	1.65	0.95
31:4:73:GLU:HB3	39:4:8561:HOH:O	1.66	0.95
2:B:3023:U:H4'	2:B:3024:U:OP2	1.67	0.94
1:A:1559:A:H1'	39:A:5341:HOH:O	1.67	0.94
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.29	0.94
11:J:163:PRO:HG2	39:J:8337:HOH:O	1.67	0.94
1:A:2890:A:H1'	23:V:56:ARG:NH2	1.83	0.94
1:A:513:A:N3	39:A:3154:HOH:O	1.99	0.94
1:A:962:C:H1'	16:O:5:ARG:HH12	1.30	0.94
39:A:9845:HOH:O	19:R:16:ASN:HB2	1.66	0.94
1:A:1863:G:H3'	39:A:4662:HOH:O	1.67	0.94
5:D:258:GLY:H	5:D:260:HIS:CE1	1.87	0.93
1:A:31:C:H4'	39:A:6884:HOH:O	1.68	0.93
1:A:2256:G:H2'	1:A:2257:G:H5'	1.50	0.93
1:A:1080:C:H4'	1:A:1081:A:OP1	1.68	0.93
6:E:236:THR:HG22	6:E:239:ALA:N	1.84	0.93
25:X:88:THR:HB	39:X:6679:HOH:O	1.68	0.93
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.51	0.93
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.50	0.93
18:Q:143:ALA:HA	39:Q:5521:HOH:O	1.67	0.93
31:4:60:LYS:HG3	31:4:61:PRO:HD2	1.48	0.93
31:4:56:PRO:HA	39:4:8549:HOH:O	1.67	0.92
1:A:2004:U:H4'	39:A:4781:HOH:O	1.69	0.92
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.33	0.92
20:S:9:ASP:O	20:S:13:THR:HB	1.69	0.92
8:G:97:VAL:HG12	39:G:4191:HOH:O	1.68	0.92
9:H:91:VAL:HG12	9:H:92:GLY:H	1.32	0.92
25:X:154:ARG:C	39:X:4276:HOH:O	2.08	0.92
1:A:1116:U:O2'	1:A:1118:A:H2	1.52	0.92
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.50	0.92
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.09	0.91
1:A:1667:A:H5'	1:A:1667:A:C8	2.05	0.91
2:B:3107:C:C5	39:B:8439:HOH:O	2.22	0.91
11:J:59:ASN:H	11:J:59:ASN:HD22	0.98	0.91
2:B:3006:C:C5'	16:O:37:ARG:HH12	1.81	0.91
11:J:141:ASN:HA	39:J:8366:HOH:O	1.69	0.91
16:O:89:GLY:O	16:O:92:ALA:HB3	1.70	0.91
1:A:1118:A:H62	1:A:1244:U:H3	1.16	0.90
15:N:30:GLU:O	15:N:34:GLU:HG3	1.71	0.90
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.51	0.90
6:E:236:THR:HG21	39:E:8378:HOH:O	1.70	0.90
1:A:542:A:H5'	1:A:542:A:C8	2.07	0.89
15:N:60:ILE:C	15:N:61:ILE:HD12	1.91	0.89
1:A:21:G:H5'	20:S:2:ILE:HA	1.54	0.89
8:G:37:ASP:OD1	12:K:125:SER:HB3	1.71	0.89
1:A:871:G:H8	1:A:871:G:C5'	1.83	0.89
4:C:161:GLY:O	28:1:68:CYS:SG	2.31	0.89
11:J:162:SER:HB2	11:J:163:PRO:CD	2.03	0.89
29:2:25:LYS:HG2	29:2:25:LYS:O	1.73	0.89
24:W:1:THR:HG23	24:W:2:VAL:H	1.36	0.89
7:F:154:LYS:H	7:F:154:LYS:HD2	1.38	0.89
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.38	0.89
5:D:321:PRO:HA	39:D:8660:HOH:O	1.71	0.88
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.85	0.88
5:D:152:PRO:HD2	39:D:8633:HOH:O	1.71	0.88
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.56	0.88
23:V:4:ARG:N	39:V:5334:HOH:O	2.06	0.88
14:M:133:VAL:HA	39:M:8452:HOH:O	1.74	0.88
1:A:645:U:OP2	14:M:4:LYS:HE2	1.74	0.87
1:A:383:A:H4'	39:A:4802:HOH:O	1.74	0.87
15:N:139:PRO:O	15:N:140:ALA:HB3	1.72	0.87
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.56	0.87
1:A:1256:C:OP2	39:A:6621:HOH:O	1.91	0.87
11:J:139:ASP:N	11:J:140:PRO:HD3	1.89	0.87
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.55	0.87
1:A:346:U:H4'	39:A:6305:HOH:O	1.72	0.87
2:B:3056:A:C2'	2:B:3057:A:H5"	2.04	0.87
1:A:1213:C:O2'	1:A:1214:G:H5'	1.75	0.87
1:A:559:U:H6	1:A:559:U:H5'	1.40	0.86
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.08	0.86
1:A:1333:U:H2'	1:A:1334:C:H6	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:12:ILE:HB	39:I:4714:HOH:O	1.74	0.86
15:N:60:ILE:O	15:N:61:ILE:HD12	1.75	0.86
1:A:1474:C:H6	1:A:1474:C:H5'	1.39	0.86
15:N:52:LEU:HD11	39:N:8613:HOH:O	1.74	0.86
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.74	0.86
1:A:31:C:H2'	39:A:7150:HOH:O	1.75	0.86
14:M:42:ASN:HB2	39:M:8424:HOH:O	1.72	0.86
20:S:99:ALA:HB1	20:S:109:MET:CE	2.04	0.86
1:A:1160:G:C5'	1:A:1161:A:H5'	2.04	0.86
1:A:1751:G:H2'	1:A:1752:G:H5"	1.58	0.86
1:A:1835:U:C5	1:A:1840:A:N7	2.41	0.86
5:D:238:ASN:HD22	5:D:240:GLY:H	1.19	0.86
25:X:88:THR:HG22	25:X:89:ASP:H	1.39	0.86
1:A:289:G:H22	1:A:363:A:H2	1.24	0.86
7:F:19:GLU:HG3	39:F:6165:HOH:O	1.76	0.86
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.74	0.86
11:J:26:LYS:HG2	11:J:28:ILE:H	1.40	0.85
15:N:80:GLY:O	15:N:81:ARG:HD3	1.75	0.85
27:Z:186:ARG:HG2	27:Z:186:ARG:HH11	1.40	0.85
8:G:100:ASP:HB2	39:G:2789:HOH:O	1.74	0.85
1:A:1160:G:H5'	1:A:1161:A:C5'	2.04	0.85
1:A:1328:A:OP1	27:Z:169:ARG:HD2	1.76	0.85
1:A:1594:C:OP2	18:Q:120:ARG:HD2	1.77	0.85
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.40	0.85
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.59	0.85
1:A:1634:G:OP2	39:A:5594:HOH:O	1.93	0.85
1:A:2346:C:O2'	7:F:52:THR:HG21	1.77	0.85
1:A:21:G:C5'	20:S:2:ILE:HA	2.05	0.85
1:A:1701:A:H5'	39:A:5748:HOH:O	1.75	0.85
7:F:20:LYS:HA	7:F:75:LEU:O	1.76	0.85
6:E:132:ASP:HB3	39:E:8369:HOH:O	1.76	0.85
16:O:4:PRO:HD2	39:O:8555:HOH:O	1.76	0.85
1:A:2256:G:C2'	1:A:2257:G:H5'	2.07	0.84
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.58	0.84
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.57	0.84
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.58	0.84
1:A:544:G:H2'	1:A:545:G:H5"	1.57	0.84
1:A:1168:C:O2'	39:A:5829:HOH:O	1.93	0.84
9:H:91:VAL:HG12	9:H:92:GLY:N	1.92	0.84
9:H:100:ASP:HB3	39:H:5691:HOH:O	1.77	0.84
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:C:H4'	39:T:8322:HOH:O	1.76	0.84
1:A:2469:A:OP2	39:A:6936:HOH:O	1.94	0.84
11:J:27:LYS:H	11:J:58:HIS:HD2	1.25	0.84
17:P:22:GLY:O	39:P:2823:HOH:O	1.95	0.84
1:A:1936:C:H3'	39:A:6643:HOH:O	1.78	0.84
1:A:2812:A:H2	1:A:2814:A:H62	1.22	0.84
4:C:228:ILE:HG13	39:C:8518:HOH:O	1.78	0.84
16:O:181:ASP:HA	39:O:8567:HOH:O	1.78	0.84
29:2:29:THR:O	29:2:32:LYS:HE2	1.78	0.84
1:A:1242:A:H5'	12:K:82:THR:HG23	1.60	0.84
16:O:113:SER:HB2	39:O:8556:HOH:O	1.78	0.84
6:E:236:THR:CG2	6:E:239:ALA:H	1.89	0.83
15:N:164:THR:CG2	15:N:167:GLY:H	1.90	0.83
1:A:1119:G:H22	1:A:1246:A:H2	1.25	0.83
10:I:23:ILE:CD1	10:I:67:LEU:HD23	2.07	0.83
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.26	0.83
1:A:214:U:H5'	39:A:5610:HOH:O	1.77	0.83
1:A:1191:A:H3'	1:A:1192:A:H5"	1.59	0.83
16:O:169:PRO:O	16:O:172:PHE:HB3	1.78	0.83
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.42	0.83
1:A:1702:U:H5'	39:A:9920:HOH:O	1.78	0.83
12:K:74:ARG:HD3	39:K:5061:HOH:O	1.77	0.83
1:A:57:C:H5"	39:A:6221:HOH:O	1.79	0.83
16:O:7:LYS:HE3	19:R:21:ARG:O	1.78	0.83
1:A:1151:G:H5"	39:A:4487:HOH:O	1.78	0.83
1:A:2506:A:H1'	39:A:3241:HOH:O	1.78	0.83
1:A:2508:C:H2'	39:A:6216:HOH:O	1.77	0.83
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.61	0.83
4:C:101:GLU:OE2	4:C:131:HIS:HB2	1.79	0.83
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.61	0.83
1:A:1666:C:O2'	1:A:1667:A:H5"	1.78	0.82
6:E:214:THR:HG21	39:E:8409:HOH:O	1.79	0.82
25:X:129:LYS:HG2	39:X:1990:HOH:O	1.79	0.82
2:B:3025:G:H3'	2:B:3026:C:H5'	1.60	0.82
1:A:157:G:H4'	15:N:95:LYS:HE3	1.61	0.82
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.61	0.82
1:A:2717:C:H2'	1:A:2718:C:H5"	1.61	0.82
1:A:2815:G:H2'	39:A:5194:HOH:O	1.79	0.82
2:B:3076:G:H3'	2:B:3077:A:H5"	1.59	0.82
13:L:81:ARG:HB2	13:L:87:ARG:NH1	1.93	0.82
1:A:2036:C:OP1	39:A:6165:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:190:MET:HE2	5:D:194:PHE:HD1	1.43	0.82
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.06	0.82
27:Z:187:VAL:HB	39:Z:8572:HOH:O	1.79	0.82
8:G:7:ILE:HD11	8:G:11:VAL:C	2.00	0.82
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.09	0.82
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.61	0.82
1:A:541:C:H2'	1:A:542:A:H5"	1.60	0.82
6:E:107:ARG:NH1	6:E:107:ARG:HB3	1.95	0.82
11:J:59:ASN:HD22	11:J:59:ASN:N	1.74	0.82
1:A:870:G:C2'	1:A:871:G:H5"	2.10	0.81
24:W:12:THR:HG22	24:W:15:GLU:CG	2.04	0.81
1:A:639:A:H2'	1:A:640:G:C8	2.15	0.81
1:A:733:U:H5"	39:A:9352:HOH:O	1.78	0.81
1:A:871:G:C8	1:A:871:G:C5'	2.59	0.81
1:A:1333:U:H2'	1:A:1334:C:C6	2.15	0.81
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.10	0.81
23:V:14:GLU:OE1	23:V:15:PRO:CD	2.28	0.81
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.46	0.81
5:D:297:VAL:HB	39:D:8608:HOH:O	1.80	0.81
15:N:139:PRO:O	15:N:140:ALA:CB	2.28	0.81
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.45	0.81
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.61	0.81
11:J:140:PRO:HB3	39:J:8380:HOH:O	1.80	0.81
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.63	0.81
1:A:960:G:H4'	39:A:6891:HOH:O	1.79	0.81
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.61	0.81
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.63	0.81
11:J:59:ASN:H	11:J:59:ASN:ND2	1.77	0.81
24:W:49:LEU:O	24:W:53:ILE:HG13	1.81	0.81
20:S:150:PRO:O	39:S:8527:HOH:O	1.99	0.81
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.45	0.81
5:D:36:PRO:HA	5:D:168:GLY:CA	2.10	0.80
29:2:10:LYS:HG3	39:2:2979:HOH:O	1.82	0.80
17:P:26:TRP:HB2	39:P:3062:HOH:O	1.81	0.80
1:A:1692:C:H1'	39:A:8969:HOH:O	1.80	0.80
1:A:2054:A:N3	20:S:128:ARG:NH2	2.29	0.80
15:N:154:ARG:O	39:N:8552:HOH:O	2.00	0.80
20:S:34:GLU:HG2	20:S:46:TYR:OH	1.79	0.80
1:A:564:G:H1'	39:A:5774:HOH:O	1.81	0.80
6:E:139:VAL:HG13	39:E:8456:HOH:O	1.79	0.80
26:Y:41:PHE:O	26:Y:43:VAL:HG23	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.82	0.80
8:G:166:VAL:HG12	39:G:3134:HOH:O	1.81	0.80
1:A:92:G:H5'	39:W:7247:HOH:O	1.81	0.80
1:A:447:A:OP1	22:U:2:LYS:HG2	1.82	0.80
1:A:553:G:P	27:Z:204:ARG:HH22	2.04	0.80
1:A:1159:G:P	39:A:3774:HOH:O	2.40	0.80
5:D:238:ASN:ND2	5:D:240:GLY:H	1.80	0.80
1:A:1116:U:H3	1:A:1246:A:H62	1.29	0.80
1:A:1151:G:P	10:I:16:LYS:HZ3	2.03	0.80
4:C:177:HIS:HE1	39:C:8618:HOH:O	1.63	0.80
1:A:2064:U:H5'	1:A:2652:U:O3'	1.82	0.79
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.47	0.79
24:W:16:ARG:NH2	24:W:63:GLU:HG3	1.97	0.79
1:A:2426:G:H1'	39:A:5562:HOH:O	1.81	0.79
1:A:1615:A:H4'	39:A:5362:HOH:O	1.81	0.79
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.64	0.79
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.16	0.79
25:X:122:ARG:NH2	25:X:154:ARG:HD2	1.97	0.79
1:A:2073:G:OP1	39:A:4224:HOH:O	2.00	0.79
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.64	0.79
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.83	0.79
12:K:76:ASP:HA	39:K:5907:HOH:O	1.83	0.79
1:A:545:G:H5'	1:A:545:G:H8	1.44	0.79
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.97	0.79
27:Z:142:SER:OG	39:Z:8613:HOH:O	2.00	0.79
1:A:2590:U:O4	39:A:5097:HOH:O	2.01	0.79
7:F:27:ILE:HG22	7:F:28:GLY:H	1.47	0.79
1:A:1120:U:H6	1:A:1120:U:H5"	1.47	0.79
6:E:246:ARG:HB3	6:E:246:ARG:NH1	1.97	0.79
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.12	0.79
28:1:58:GLY:HA3	39:1:7239:HOH:O	1.83	0.79
1:A:1735:C:O2'	1:A:1736:A:H5'	1.82	0.79
1:A:2612:A:H4'	39:A:3175:HOH:O	1.83	0.79
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.63	0.79
11:J:65:ARG:NH1	39:J:8384:HOH:O	2.14	0.79
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.47	0.79
15:N:172:GLY:O	15:N:183:VAL:HG11	1.82	0.79
1:A:1166:A:H1'	1:A:1192:A:C2	2.18	0.78
1:A:1470:A:OP1	15:N:93:ARG:HD2	1.83	0.78
2:B:3025:G:H3'	2:B:3026:C:C5'	2.13	0.78
2:B:3014:G:H5'	2:B:3014:G:H8	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3028:U:H2'	2:B:3029:C:C6	2.17	0.78
1:A:316:A:H5'	22:U:54:ASP:OD2	1.84	0.78
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.65	0.78
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.47	0.78
1:A:428:G:OP1	39:A:5688:HOH:O	2.01	0.78
8:G:132:THR:HB	39:G:2227:HOH:O	1.83	0.78
10:I:64:ASN:HD22	10:I:64:ASN:N	1.80	0.78
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.13	0.78
1:A:1187:U:H3'	39:A:6358:HOH:O	1.84	0.78
1:A:1401:G:O6	39:A:5896:HOH:O	2.01	0.78
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.47	0.78
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.64	0.78
12:K:59:LYS:O	12:K:63:ILE:HG13	1.83	0.78
1:A:790:A:H1'	1:A:1710:A:H2'	1.64	0.78
1:A:1202:A:N7	39:A:5699:HOH:O	2.16	0.78
1:A:2322:U:O3'	39:A:6484:HOH:O	2.00	0.78
1:A:2659:U:H3'	39:A:3878:HOH:O	1.83	0.78
5:D:43:GLY:O	5:D:308:LEU:HD12	1.82	0.78
1:A:1187:U:H2'	39:A:6358:HOH:O	1.83	0.78
1:A:1353:C:P	39:A:4154:HOH:O	2.42	0.78
39:A:3942:HOH:O	15:N:146:GLN:HG2	1.83	0.78
39:A:5973:HOH:O	30:3:1:GLY:HA3	1.84	0.78
1:A:2121:G:OP2	39:A:3005:HOH:O	2.02	0.78
39:A:6921:HOH:O	6:E:188:ARG:HD2	1.83	0.78
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.19	0.78
12:K:16:ASP:OD1	39:K:2858:HOH:O	2.01	0.78
17:P:87:THR:O	17:P:91:GLN:HG3	1.85	0.78
1:A:2256:G:H2'	1:A:2257:G:C5'	2.13	0.77
10:I:63:ARG:N	39:I:2569:HOH:O	2.15	0.77
18:Q:143:ALA:CA	39:Q:5521:HOH:O	2.28	0.77
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.18	0.77
14:M:26:HIS:HB2	39:M:8383:HOH:O	1.83	0.77
31:4:87:ARG:HG3	39:4:8573:HOH:O	1.82	0.77
1:A:639:A:H2'	1:A:640:G:H8	1.48	0.77
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.84	0.77
39:A:4699:HOH:O	13:L:39:GLY:HA2	1.84	0.77
4:C:140:LEU:HB3	4:C:141:PRO:HD2	1.67	0.77
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.66	0.77
27:Z:220:GLU:HG2	39:Z:8548:HOH:O	1.83	0.77
1:A:1118:A:H8	1:A:1118:A:H3'	1.49	0.77
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:G:N3	39:A:8644:HOH:O	2.17	0.77
1:A:1119:G:N2	1:A:1246:A:C2	2.53	0.77
1:A:2660:G:OP2	39:A:3878:HOH:O	2.01	0.77
39:A:6921:HOH:O	6:E:188:ARG:CD	2.33	0.77
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.66	0.77
1:A:1160:G:N3	39:A:5110:HOH:O	2.18	0.77
1:A:1204:C:O2	39:A:4219:HOH:O	1.99	0.77
15:N:169:ARG:HD2	39:N:8587:HOH:O	1.84	0.77
2:B:3024:U:C6	39:B:8490:HOH:O	2.36	0.77
1:A:1377:C:H6	1:A:1377:C:H5'	1.50	0.77
1:A:2261:C:O2	39:A:4457:HOH:O	2.02	0.77
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.67	0.77
18:Q:16:VAL:HG12	18:Q:17:GLY:N	1.99	0.77
1:A:2435:U:H1'	39:A:4905:HOH:O	1.85	0.77
4:C:173:GLY:O	4:C:176:HIS:HB3	1.84	0.77
12:K:107:ASN:ND2	12:K:109:TYR:H	1.82	0.77
17:P:32:ARG:HB2	39:P:4656:HOH:O	1.83	0.77
17:P:37:ARG:HG3	39:P:3002:HOH:O	1.84	0.77
1:A:272:A:H5'	1:A:273:G:OP2	1.84	0.76
19:R:93:ARG:HH11	19:R:93:ARG:HG3	1.51	0.76
39:A:5265:HOH:O	15:N:170:CYS:SG	2.43	0.76
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.50	0.76
1:A:236:A:H4'	1:A:237:G:H5'	1.68	0.76
1:A:1603:A:H5'	1:A:1605:G:O4'	1.86	0.76
4:C:35:GLY:O	4:C:36:ASP:HB3	1.84	0.76
11:J:137:ASN:O	11:J:139:ASP:N	2.19	0.76
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.48	0.76
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.20	0.76
6:E:111:VAL:HB	39:E:8324:HOH:O	1.84	0.76
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.84	0.76
1:A:1441:G:O2'	1:A:1442:A:H5'	1.84	0.76
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.21	0.76
2:B:3064:C:C2'	2:B:3065:A:H5'	2.15	0.76
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.68	0.76
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.00	0.76
31:4:70:ARG:HD3	39:4:8539:HOH:O	1.84	0.76
1:A:284:C:H4'	1:A:285:A:O5'	1.85	0.76
6:E:237:GLU:HB2	39:E:8438:HOH:O	1.86	0.76
13:L:72:VAL:O	13:L:95:ALA:HB1	1.85	0.76
14:M:148:GLU:HA	39:M:8451:HOH:O	1.84	0.76
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:25:LYS:HE2	39:2:7213:HOH:O	1.85	0.76
5:D:162:MET:CE	5:D:308:LEU:HD21	2.14	0.76
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.67	0.76
11:J:150:LYS:HE2	39:J:8382:HOH:O	1.84	0.76
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.80	0.76
20:S:111:ILE:O	20:S:111:ILE:HG22	1.82	0.76
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.31	0.76
1:A:1118:A:H3'	1:A:1118:A:C8	2.20	0.75
1:A:2813:A:OP2	39:A:3765:HOH:O	2.02	0.75
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.81	0.75
22:U:25:ALA:O	22:U:39:ASN:HB2	1.86	0.75
25:X:13:MET:CE	25:X:17:ILE:HG22	2.16	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
1:A:2533:C:H6	1:A:2533:C:H5'	1.51	0.75
29:2:31:LYS:O	29:2:33:VAL:HG23	1.85	0.75
1:A:693:A:H5"	35:A:8510:CL:CL	2.22	0.75
1:A:1080:C:O2	39:A:6081:HOH:O	2.05	0.75
1:A:2039:A:OP1	39:A:4553:HOH:O	2.05	0.75
1:A:2120:U:H3'	39:A:3005:HOH:O	1.86	0.75
12:K:19:MET:HE1	12:K:79:PHE:HA	1.68	0.75
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.69	0.75
6:E:1:MET:HG2	6:E:2:GLN:H	1.50	0.75
15:N:57:LYS:HB3	15:N:60:ILE:HD12	1.67	0.75
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.86	0.75
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.68	0.75
16:O:33:ARG:NH1	16:O:103:ASP:OD2	2.18	0.75
27:Z:115:ARG:NE	39:Z:8556:HOH:O	2.19	0.75
1:A:1564:C:H4'	39:A:6296:HOH:O	1.84	0.75
1:A:2768:A:H2'	1:A:2769:C:O4'	1.86	0.75
6:E:246:ARG:HB3	6:E:246:ARG:HH11	1.51	0.75
6:E:67:GLN:OE1	39:E:8432:HOH:O	2.05	0.75
7:F:19:GLU:O	7:F:20:LYS:HG2	1.87	0.75
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.67	0.75
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.17	0.75
1:A:2586:U:H3	1:A:2592:G:H22	1.34	0.75
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.69	0.75
5:D:175:LEU:HD23	5:D:175:LEU:C	2.07	0.75
1:A:1919:A:H4'	39:A:4327:HOH:O	1.87	0.74
1:A:603:A:H5"	1:A:604:G:OP1	1.87	0.74
5:D:85:ARG:NH1	39:D:8636:HOH:O	2.19	0.74
12:K:74:ARG:O	12:K:78:ILE:HG12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:94:LYS:CE	39:N:8581:HOH:O	2.27	0.74
27:Z:154:ARG:O	27:Z:154:ARG:HG2	1.87	0.74
1:A:1666:C:H2'	1:A:1667:A:H5'	1.69	0.74
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.20	0.74
6:E:78:ARG:HH11	6:E:78:ARG:CG	1.97	0.74
1:A:1164:U:H3	1:A:1192:A:H2	1.34	0.74
1:A:1450:C:H4'	1:A:1451:C:OP2	1.88	0.74
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.17	0.74
29:2:46:ARG:HB2	39:2:6935:HOH:O	1.86	0.74
1:A:2912:C:OP2	39:A:5028:HOH:O	2.05	0.74
12:K:70:PHE:O	39:K:6807:HOH:O	2.06	0.74
1:A:514:G:H8	1:A:514:G:O5'	1.69	0.74
14:M:77:ALA:HB3	39:M:8405:HOH:O	1.88	0.74
23:V:39:ASN:ND2	23:V:44:ARG:HH11	1.86	0.74
31:4:60:LYS:CG	31:4:61:PRO:HD2	2.17	0.74
31:4:75:GLY:HA2	39:4:8560:HOH:O	1.87	0.74
7:F:128:LEU:N	39:F:5495:HOH:O	2.20	0.74
1:A:821:U:O2'	1:A:822:C:H5'	1.88	0.74
10:I:73:ASP:C	39:I:2994:HOH:O	2.25	0.74
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.68	0.74
31:4:56:PRO:CA	39:4:8549:HOH:O	2.32	0.74
7:F:135:VAL:HG22	7:F:136:ARG:H	1.53	0.74
20:S:92:LEU:HD23	20:S:145:LEU:HD21	1.69	0.74
26:Y:73:ARG:O	26:Y:85:VAL:HG13	1.88	0.74
1:A:1909:A:H2'	1:A:1910:A:C8	2.23	0.73
12:K:52:GLN:HG3	12:K:53:ILE:N	2.02	0.73
16:O:171:HIS:CE1	39:O:8562:HOH:O	2.41	0.73
1:A:1936:C:O5'	39:A:6643:HOH:O	2.06	0.73
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.19	0.73
24:W:56:ILE:O	24:W:60:GLN:HG3	1.87	0.73
1:A:182:G:H5'	39:A:4633:HOH:O	1.86	0.73
1:A:1625:U:H4'	39:A:4142:HOH:O	1.88	0.73
1:A:2546:U:OP1	39:A:3338:HOH:O	2.05	0.73
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.69	0.73
15:N:67:ILE:HG21	15:N:97:ILE:HG23	1.69	0.73
16:O:181:ASP:CA	39:O:8567:HOH:O	2.35	0.73
21:T:51:GLN:NE2	21:T:53:ASN:HD21	1.86	0.73
25:X:88:THR:HG22	25:X:89:ASP:N	2.03	0.73
1:A:501:G:OP2	39:A:4492:HOH:O	2.06	0.73
1:A:1209:C:O2	1:A:1210:G:C8	2.41	0.73
1:A:2265:U:H2'	1:A:2266:A:C8	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:27:ARG:HD2	39:L:4747:HOH:O	1.86	0.73
14:M:134:GLU:HA	14:M:138:GLY:O	1.88	0.73
1:A:415:A:O2'	39:A:3791:HOH:O	2.07	0.73
1:A:1474:C:H5'	1:A:1474:C:C6	2.21	0.73
15:N:59:GLY:HA3	15:N:141:ILE:HD12	1.69	0.73
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.04	0.73
27:Z:151:SER:HB3	27:Z:154:ARG:HB3	1.70	0.73
1:A:1167:G:O2'	39:A:6872:HOH:O	2.06	0.73
2:B:3002:U:OP2	2:B:3002:U:H4'	1.89	0.73
7:F:136:ARG:HD2	7:F:155:HIS:O	1.88	0.73
2:B:3010:C:OP2	39:B:8521:HOH:O	2.07	0.73
1:A:1589:G:N2	1:A:1605:G:H1'	2.03	0.73
6:E:235:PHE:CE2	6:E:243:VAL:HG21	2.21	0.73
1:A:745:G:H4'	39:A:4625:HOH:O	1.88	0.73
1:A:2089:A:OP1	39:A:6535:HOH:O	2.07	0.73
7:F:105:SER:HB2	7:F:131:THR:HG23	1.69	0.73
11:J:41:THR:HA	39:J:8393:HOH:O	1.88	0.73
15:N:46:LEU:CD2	15:N:50:ARG:HG3	2.18	0.73
15:N:164:THR:HG23	15:N:165:SER:N	2.02	0.73
23:V:37:GLU:O	23:V:40:ALA:HB3	1.87	0.73
27:Z:141:THR:HG23	39:Z:8590:HOH:O	1.89	0.73
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.70	0.73
21:T:51:GLN:HE21	21:T:53:ASN:ND2	1.87	0.73
1:A:1221:G:N7	39:A:5461:HOH:O	2.22	0.72
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.24	0.72
22:U:71:VAL:HG13	22:U:91:LEU:O	1.89	0.72
1:A:2251:G:H4'	39:A:6868:HOH:O	1.90	0.72
5:D:175:LEU:HD23	5:D:175:LEU:O	1.89	0.72
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.70	0.72
7:F:101:THR:HG22	39:F:7400:HOH:O	1.88	0.72
1:A:1120:U:H5"	1:A:1120:U:C6	2.24	0.72
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.72
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.71	0.72
1:A:584:U:H3'	39:A:5565:HOH:O	1.89	0.72
1:A:1321:A:N3	39:A:9721:HOH:O	2.22	0.72
27:Z:235:GLU:H	27:Z:235:GLU:CD	1.92	0.72
1:A:349:U:O2'	1:A:350:C:H5'	1.90	0.72
1:A:485:A:O2'	1:A:487:G:H5'	1.90	0.72
1:A:557:C:H1'	39:A:5139:HOH:O	1.90	0.72
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.71	0.72
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:C:O2'	1:A:283:U:H5'	1.90	0.72
1:A:960:G:H2'	1:A:960:G:N3	2.04	0.72
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.70	0.72
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.70	0.72
14:M:73:VAL:HG21	14:M:116:HIS:CD2	2.23	0.72
1:A:1589:G:H22	1:A:1605:G:H1'	1.54	0.72
1:A:2783:A:O5'	39:A:4710:HOH:O	2.07	0.72
5:D:146:THR:O	5:D:148:PRO:HD3	1.90	0.72
8:G:11:VAL:HG12	8:G:12:ASP:N	2.04	0.72
1:A:2346:C:O5'	1:A:2346:C:H6	1.73	0.72
1:A:2506:A:O2'	1:A:2507:G:H8	1.73	0.72
2:B:3064:C:H2'	2:B:3065:A:H5'	1.70	0.72
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.72
1:A:777:U:OP1	39:A:6961:HOH:O	2.08	0.71
1:A:2831:C:H2'	1:A:2832:C:H5'	1.72	0.71
39:A:7044:HOH:O	28:1:31:ILE:HG13	1.90	0.71
6:E:69:HIS:O	39:E:8313:HOH:O	2.07	0.71
9:H:99:THR:HA	39:H:3461:HOH:O	1.90	0.71
13:L:55:VAL:HG12	13:L:56:SER:H	1.55	0.71
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.05	0.71
20:S:132:ARG:NH1	39:S:8587:HOH:O	2.23	0.71
28:1:59:HIS:HA	39:1:7607:HOH:O	1.87	0.71
1:A:240:C:C5'	15:N:146:GLN:NE2	2.54	0.71
1:A:1308:A:H5'	39:A:6398:HOH:O	1.90	0.71
1:A:1629:G:N2	1:A:1632:A:OP2	2.23	0.71
4:C:199:HIS:CD2	4:C:201:PHE:H	2.09	0.71
7:F:99:ASP:CB	7:F:103:ASN:H	2.03	0.71
11:J:140:PRO:O	39:J:8366:HOH:O	2.07	0.71
1:A:1116:U:H1'	39:A:4006:HOH:O	1.89	0.71
39:A:3276:HOH:O	15:N:189:VAL:HG21	1.90	0.71
5:D:179:LEU:O	5:D:183:GLU:HG2	1.88	0.71
16:O:82:TYR:C	16:O:82:TYR:CD2	2.64	0.71
1:A:1634:G:H3'	39:A:3385:HOH:O	1.91	0.71
5:D:238:ASN:HD22	5:D:240:GLY:N	1.87	0.71
6:E:25:PRO:HD2	39:E:8436:HOH:O	1.91	0.71
20:S:132:ARG:CZ	39:S:8587:HOH:O	2.37	0.71
1:A:1127:C:C2'	1:A:1128:U:H5'	2.18	0.71
1:A:1901:G:O2'	1:A:1902:G:H5'	1.91	0.71
1:A:2605:G:N7	39:A:6957:HOH:O	2.22	0.71
7:F:146:LYS:HZ3	16:O:107:ASN:HD21	1.39	0.71
17:P:73:ASP:HA	17:P:92:VAL:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:U:H5"	1:A:1044:C:N4	2.05	0.71
1:A:1778:A:H2'	1:A:1779:A:H5'	1.72	0.71
1:A:2359:G:O5'	39:A:5169:HOH:O	2.08	0.71
23:V:14:GLU:O	23:V:17:THR:HB	1.91	0.71
28:1:58:GLY:CA	39:1:7239:HOH:O	2.38	0.71
1:A:1170:U:O2'	1:A:1172:G:N7	2.21	0.71
1:A:2760:C:H5"	39:A:4801:HOH:O	1.91	0.71
5:D:75:GLU:C	5:D:77:PRO:HD3	2.11	0.71
6:E:140:VAL:O	39:E:8459:HOH:O	2.08	0.71
20:S:44:VAL:O	20:S:48:GLU:HG3	1.91	0.71
1:A:204:A:H2'	1:A:205:U:H5'	1.73	0.71
1:A:2729:C:H2'	1:A:2730:G:H8	1.53	0.71
7:F:25:MET:CE	7:F:41:LEU:HG	2.14	0.71
13:L:55:VAL:HG12	13:L:56:SER:N	2.05	0.71
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.05	0.71
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.71	0.71
1:A:1165:G:O2'	1:A:1166:A:OP1	2.07	0.71
1:A:1909:A:N1	1:A:2128:G:H1'	2.05	0.71
1:A:2401:A:H5'	39:A:8998:HOH:O	1.91	0.71
4:C:121:ALA:O	4:C:124:VAL:HG22	1.91	0.71
11:J:139:ASP:H	11:J:140:PRO:HD3	1.55	0.71
16:O:92:ALA:O	16:O:95:ALA:HB3	1.90	0.71
1:A:306:A:P	22:U:38:ARG:HH21	2.14	0.70
1:A:308:U:OP2	39:A:6151:HOH:O	2.09	0.70
39:A:6694:HOH:O	15:N:13:LYS:HE2	1.91	0.70
13:L:87:ARG:CZ	39:L:4854:HOH:O	2.38	0.70
4:C:223:ARG:HG3	39:C:8604:HOH:O	1.90	0.70
5:D:82:VAL:O	5:D:83:ALA:HB2	1.90	0.70
1:A:21:G:H5"	20:S:1:GLY:O	1.92	0.70
1:A:516:A:OP2	39:A:5123:HOH:O	2.08	0.70
1:A:1751:G:C2'	1:A:1752:G:H5"	2.20	0.70
1:A:1834:C:H2'	1:A:1840:A:N6	2.06	0.70
13:L:20:CYS:HB3	13:L:26:ALA:O	1.91	0.70
8:G:157:LYS:NZ	39:G:2401:HOH:O	2.23	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.74	0.70
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.72	0.70
1:A:283:U:H5	1:A:284:C:N4	1.89	0.70
1:A:1494:A:N3	39:A:8747:HOH:O	2.24	0.70
1:A:2064:U:H4'	1:A:2653:A:OP1	1.91	0.70
1:A:2851:G:O2'	1:A:2852:A:H5'	1.92	0.70
14:M:148:GLU:HG3	39:M:8429:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:U:C5	39:A:3497:HOH:O	2.44	0.70
1:A:193:A:H3'	39:A:8839:HOH:O	1.92	0.70
1:A:2638:G:H1'	39:A:7219:HOH:O	1.90	0.70
14:M:79:ASP:HB3	39:M:8437:HOH:O	1.89	0.70
24:W:12:THR:O	24:W:15:GLU:N	2.23	0.70
39:A:9783:HOH:O	13:L:9:THR:HA	1.92	0.70
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.72	0.70
7:F:135:VAL:HG22	7:F:136:ARG:N	2.07	0.70
16:O:141:ARG:N	39:O:8565:HOH:O	2.24	0.70
17:P:115:ARG:NH1	39:P:6194:HOH:O	2.25	0.70
28:1:28:ASP:O	28:1:31:ILE:HG22	1.90	0.70
1:A:2400:G:O2'	39:A:4620:HOH:O	2.10	0.70
2:B:3014:G:H5'	2:B:3014:G:C8	2.26	0.70
6:E:7:ASP:OD1	6:E:11:ASN:O	2.09	0.70
27:Z:216:ARG:HD3	39:Z:8571:HOH:O	1.90	0.70
1:A:2594:C:O2'	1:A:2595:U:H5'	1.92	0.70
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.40	0.70
1:A:541:C:C2'	1:A:542:A:H5"	2.22	0.70
9:H:46:GLU:N	39:H:3461:HOH:O	2.24	0.70
14:M:42:ASN:O	39:M:8454:HOH:O	2.10	0.70
31:4:62:THR:HB	39:4:8550:HOH:O	1.92	0.70
1:A:430:A:H4'	39:A:9525:HOH:O	1.91	0.69
1:A:1184:C:C6	39:A:5710:HOH:O	2.44	0.69
1:A:1209:C:C2	1:A:1210:G:C8	2.80	0.69
39:A:9129:HOH:O	9:H:38:LYS:HD2	1.91	0.69
6:E:238:SER:O	39:E:8386:HOH:O	2.10	0.69
13:L:45:PRO:HB2	39:L:7169:HOH:O	1.92	0.69
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.90	0.69
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.57	0.69
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.27	0.69
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.21	0.69
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.22	0.69
1:A:78:G:C6	1:A:79:G:C6	2.80	0.69
1:A:401:C:H5'	39:A:5265:HOH:O	1.91	0.69
11:J:57:ARG:O	11:J:61:LEU:HD22	1.91	0.69
21:T:57:THR:HG22	21:T:59:ASP:H	1.58	0.69
1:A:411:A:O2'	39:A:6772:HOH:O	2.09	0.69
1:A:2243:C:O5'	39:A:3245:HOH:O	2.10	0.69
39:A:4994:HOH:O	5:D:298:LYS:HD3	1.93	0.69
6:E:16:VAL:HG12	6:E:17:ASP:N	2.08	0.69
6:E:236:THR:HA	39:E:8459:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:23:ASN:OD1	39:L:5264:HOH:O	2.10	0.69
16:O:164:ASP:CG	16:O:167:ASP:HA	2.12	0.69
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.74	0.69
31:4:87:ARG:HD2	39:4:8523:HOH:O	1.92	0.69
2:B:3026:C:H1'	39:B:8421:HOH:O	1.91	0.69
22:U:25:ALA:O	22:U:39:ASN:CB	2.40	0.69
1:A:710:G:OP1	17:P:24:ALA:HB3	1.92	0.69
1:A:1653:A:N7	39:A:6411:HOH:O	2.25	0.69
1:A:1810:C:OP1	23:V:44:ARG:NE	2.17	0.69
5:D:81:ALA:HB1	5:D:142:LEU:HD13	1.74	0.69
22:U:4:PRO:O	22:U:8:ARG:HG3	1.92	0.69
30:3:41:HIS:H	30:3:45:ASN:HD22	1.40	0.69
1:A:506:G:H22	1:A:509:A:H5'	1.56	0.69
1:A:514:G:O5'	1:A:514:G:C8	2.46	0.69
1:A:1289:C:H3'	39:A:5873:HOH:O	1.91	0.69
39:A:6107:HOH:O	17:P:24:ALA:N	2.25	0.69
39:A:9204:HOH:O	5:D:254:GLN:HG3	1.91	0.69
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.73	0.69
1:A:111:C:O2'	1:A:112:G:H5'	1.91	0.69
1:A:130:C:H5'	39:A:4691:HOH:O	1.93	0.69
1:A:1187:U:C3'	39:A:6358:HOH:O	2.39	0.69
1:A:1676:G:O2'	39:A:8934:HOH:O	2.11	0.69
1:A:1891:G:OP2	39:A:4453:HOH:O	2.11	0.69
1:A:2672:C:P	5:D:25:ARG:NH1	2.66	0.69
6:E:233:THR:HG22	6:E:234:VAL:N	2.06	0.69
15:N:35:PRO:HD2	15:N:38:VAL:CG2	2.22	0.69
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.23	0.69
1:A:746:A:OP1	39:A:4988:HOH:O	2.11	0.69
1:A:1135:G:H5'	39:A:5402:HOH:O	1.92	0.69
1:A:1993:C:N3	39:A:9428:HOH:O	2.26	0.69
1:A:2866:U:H4'	1:A:2867:G:H5'	1.75	0.69
2:B:3029:C:H2'	2:B:3030:C:H5'	1.75	0.69
2:B:3042:C:H2'	39:B:8512:HOH:O	1.93	0.69
5:D:41:PHE:CD2	5:D:190:MET:HE3	2.27	0.69
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.22	0.69
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.63	0.69
16:O:151:ASP:HB3	39:O:8527:HOH:O	1.92	0.69
1:A:1669:A:H2	39:A:3196:HOH:O	1.75	0.69
7:F:37:ALA:O	7:F:40:ILE:HG12	1.93	0.69
11:J:49:VAL:O	11:J:157:ILE:HG23	1.93	0.69
13:L:63:GLU:HG3	39:L:6344:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.74	0.69
16:O:142:THR:N	39:O:8565:HOH:O	2.25	0.69
22:U:37:GLN:HB3	39:U:6711:HOH:O	1.91	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.93	0.68
1:A:1008:C:H5"	11:J:16:ARG:HH12	1.58	0.68
4:C:105:VAL:HG12	4:C:106:CYS:N	2.07	0.68
25:X:110:GLN:NE2	25:X:110:GLN:HA	2.08	0.68
25:X:139:GLY:O	25:X:141:HIS:HD2	1.75	0.68
1:A:240:C:H5'	15:N:146:GLN:NE2	2.07	0.68
7:F:21:VAL:HG13	7:F:131:THR:O	1.94	0.68
15:N:113:ARG:NH1	15:N:152:ARG:O	2.22	0.68
20:S:15:LYS:HE3	39:S:8582:HOH:O	1.92	0.68
27:Z:188:HIS:NE2	39:Z:8579:HOH:O	2.26	0.68
1:A:1505:U:H6	1:A:1505:U:H5'	1.56	0.68
1:A:2468:A:H61	31:4:48:ASN:HD21	1.42	0.68
15:N:46:LEU:HB2	39:N:8604:HOH:O	1.92	0.68
1:A:1185:U:H2'	1:A:1186:C:C6	2.27	0.68
1:A:1271:A:C2	1:A:1286:A:C2	2.81	0.68
1:A:1500:U:O4'	39:A:4232:HOH:O	2.11	0.68
39:A:4426:HOH:O	2:B:3103:A:H4'	1.93	0.68
17:P:21:SER:CB	17:P:106:PRO:O	2.42	0.68
31:4:49:ASP:OD2	39:4:8524:HOH:O	2.11	0.68
1:A:119:A:H2'	1:A:120:A:H5"	1.73	0.68
4:C:55:VAL:HG13	4:C:67:LEU:HD22	1.74	0.68
5:D:119:HIS:O	5:D:121:PRO:HD3	1.92	0.68
10:I:12:ILE:N	10:I:13:PRO:HD3	2.07	0.68
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.28	0.68
1:A:593:A:OP2	39:A:3881:HOH:O	2.10	0.68
1:A:635:A:OP1	1:A:1359:U:O2'	2.11	0.68
1:A:1200:A:H4'	39:A:6805:HOH:O	1.93	0.68
1:A:1422:U:H2'	1:A:1423:C:C6	2.28	0.68
1:A:1494:A:O2'	1:A:1505:U:O2	2.09	0.68
1:A:2269:C:H2'	1:A:2270:G:H5'	1.75	0.68
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.27	0.68
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.74	0.68
22:U:48:VAL:HG22	22:U:97:ARG:C	2.14	0.68
28:1:50:ALA:HB3	28:1:54:ILE:HG22	1.74	0.68
1:A:1497:G:P	39:A:6011:HOH:O	2.52	0.68
1:A:1759:A:N7	39:A:9062:HOH:O	2.27	0.68
5:D:267:LYS:NZ	5:D:300:SER:O	2.21	0.68
17:P:99:GLU:HG3	39:P:6044:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:149:LEU:HG	25:X:153:MET:HE2	1.75	0.68
31:4:74:CYS:N	39:4:8561:HOH:O	2.27	0.68
1:A:160:A:OP1	39:A:6112:HOH:O	2.11	0.68
2:B:3024:U:O2'	2:B:3025:G:H4'	1.94	0.68
35:K:8501:CL:CL	39:K:4038:HOH:O	2.48	0.68
20:S:18:LEU:HG	20:S:91:LEU:HD13	1.75	0.68
1:A:786:G:N7	39:A:9305:HOH:O	2.26	0.68
1:A:2466:G:H8	39:A:9036:HOH:O	1.76	0.68
1:A:2716:G:H5"	5:D:206:THR:HG21	1.74	0.68
5:D:329:TYR:CE2	23:V:15:PRO:HG3	2.29	0.68
6:E:242:GLU:HG3	39:E:8386:HOH:O	1.93	0.68
7:F:99:ASP:HB3	7:F:103:ASN:H	1.59	0.68
11:J:139:ASP:HA	39:J:8370:HOH:O	1.94	0.68
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.74	0.68
1:A:1186:C:N4	1:A:1187:U:C4	2.61	0.68
1:A:1209:C:H4'	39:A:4755:HOH:O	1.93	0.68
8:G:118:ILE:HG23	8:G:144:THR:HG21	1.76	0.68
13:L:115:ARG:HG3	13:L:116:GLU:N	2.07	0.68
1:A:1329:A:H2	39:A:4159:HOH:O	1.77	0.67
1:A:2672:C:OP2	5:D:25:ARG:NH1	2.27	0.67
39:A:8902:HOH:O	15:N:94:LYS:HE2	1.94	0.67
9:H:57:GLU:O	9:H:61:MET:HG3	1.93	0.67
22:U:65:VAL:HG22	22:U:72:ILE:HG22	1.75	0.67
31:4:17:HIS:O	31:4:18:GLN:HG3	1.94	0.67
31:4:30:GLN:HB3	39:4:8554:HOH:O	1.92	0.67
1:A:541:C:H5	39:A:9778:HOH:O	1.75	0.67
1:A:2292:C:OP1	39:A:6364:HOH:O	2.11	0.67
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.74	0.67
1:A:2040:C:OP1	39:A:4047:HOH:O	2.11	0.67
1:A:2430:A:OP2	39:A:9464:HOH:O	2.11	0.67
4:C:170:VAL:HG22	28:1:22:ILE:HG23	1.77	0.67
1:A:1316:G:H1'	1:A:1340:G:N2	2.10	0.67
1:A:2252:A:C5	1:A:2253:G:H1'	2.30	0.67
7:F:23:VAL:HG23	7:F:23:VAL:O	1.93	0.67
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.76	0.67
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.76	0.67
29:2:46:ARG:HD2	39:2:6935:HOH:O	1.94	0.67
1:A:1370:G:C4	39:A:9638:HOH:O	2.48	0.67
1:A:1641:A:H2'	1:A:1642:A:H5'	1.76	0.67
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.75	0.67
5:D:82:VAL:O	5:D:82:VAL:HG12	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:56:ILE:HG22	11:J:61:LEU:HD21	1.77	0.67
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.29	0.67
23:V:33:SER:O	23:V:37:GLU:HG3	1.95	0.67
1:A:558:C:H5'	39:A:4735:HOH:O	1.95	0.67
39:A:8729:HOH:O	4:C:11:ARG:HD3	1.94	0.67
5:D:336:GLN:NE2	39:D:8525:HOH:O	2.28	0.67
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.10	0.67
15:N:72:SER:HB2	15:N:93:ARG:HG2	1.75	0.67
22:U:48:VAL:HG23	22:U:98:VAL:HA	1.77	0.67
22:U:106:GLU:HG3	39:U:4913:HOH:O	1.94	0.67
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.76	0.67
28:1:31:ILE:HG23	28:1:32:LYS:N	2.10	0.67
1:A:125:U:H2'	39:A:3259:HOH:O	1.93	0.67
1:A:241:A:C2	1:A:378:A:H4'	2.29	0.67
1:A:2067:A:N7	39:A:6115:HOH:O	2.28	0.67
7:F:86:THR:HG23	39:F:7477:HOH:O	1.95	0.67
12:K:93:ARG:HB3	12:K:93:ARG:HH11	1.60	0.67
20:S:99:ALA:CB	20:S:109:MET:HE1	2.18	0.67
23:V:39:ASN:HD22	23:V:44:ARG:HH11	1.40	0.67
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.75	0.67
27:Z:187:VAL:HG23	27:Z:192:ASP:HB3	1.75	0.67
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.25	0.67
1:A:88:G:H5'	1:A:88:G:H8	1.59	0.67
1:A:581:G:H5'	39:A:7144:HOH:O	1.94	0.67
1:A:1200:A:C4'	39:A:6805:HOH:O	2.42	0.67
1:A:2502:C:C2'	1:A:2503:A:H5'	2.25	0.67
2:B:3020:G:O2'	2:B:3021:G:H5'	1.94	0.67
7:F:25:MET:CE	7:F:37:ALA:HB1	2.25	0.67
1:A:2594:C:C2'	1:A:2595:U:H5'	2.25	0.67
39:A:6060:HOH:O	31:4:79:LEU:HD12	1.92	0.67
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.76	0.67
8:G:101:GLU:HB2	8:G:116:THR:O	1.95	0.67
20:S:39:THR:HG23	20:S:107:GLU:O	1.93	0.67
1:A:20:G:H21	20:S:117:HIS:HD2	1.43	0.66
1:A:290:C:O2'	1:A:291:C:H5'	1.95	0.66
1:A:544:G:C2'	1:A:545:G:H5"	2.24	0.66
1:A:1558:C:O2	1:A:1563:G:N2	2.23	0.66
1:A:2487:C:OP2	39:A:5708:HOH:O	2.13	0.66
15:N:35:PRO:HD2	15:N:38:VAL:HG21	1.75	0.66
25:X:142:ASP:HB2	39:X:2729:HOH:O	1.95	0.66
27:Z:186:ARG:HG2	27:Z:186:ARG:NH1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.66
1:A:2635:A:H2'	1:A:2636:C:C6	2.31	0.66
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.25	0.66
11:J:57:ARG:HG3	39:J:8353:HOH:O	1.95	0.66
25:X:64:THR:O	25:X:68:THR:HG22	1.95	0.66
1:A:537:G:OP2	39:A:4524:HOH:O	2.14	0.66
1:A:1191:A:C3'	1:A:1192:A:H5"	2.25	0.66
1:A:2635:A:H2'	1:A:2636:C:H6	1.60	0.66
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.59	0.66
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.78	0.66
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.11	0.66
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.41	0.66
27:Z:155:ARG:NH1	39:Z:8558:HOH:O	2.28	0.66
1:A:1089:G:H1'	39:A:6170:HOH:O	1.94	0.66
1:A:1934:A:C8	1:A:1935:C:C5	2.84	0.66
1:A:2249:G:OP2	39:A:4916:HOH:O	2.12	0.66
27:Z:122:ARG:NH2	39:Z:8533:HOH:O	2.26	0.66
30:3:24:TRP:CD1	39:3:6863:HOH:O	2.48	0.66
1:A:100:C:O5'	39:A:3593:HOH:O	2.12	0.66
1:A:702:G:O2'	1:A:703:G:H5'	1.95	0.66
1:A:758:A:OP2	39:A:3043:HOH:O	2.13	0.66
1:A:1427:A:N3	39:A:4280:HOH:O	2.29	0.66
1:A:2631:U:OP2	39:A:9589:HOH:O	2.13	0.66
8:G:7:ILE:HD11	8:G:11:VAL:O	1.96	0.66
1:A:130:C:H2'	39:A:9657:HOH:O	1.96	0.66
1:A:399:C:H5'	15:N:179:GLY:O	1.96	0.66
1:A:629:A:N7	39:A:9357:HOH:O	2.27	0.66
1:A:681:G:H5'	1:A:681:G:N3	2.11	0.66
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.10	0.66
1:A:82:C:OP1	22:U:67:LEU:HB2	1.95	0.66
1:A:963:C:O5'	1:A:963:C:H6	1.78	0.66
1:A:1165:G:OP1	1:A:1165:G:H3'	1.95	0.66
1:A:1328:A:C8	27:Z:169:ARG:HD3	2.31	0.66
1:A:1377:C:H1'	39:A:6740:HOH:O	1.95	0.66
2:B:3023:U:H6	2:B:3023:U:H5"	1.60	0.66
4:C:179:MET:HG2	4:C:186:TRP:CG	2.31	0.66
5:D:48:MET:N	39:D:8563:HOH:O	2.29	0.66
15:N:144:ASP:O	15:N:148:SER:HB3	1.96	0.66
20:S:79:ARG:C	20:S:81:PRO:HD3	2.15	0.66
1:A:195:C:H2'	1:A:196:G:H5'	1.78	0.66
1:A:506:G:H22	1:A:509:A:C5'	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:U:H2'	1:A:1057:A:O4'	1.96	0.66
1:A:1306:U:C5'	6:E:184:ARG:NH1	2.59	0.66
1:A:1187:U:O2'	1:A:1189:A:H2	1.79	0.66
1:A:2278:U:H3'	39:A:4569:HOH:O	1.96	0.66
1:A:2825:C:O2'	39:A:5457:HOH:O	2.14	0.66
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.78	0.66
30:3:48:ASP:O	39:3:719:HOH:O	2.14	0.66
1:A:1270:U:OP1	39:A:7308:HOH:O	2.13	0.65
1:A:1986:G:H2'	1:A:1987:C:C6	2.31	0.65
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.25	0.65
7:F:105:SER:CB	7:F:131:THR:HG23	2.25	0.65
11:J:162:SER:CB	11:J:163:PRO:HD3	2.18	0.65
16:O:58:LEU:HD12	16:O:58:LEU:N	2.10	0.65
1:A:332:G:H4'	22:U:2:LYS:O	1.95	0.65
1:A:338:C:H4'	6:E:174:ILE:HD11	1.79	0.65
1:A:926:A:H5'	14:M:39:GLU:OE2	1.96	0.65
1:A:1362:U:H5'	39:A:9762:HOH:O	1.94	0.65
1:A:2311:A:OP2	39:A:7205:HOH:O	2.14	0.65
1:A:2717:C:C2'	1:A:2718:C:H5"	2.27	0.65
5:D:132:HIS:HB2	5:D:137:LEU:HD22	1.77	0.65
5:D:211:THR:HA	5:D:255:GLY:O	1.96	0.65
9:H:99:THR:O	9:H:99:THR:HG23	1.97	0.65
15:N:77:PHE:O	39:N:8544:HOH:O	2.15	0.65
27:Z:200:THR:HG22	27:Z:201:GLU:HG2	1.78	0.65
30:3:41:HIS:N	30:3:45:ASN:HD22	1.94	0.65
1:A:560:C:H42	1:A:597:A:H61	1.43	0.65
14:M:114:VAL:HG11	39:M:8452:HOH:O	1.94	0.65
17:P:32:ARG:O	17:P:32:ARG:HD3	1.97	0.65
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.59	0.65
1:A:473:A:O2'	1:A:474:C:H5'	1.97	0.65
1:A:2388:C:OP1	39:A:4076:HOH:O	2.14	0.65
16:O:159:TYR:HB2	39:O:8530:HOH:O	1.97	0.65
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.26	0.65
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.77	0.65
1:A:710:G:P	17:P:24:ALA:HB3	2.36	0.65
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.11	0.65
1:A:2508:C:OP1	39:A:4017:HOH:O	2.14	0.65
4:C:221:PRO:O	39:C:8591:HOH:O	2.12	0.65
7:F:69:ILE:HG22	7:F:69:ILE:O	1.95	0.65
14:M:90:ARG:O	39:M:8437:HOH:O	2.15	0.65
19:R:26:PRO:O	19:R:29:ALA:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:52:THR:CG2	23:V:54:THR:HB	2.27	0.65
24:W:39:ALA:N	24:W:40:PRO:HD2	2.12	0.65
28:1:33:HIS:NE2	39:1:5656:HOH:O	2.30	0.65
1:A:1088:A:N1	39:A:8943:HOH:O	2.29	0.65
1:A:1126:C:OP2	39:A:3133:HOH:O	2.15	0.65
1:A:2506:A:C1'	39:A:3241:HOH:O	2.40	0.65
5:D:74:ILE:HG22	5:D:76:THR:HG23	1.79	0.65
6:E:198:ASP:O	39:E:8478:HOH:O	2.13	0.65
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.78	0.65
9:H:91:VAL:CG1	9:H:92:GLY:H	2.07	0.65
11:J:71:TYR:C	11:J:73:GLN:H	1.98	0.65
12:K:103:VAL:HG12	39:K:5907:HOH:O	1.96	0.65
16:O:170:GLU:O	16:O:174:GLU:HG3	1.97	0.65
17:P:39:THR:HB	39:P:3360:HOH:O	1.97	0.65
22:U:55:PHE:HB2	39:U:6384:HOH:O	1.96	0.65
1:A:677:C:OP2	39:A:8705:HOH:O	2.14	0.65
1:A:1819:G:H2'	1:A:1820:G:H4'	1.77	0.65
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.78	0.65
23:V:6:CYS:HA	23:V:13:ILE:HD11	1.77	0.65
1:A:401:C:C5'	39:A:5265:HOH:O	2.44	0.65
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.30	0.65
1:A:1693:A:OP1	39:A:9932:HOH:O	2.14	0.65
1:A:2436:U:H5'	31:4:68:LYS:HE2	1.77	0.65
1:A:2768:A:C2	39:A:3904:HOH:O	2.49	0.65
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.23	0.65
15:N:61:ILE:HG13	39:N:8623:HOH:O	1.96	0.65
26:Y:30:MET:HE1	26:Y:55:ASN:HA	1.78	0.65
1:A:801:U:H2'	1:A:802:G:H8	1.61	0.65
39:A:5106:HOH:O	18:Q:58:SER:HB3	1.97	0.65
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.62	0.65
14:M:133:VAL:HB	39:M:8435:HOH:O	1.96	0.65
21:T:8:PRO:HD2	24:W:32:ALA:HA	1.77	0.65
1:A:1182:C:H1'	1:A:1192:A:H8	1.62	0.65
1:A:2492:U:H5	39:A:6483:HOH:O	1.80	0.65
1:A:2630:G:O6	4:C:206:ARG:NH2	2.29	0.65
1:A:2780:C:H2'	1:A:2781:U:C6	2.32	0.65
1:A:2834:G:C4	1:A:2847:G:N2	2.65	0.65
6:E:54:LEU:HD21	6:E:87:ARG:HD2	1.77	0.65
17:P:99:GLU:HA	39:P:7481:HOH:O	1.96	0.65
25:X:80:ASP:O	25:X:84:VAL:HG23	1.97	0.65
27:Z:131:GLN:HB3	27:Z:153:GLN:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:U:O4'	39:A:6930:HOH:O	2.14	0.64
4:C:188:ASN:OD1	39:C:8562:HOH:O	2.14	0.64
5:D:76:THR:N	5:D:77:PRO:HD3	2.10	0.64
19:R:33:PHE:N	19:R:71:TYR:OH	2.25	0.64
25:X:85:ALA:HB2	25:X:91:ASP:O	1.96	0.64
27:Z:133:HIS:HD2	39:Z:8582:HOH:O	1.80	0.64
1:A:240:C:H5'	15:N:146:GLN:HE22	1.62	0.64
1:A:536:A:H3'	39:A:4524:HOH:O	1.98	0.64
1:A:962:C:C1'	16:O:5:ARG:NH1	2.58	0.64
39:A:5784:HOH:O	7:F:55:LYS:HB2	1.97	0.64
4:C:9:ARG:HD3	39:C:8524:HOH:O	1.98	0.64
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.79	0.64
12:K:48:GLY:HA3	12:K:53:ILE:HD11	1.79	0.64
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.79	0.64
29:2:10:LYS:CB	39:2:2979:HOH:O	2.46	0.64
1:A:1878:G:O3'	39:A:5591:HOH:O	2.14	0.64
13:L:10:GLN:HE21	13:L:10:GLN:N	1.86	0.64
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.33	0.64
1:A:2285:G:OP2	39:A:3729:HOH:O	2.14	0.64
15:N:154:ARG:HD3	39:N:8639:HOH:O	1.96	0.64
1:A:316:A:N3	1:A:336:G:O2'	2.30	0.64
1:A:1497:G:O2'	1:A:1498:G:H5'	1.96	0.64
4:C:177:HIS:CE1	39:C:8618:HOH:O	2.42	0.64
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.28	0.64
27:Z:212:ARG:HD2	39:Z:8602:HOH:O	1.96	0.64
1:A:1130:U:H2'	1:A:1131:G:O4'	1.98	0.64
1:A:1664:A:H8	1:A:1664:A:OP1	1.80	0.64
1:A:2326:U:H4'	1:A:2412:G:H4'	1.80	0.64
2:B:3064:C:O2'	2:B:3065:A:H5'	1.97	0.64
4:C:170:VAL:HG13	28:1:22:ILE:HG21	1.80	0.64
11:J:65:ARG:CZ	39:J:8384:HOH:O	2.44	0.64
11:J:141:ASN:CA	39:J:8366:HOH:O	2.33	0.64
12:K:99:GLU:HA	39:K:7377:HOH:O	1.97	0.64
16:O:50:LEU:HB2	39:O:8523:HOH:O	1.97	0.64
27:Z:115:ARG:CZ	39:Z:8556:HOH:O	2.46	0.64
1:A:289:G:N2	1:A:363:A:H2	1.93	0.64
1:A:545:G:H5'	1:A:545:G:C8	2.30	0.64
1:A:2243:C:C5'	39:A:3245:HOH:O	2.44	0.64
1:A:2496:C:OP2	39:A:6810:HOH:O	2.15	0.64
2:B:3103:A:H1'	39:B:8405:HOH:O	1.97	0.64
9:H:104:ALA:HA	39:H:6617:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:31:PHE:CE2	23:V:37:GLU:HA	2.32	0.64
1:A:1166:A:N3	1:A:1166:A:H2'	2.12	0.64
1:A:2831:C:C2'	1:A:2832:C:H5'	2.28	0.64
39:A:6151:HOH:O	22:U:38:ARG:NH1	2.31	0.64
11:J:27:LYS:N	11:J:58:HIS:HD2	1.95	0.64
12:K:52:GLN:HG3	12:K:53:ILE:H	1.61	0.64
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.05	0.64
21:T:57:THR:HG22	21:T:59:ASP:N	2.13	0.64
22:U:48:VAL:HG22	22:U:97:ARG:O	1.98	0.64
1:A:1211:G:O2'	1:A:1212:C:H5'	1.97	0.64
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.11	0.64
1:A:1046:G:OP1	39:A:9656:HOH:O	2.15	0.64
1:A:1543:G:HO2'	1:A:1544:U:H6	1.46	0.64
1:A:1920:C:H2'	1:A:1921:A:H5'	1.79	0.64
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.79	0.64
7:F:95:THR:O	7:F:97:GLN:N	2.26	0.64
8:G:107:PHE:CD2	8:G:108:LEU:HD13	2.32	0.64
15:N:46:LEU:HD22	15:N:50:ARG:HG3	1.79	0.64
28:1:49:ARG:HD2	39:1:5656:HOH:O	1.98	0.64
1:A:212:A:O4'	1:A:214:U:C6	2.51	0.63
1:A:877:G:H5'	1:A:878:G:OP1	1.98	0.63
1:A:2467:A:H2'	39:A:4931:HOH:O	1.98	0.63
39:A:9470:HOH:O	6:E:174:ILE:HD12	1.98	0.63
5:D:21:SER:OG	39:D:8654:HOH:O	2.05	0.63
5:D:36:PRO:HA	5:D:168:GLY:HA2	1.80	0.63
21:T:73:ASP:O	21:T:77:VAL:HG23	1.98	0.63
30:3:41:HIS:H	30:3:45:ASN:ND2	1.96	0.63
1:A:1080:C:H5'	39:A:3549:HOH:O	1.98	0.63
1:A:1450:C:O2'	1:A:1493:A:H2'	1.97	0.63
2:B:3002:U:OP2	2:B:3003:A:H5'	1.98	0.63
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.78	0.63
16:O:18:THR:HA	39:O:8524:HOH:O	1.98	0.63
1:A:558:C:O2'	1:A:559:U:H5"	1.98	0.63
1:A:1161:A:H8	1:A:1161:A:O5'	1.79	0.63
1:A:1593:C:O2'	1:A:1594:C:H5'	1.99	0.63
14:M:104:ASP:O	14:M:105:TYR:HB3	1.98	0.63
25:X:13:MET:HE1	25:X:18:GLN:HA	1.79	0.63
1:A:2723:G:H1'	39:A:4318:HOH:O	1.98	0.63
1:A:2898:G:H4'	5:D:288:GLY:HA2	1.80	0.63
1:A:2913:A:OP2	39:A:5835:HOH:O	2.15	0.63
6:E:1:MET:HG2	6:E:2:GLN:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:64:GLU:HG2	39:Q:2495:HOH:O	1.98	0.63
1:A:542:A:H8	1:A:542:A:C5'	2.05	0.63
1:A:774:C:OP2	39:A:5089:HOH:O	2.15	0.63
5:D:278:PRO:HD2	39:D:8653:HOH:O	1.99	0.63
6:E:166:ILE:HG23	6:E:208:ALA:HB3	1.80	0.63
16:O:113:SER:CB	39:O:8556:HOH:O	2.40	0.63
16:O:125:ALA:O	39:O:8554:HOH:O	2.15	0.63
30:3:5:LYS:O	30:3:9:LYS:HG3	1.98	0.63
1:A:797:A:C4'	28:1:10:ARG:N	2.61	0.63
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.64	0.63
5:D:81:ALA:CB	5:D:142:LEU:HD13	2.29	0.63
1:A:1422:U:H2'	1:A:1423:C:H6	1.63	0.63
1:A:1649:G:O2'	39:A:5009:HOH:O	2.15	0.63
1:A:2727:A:H2'	1:A:2728:C:H5'	1.80	0.63
1:A:281:U:O2'	1:A:282:C:H5'	1.99	0.63
1:A:1701:A:H4'	39:A:6685:HOH:O	1.99	0.63
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.29	0.63
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.61	0.63
31:4:3:MET:O	31:4:90:PHE:HA	1.98	0.63
31:4:31:THR:HB	31:4:33:MET:CE	2.29	0.63
1:A:1827:G:H2'	1:A:1828:G:C8	2.34	0.63
2:B:3092:G:H2'	2:B:3093:A:C8	2.34	0.63
16:O:73:ALA:N	39:O:8562:HOH:O	2.32	0.63
19:R:13:LYS:NZ	39:R:1719:HOH:O	2.32	0.63
19:R:53:HIS:CE1	19:R:55:ARG:HG3	2.34	0.63
26:Y:23:HIS:HB2	39:Y:7830:HOH:O	1.99	0.63
1:A:445:U:C1'	39:A:6800:HOH:O	2.47	0.62
1:A:1119:G:N2	1:A:1246:A:H2	1.95	0.62
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.81	0.62
18:Q:91:LYS:O	18:Q:95:GLU:HG3	1.98	0.62
26:Y:21:PRO:HD3	39:Y:6179:HOH:O	1.99	0.62
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.64	0.62
1:A:1752:G:H2'	39:A:7011:HOH:O	1.99	0.62
1:A:1947:G:N2	1:A:1966:U:C2	2.67	0.62
4:C:33:GLU:O	4:C:34:ASP:HB2	1.97	0.62
5:D:62:ARG:HA	5:D:65:MET:HE3	1.77	0.62
5:D:248:ARG:HG2	39:D:8580:HOH:O	1.97	0.62
1:A:187:A:H3'	1:A:188:C:H6	1.64	0.62
1:A:1192:A:O2'	1:A:1193:A:OP1	2.17	0.62
1:A:1312:G:H1'	39:A:3780:HOH:O	1.99	0.62
2:B:3040:C:N4	7:F:51:ARG:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:10:PHE:CD1	7:F:11:HIS:N	2.67	0.62
23:V:52:THR:HG22	23:V:54:THR:N	2.13	0.62
1:A:168:C:O2'	1:A:169:A:H5'	1.99	0.62
1:A:894:A:C2	6:E:87:ARG:NH2	2.67	0.62
1:A:1057:A:C6	1:A:1058:A:C6	2.87	0.62
1:A:1080:C:C4'	1:A:1081:A:OP1	2.47	0.62
1:A:1185:U:H5'	39:A:6930:HOH:O	1.98	0.62
1:A:2276:U:H2'	1:A:2277:U:C6	2.34	0.62
1:A:2502:C:H2'	1:A:2503:A:H5'	1.80	0.62
16:O:77:ASN:OD1	16:O:80:SER:HB2	1.99	0.62
26:Y:41:PHE:CZ	26:Y:74:ALA:HB3	2.34	0.62
1:A:381:G:H5"	39:A:3800:HOH:O	1.98	0.62
1:A:695:C:H2'	1:A:696:C:H6	1.65	0.62
1:A:1657:A:H2'	1:A:1658:A:C8	2.34	0.62
1:A:2265:U:H2'	1:A:2266:A:H8	1.63	0.62
1:A:2359:G:H3'	39:A:5169:HOH:O	1.98	0.62
12:K:45:VAL:HG23	12:K:130:VAL:O	2.00	0.62
14:M:143:THR:HG22	14:M:144:ASP:H	1.64	0.62
28:1:19:GLY:O	28:1:23:ARG:HG2	2.00	0.62
1:A:1151:G:P	10:I:16:LYS:NZ	2.71	0.62
1:A:1191:A:C2	1:A:1207:A:C2	2.88	0.62
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.30	0.62
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.64	0.62
31:4:31:THR:HB	31:4:33:MET:HE3	1.81	0.62
1:A:288:A:H61	1:A:364:C:H42	1.48	0.62
1:A:1523:G:H2'	1:A:1524:U:C6	2.35	0.62
1:A:2243:C:H5"	39:A:3245:HOH:O	1.99	0.62
1:A:2269:C:C2'	1:A:2270:G:H5'	2.30	0.62
1:A:2387:U:H2'	1:A:2388:C:C6	2.35	0.62
1:A:2547:C:H2'	1:A:2548:C:H6	1.63	0.62
4:C:125:ASN:HB3	4:C:158:VAL:HG12	1.81	0.62
13:L:49:LEU:HD21	13:L:74:VAL:O	2.00	0.62
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.81	0.62
31:4:71:CYS:SG	38:4:8404:CD:CD	2.09	0.62
1:A:1783:A:O2'	1:A:1784:U:H5'	2.00	0.62
1:A:2326:U:H4'	1:A:2412:G:C4'	2.30	0.62
1:A:2346:C:O3'	7:F:52:THR:HG23	2.00	0.62
1:A:2748:G:H5'	39:A:7005:HOH:O	2.00	0.62
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.34	0.62
7:F:86:THR:CG2	39:F:7477:HOH:O	2.48	0.62
8:G:69:ILE:O	8:G:72:MET:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:74:ASN:ND2	11:J:141:ASN:OD1	2.32	0.62
15:N:137:ASP:O	15:N:142:LYS:HE3	1.99	0.62
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.82	0.62
28:1:53:GLY:HA2	28:1:67:GLY:O	1.99	0.62
1:A:484:A:N1	1:A:506:G:H4'	2.14	0.62
1:A:514:G:OP1	1:A:514:G:H2'	2.00	0.62
1:A:1164:U:C4'	1:A:1165:G:OP1	2.46	0.62
4:C:131:HIS:O	4:C:132:ASP:HB2	1.98	0.62
5:D:16:ARG:HB3	5:D:217:ARG:NH2	2.15	0.62
17:P:21:SER:HB3	17:P:106:PRO:O	1.99	0.62
1:A:263:U:O4'	9:H:59:ILE:HD13	2.00	0.62
1:A:328:U:O4'	6:E:202:THR:HG22	1.99	0.62
5:D:129:ARG:NH2	5:D:176:ASP:OD1	2.31	0.62
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.15	0.62
9:H:96:ALA:HA	39:H:3111:HOH:O	2.00	0.62
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.15	0.62
1:A:812:A:H1'	39:A:3448:HOH:O	1.99	0.61
1:A:1189:A:H1'	1:A:1209:C:C1'	2.31	0.61
39:A:3143:HOH:O	17:P:3:THR:HG21	2.00	0.61
12:K:70:PHE:C	39:K:6807:HOH:O	2.37	0.61
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	1.81	0.61
31:4:65:THR:HG23	31:4:67:LEU:HG	1.81	0.61
1:A:347:A:C2'	1:A:348:C:H5'	2.29	0.61
1:A:395:A:H4'	39:A:9466:HOH:O	2.00	0.61
1:A:638:C:H2'	1:A:639:A:C8	2.35	0.61
1:A:1123:A:C6	1:A:1238:C:H5'	2.36	0.61
1:A:1682:A:H5"	39:A:8958:HOH:O	1.99	0.61
4:C:199:HIS:HD2	4:C:201:PHE:H	1.45	0.61
6:E:154:VAL:O	6:E:158:GLU:HG3	2.00	0.61
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.82	0.61
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	1.99	0.61
30:3:49:GLU:HB2	39:3:719:HOH:O	2.00	0.61
1:A:92:G:C5'	39:W:7247:HOH:O	2.44	0.61
1:A:445:U:H1'	39:A:6800:HOH:O	2.00	0.61
1:A:2836:G:C6	1:A:2838:A:C2	2.88	0.61
6:E:115:LEU:HD13	6:E:223:LEU:CD2	2.28	0.61
6:E:214:THR:HB	39:E:8327:HOH:O	1.99	0.61
11:J:48:LEU:CD1	11:J:157:ILE:HG21	2.31	0.61
14:M:136:ALA:HB3	39:M:8452:HOH:O	1.99	0.61
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.14	0.61
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:22:PRO:HB2	30:3:24:TRP:CD1	2.35	0.61
1:A:288:A:O3'	39:A:4082:HOH:O	2.16	0.61
12:K:42:GLU:HG3	12:K:145:TRP:CD1	2.35	0.61
26:Y:25:ARG:HD2	39:Y:3861:HOH:O	2.00	0.61
1:A:255:A:H2'	1:A:256:C:C6	2.36	0.61
5:D:16:ARG:NH2	39:D:8558:HOH:O	2.31	0.61
5:D:86:ALA:HA	39:D:8584:HOH:O	2.01	0.61
5:D:258:GLY:H	5:D:260:HIS:HE1	1.46	0.61
6:E:39:GLN:O	6:E:43:LYS:HD3	2.00	0.61
6:E:79:ARG:O	6:E:87:ARG:HG2	2.01	0.61
6:E:162:VAL:CG1	6:E:192:ILE:HD11	2.30	0.61
11:J:75:SER:O	11:J:79:ALA:HB2	2.00	0.61
16:O:24:LEU:HD13	19:R:26:PRO:HB3	1.80	0.61
26:Y:76:ARG:HH11	26:Y:76:ARG:CG	2.05	0.61
1:A:939:A:OP1	39:A:4886:HOH:O	2.16	0.61
1:A:1423:C:O2'	1:A:1424:A:H5'	2.01	0.61
1:A:1641:A:C2'	1:A:1642:A:H5'	2.30	0.61
1:A:2252:A:C6	1:A:2253:G:H1'	2.35	0.61
39:A:5386:HOH:O	15:N:189:VAL:HG23	2.00	0.61
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.35	0.61
17:P:112:ARG:HA	39:P:1484:HOH:O	1.98	0.61
22:U:32:ARG:NH1	22:U:38:ARG:HH12	1.98	0.61
1:A:299:U:H5'	39:A:6800:HOH:O	2.00	0.61
1:A:338:C:H5"	39:A:5311:HOH:O	2.00	0.61
1:A:417:G:P	39:A:6878:HOH:O	2.58	0.61
1:A:1614:G:H2'	39:A:4101:HOH:O	2.01	0.61
1:A:1878:G:O2'	1:A:1879:U:H6	1.84	0.61
1:A:2047:C:H5'	39:A:9321:HOH:O	1.99	0.61
13:L:81:ARG:HD3	13:L:87:ARG:NH1	2.15	0.61
25:X:125:HIS:HE1	39:X:3071:HOH:O	1.83	0.61
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.15	0.61
1:A:775:G:OP2	39:A:5062:HOH:O	2.16	0.61
1:A:1920:C:C2'	1:A:1921:A:H5'	2.31	0.61
1:A:2748:G:H2'	39:A:7005:HOH:O	2.00	0.61
6:E:133:ARG:NH1	39:E:8417:HOH:O	2.17	0.61
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.16	0.61
12:K:142:ASN:O	12:K:144:THR:N	2.34	0.61
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.31	0.61
27:Z:107:PRO:HD3	27:Z:182:PHE:CE1	2.36	0.61
1:A:338:C:H4'	6:E:174:ILE:CD1	2.31	0.61
11:J:150:LYS:CD	39:J:8382:HOH:O	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:G:H4'	11:J:151:MET:CE	2.26	0.61
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.36	0.61
4:C:135:VAL:HG21	4:C:147:ARG:NH1	2.16	0.61
4:C:168:PRO:O	4:C:170:VAL:HG23	2.01	0.61
6:E:177:GLY:HA3	39:E:8314:HOH:O	2.01	0.61
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.98	0.61
1:A:514:G:O5'	1:A:514:G:H2'	2.01	0.60
1:A:1380:U:H5'	39:A:8730:HOH:O	2.00	0.60
6:E:114:ALA:HB1	6:E:223:LEU:HB3	1.82	0.60
8:G:6:GLU:HA	8:G:46:THR:HG22	1.81	0.60
12:K:45:VAL:HG22	12:K:46:ILE:N	2.16	0.60
25:X:142:ASP:CB	39:X:2729:HOH:O	2.49	0.60
1:A:1008:C:OP1	11:J:16:ARG:NH2	2.35	0.60
1:A:1184:C:H1'	39:A:6930:HOH:O	2.01	0.60
1:A:1434:A:H2'	1:A:1436:C:C5	2.35	0.60
1:A:2320:U:H4'	1:A:2321:A:O4'	2.02	0.60
2:B:3025:G:H5"	2:B:3026:C:C6	2.36	0.60
20:S:8:ALA:HB3	39:S:8582:HOH:O	2.01	0.60
1:A:80:A:H3'	22:U:43:ASN:OD1	2.01	0.60
1:A:380:A:H5"	15:N:48:ARG:NH2	2.15	0.60
1:A:1316:G:H1'	1:A:1340:G:H22	1.65	0.60
39:A:4048:HOH:O	15:N:86:MET:HE3	1.99	0.60
17:P:7:LEU:HD22	39:P:5650:HOH:O	2.00	0.60
1:A:354:A:H3'	39:A:6626:HOH:O	2.00	0.60
1:A:2310:G:OP2	11:J:114:PRO:HD2	2.00	0.60
5:D:329:TYR:CE2	23:V:15:PRO:CG	2.85	0.60
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.83	0.60
25:X:139:GLY:O	25:X:141:HIS:CD2	2.54	0.60
1:A:266:G:C2	1:A:267:G:C8	2.89	0.60
1:A:331:A:N6	1:A:332:G:C2	2.69	0.60
1:A:820:G:O2'	1:A:856:G:H4'	2.02	0.60
1:A:2827:A:H2'	1:A:2828:G:O4'	2.01	0.60
39:A:6060:HOH:O	31:4:79:LEU:HB2	2.00	0.60
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.36	0.60
6:E:29:ASP:OD1	17:P:5:PRO:HD3	2.02	0.60
15:N:119:SER:OG	39:N:8572:HOH:O	2.16	0.60
16:O:43:VAL:HG13	16:O:118:ILE:HD11	1.82	0.60
1:A:324:G:O2'	1:A:325:U:H5'	2.01	0.60
1:A:1187:U:HO2'	1:A:1189:A:H2	1.47	0.60
1:A:1306:U:H5"	6:E:184:ARG:NH1	2.17	0.60
1:A:2464:C:H5"	1:A:2465:A:OP1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2541:U:O2'	1:A:2542:C:H5'	2.01	0.60
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.37	0.60
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.82	0.60
1:A:1213:C:N4	1:A:1214:G:N1	2.49	0.60
1:A:2125:G:O6	39:A:9909:HOH:O	2.12	0.60
6:E:133:ARG:HD2	39:E:8417:HOH:O	2.02	0.60
7:F:65:GLU:HG3	39:F:6752:HOH:O	2.01	0.60
11:J:136:VAL:HG22	11:J:137:ASN:O	2.02	0.60
26:Y:36:HIS:CE1	26:Y:40:HIS:CD2	2.90	0.60
1:A:135:G:O2'	15:N:135:ASP:OD2	2.19	0.60
1:A:154:C:H2'	1:A:155:C:H6	1.66	0.60
1:A:1185:U:C5'	39:A:6930:HOH:O	2.50	0.60
1:A:1687:C:H1'	29:2:8:GLN:O	2.02	0.60
1:A:2323:G:H5'	39:A:6484:HOH:O	2.02	0.60
4:C:105:VAL:CG1	4:C:106:CYS:N	2.65	0.60
5:D:102:THR:HG23	5:D:182:VAL:HG12	1.83	0.60
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.32	0.60
30:3:40:ARG:HG2	30:3:40:ARG:HH11	1.66	0.60
1:A:283:U:H5"	1:A:284:C:P	2.41	0.60
1:A:2371:G:H5'	39:A:4484:HOH:O	2.00	0.60
1:A:2780:C:H2'	1:A:2781:U:H6	1.65	0.60
2:B:3024:U:H1'	39:B:8438:HOH:O	2.00	0.60
6:E:107:ARG:HB3	6:E:107:ARG:CZ	2.31	0.60
7:F:144:ARG:NH2	39:F:3839:HOH:O	2.30	0.60
13:L:50:GLY:O	13:L:120:ARG:NH1	2.35	0.60
17:P:25:VAL:HG23	17:P:26:TRP:N	2.17	0.60
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.83	0.60
1:A:1003:U:HO2'	11:J:90:PHE:HE1	1.50	0.60
1:A:1195:G:C2	1:A:1205:U:O2	2.54	0.60
1:A:1329:A:N1	35:A:8513:CL:CL	2.72	0.60
1:A:2443:C:H5'	14:M:57:VAL:HG21	1.83	0.60
2:B:3078:G:O2'	2:B:3079:U:OP2	2.20	0.60
4:C:200:PRO:HG2	4:C:225:VAL:HG21	1.84	0.60
8:G:146:ALA:O	8:G:150:GLN:HG2	2.02	0.60
11:J:127:GLY:O	11:J:128:ALA:HB3	2.01	0.60
19:R:50:GLY:HA3	19:R:87:THR:CG2	2.32	0.60
21:T:57:THR:C	21:T:59:ASP:H	2.05	0.60
1:A:273:G:OP2	39:A:6481:HOH:O	2.16	0.59
1:A:2073:G:OP2	1:A:2490:A:H5'	2.02	0.59
1:A:2792:A:O2'	39:A:4031:HOH:O	2.17	0.59
5:D:190:MET:CE	5:D:194:PHE:CD1	2.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:163:VAL:HA	39:F:6326:HOH:O	2.01	0.59
8:G:11:VAL:HG11	8:G:22:VAL:HG13	1.83	0.59
11:J:26:LYS:HD2	11:J:28:ILE:HB	1.84	0.59
11:J:132:PHE:O	11:J:133:ILE:HD13	2.02	0.59
22:U:6:LYS:NZ	39:U:644:HOH:O	2.24	0.59
1:A:223:G:O2'	39:A:6555:HOH:O	2.17	0.59
1:A:884:C:O2	39:A:3312:HOH:O	2.14	0.59
1:A:1081:A:C6	1:A:1082:A:N1	2.70	0.59
1:A:1503:U:H2'	1:A:1504:A:O4'	2.02	0.59
6:E:174:ILE:HG12	6:E:186:TYR:CE2	2.38	0.59
7:F:140:ARG:O	7:F:144:ARG:HG2	2.02	0.59
7:F:169:THR:O	7:F:170:TYR:HB2	2.02	0.59
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.83	0.59
1:A:169:A:C5'	39:A:9115:HOH:O	2.50	0.59
1:A:283:U:H5"	1:A:284:C:OP2	2.03	0.59
1:A:1535:G:H2'	1:A:1536:C:C6	2.37	0.59
1:A:1989:G:O2'	1:A:1990:C:H5'	2.03	0.59
1:A:2769:C:C2'	1:A:2770:G:H5'	2.33	0.59
1:A:2890:A:C1'	23:V:56:ARG:NH2	2.63	0.59
9:H:22:VAL:HG21	9:H:104:ALA:HB2	1.84	0.59
9:H:49:PHE:HE1	9:H:98:VAL:HG23	1.68	0.59
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.83	0.59
20:S:132:ARG:HG2	20:S:133:ALA:N	2.16	0.59
24:W:44:GLY:O	24:W:48:GLU:HG2	2.01	0.59
1:A:240:C:H4'	15:N:146:GLN:NE2	2.17	0.59
1:A:2281:C:C2'	1:A:2282:U:H5'	2.31	0.59
8:G:26:ASN:CG	39:G:7046:HOH:O	2.41	0.59
16:O:3:GLY:HA3	39:O:8512:HOH:O	2.02	0.59
19:R:22:GLY:O	19:R:23:THR:O	2.19	0.59
22:U:87:VAL:HB	39:U:5545:HOH:O	2.02	0.59
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.38	0.59
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.17	0.59
1:A:229:G:O2'	1:A:230:C:H5'	2.03	0.59
1:A:886:A:P	39:A:3976:HOH:O	2.60	0.59
1:A:1409:G:H5'	39:A:3219:HOH:O	2.02	0.59
1:A:1477:C:H4'	1:A:1868:G:OP1	2.03	0.59
1:A:2256:G:O2'	1:A:2257:G:H5'	2.03	0.59
5:D:41:PHE:N	39:D:8651:HOH:O	2.35	0.59
7:F:64:ARG:O	7:F:67:ASP:OD2	2.18	0.59
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.85	0.59
11:J:71:TYR:O	11:J:73:GLN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:75:THR:HG21	39:N:8539:HOH:O	2.01	0.59
17:P:39:THR:O	17:P:115:ARG:NH2	2.35	0.59
20:S:8:ALA:CB	20:S:13:THR:HG21	2.17	0.59
1:A:669:G:O2'	1:A:670:G:H5'	2.03	0.59
1:A:2325:C:H1'	39:A:3635:HOH:O	2.02	0.59
1:A:2815:G:N7	12:K:80:LYS:NZ	2.49	0.59
1:A:2859:C:H6	1:A:2859:C:H5"	1.66	0.59
39:A:3476:HOH:O	22:U:82:THR:HA	2.00	0.59
39:A:9543:HOH:O	29:2:32:LYS:HD2	2.02	0.59
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.38	0.59
15:N:35:PRO:CD	15:N:38:VAL:HG23	2.31	0.59
17:P:4:ASN:HB3	17:P:7:LEU:HB3	1.84	0.59
29:2:10:LYS:CG	39:2:2979:HOH:O	2.45	0.59
29:2:25:LYS:O	29:2:25:LYS:CG	2.47	0.59
1:A:431:G:P	15:N:48:ARG:HH12	2.25	0.59
1:A:2570:G:OP2	39:A:4390:HOH:O	2.17	0.59
1:A:2763:G:H2'	1:A:2764:C:H6	1.68	0.59
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.83	0.59
20:S:106:GLY:HA2	20:S:109:MET:CE	2.33	0.59
25:X:31:HIS:ND1	39:X:2229:HOH:O	2.31	0.59
1:A:2415:A:O2'	16:O:29:SER:HB3	2.02	0.59
1:A:2777:G:O2'	1:A:2778:A:H5'	2.02	0.59
1:A:2819:C:H2'	1:A:2820:A:C8	2.37	0.59
25:X:110:GLN:HA	25:X:110:GLN:HE21	1.67	0.59
1:A:435:A:O2'	1:A:436:A:H5'	2.02	0.59
1:A:1730:G:H5'	1:A:1731:C:C5	2.38	0.59
1:A:1896:G:H1'	39:A:3741:HOH:O	2.01	0.59
1:A:2526:C:O2'	1:A:2527:U:H5'	2.02	0.59
2:B:3007:G:OP1	16:O:23:ARG:NE	2.35	0.59
5:D:146:THR:C	5:D:148:PRO:HD3	2.23	0.59
21:T:6:LYS:HB2	21:T:27:ALA:O	2.02	0.59
22:U:71:VAL:HG12	22:U:72:ILE:N	2.16	0.59
1:A:1477:C:H5'	1:A:1868:G:C5'	2.33	0.59
1:A:1855:G:H8	4:C:144:GLU:OE2	1.86	0.59
1:A:2610:U:H4'	39:D:8531:HOH:O	2.03	0.59
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.68	0.59
39:A:5416:HOH:O	28:1:34:LYS:HE2	2.03	0.59
39:A:6762:HOH:O	15:N:152:ARG:HB3	2.01	0.59
2:B:3025:G:C3'	2:B:3026:C:H5'	2.30	0.59
4:C:188:ASN:HA	39:C:8571:HOH:O	2.02	0.59
7:F:10:PHE:CG	7:F:11:HIS:N	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:174:VAL:HG13	39:F:6555:HOH:O	2.03	0.59
9:H:79:GLN:HG3	9:H:82:ASP:OD2	2.01	0.59
31:4:11:CYS:HB2	31:4:20:HIS:NE2	2.18	0.59
1:A:12:U:H2'	1:A:13:G:H5'	1.85	0.58
1:A:1189:A:H1'	1:A:1209:C:H1'	1.85	0.58
39:A:4487:HOH:O	10:I:16:LYS:NZ	2.35	0.58
34:C:8345:NA:NA	39:C:8602:HOH:O	1.73	0.58
6:E:2:GLN:HB3	39:E:8340:HOH:O	2.03	0.58
6:E:107:ARG:NH1	6:E:107:ARG:CB	2.64	0.58
14:M:63:THR:O	39:M:8460:HOH:O	2.17	0.58
24:W:23:LEU:HD12	24:W:56:ILE:HD12	1.85	0.58
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.58
1:A:558:C:C2'	1:A:559:U:H5"	2.33	0.58
1:A:1878:G:HO2'	1:A:1879:U:H6	1.51	0.58
2:B:3114:G:O6	16:O:11:ARG:HD3	2.02	0.58
6:E:197:SER:HB3	39:E:8378:HOH:O	2.03	0.58
8:G:149:GLU:OE1	8:G:168:ILE:HG12	2.02	0.58
10:I:64:ASN:N	10:I:64:ASN:ND2	2.50	0.58
15:N:59:GLY:HA3	15:N:141:ILE:CD1	2.32	0.58
15:N:74:ARG:NH1	39:N:8579:HOH:O	2.36	0.58
16:O:74:PRO:HG2	16:O:159:TYR:CZ	2.38	0.58
16:O:116:PHE:O	16:O:119:GLN:HB3	2.03	0.58
22:U:37:GLN:HG2	39:U:2876:HOH:O	2.03	0.58
28:1:55:TRP:CZ2	28:1:70:GLN:C	2.77	0.58
31:4:57:GLY:HA2	39:4:8525:HOH:O	2.02	0.58
1:A:1603:A:H5"	1:A:1605:G:H5'	1.84	0.58
1:A:1675:C:H5"	30:3:5:LYS:HD2	1.83	0.58
1:A:1730:G:OP2	39:A:4523:HOH:O	2.17	0.58
1:A:1820:G:C6	1:A:2030:A:C2	2.91	0.58
5:D:144:THR:HG22	5:D:145:HIS:N	2.17	0.58
6:E:140:VAL:HB	39:E:8459:HOH:O	2.01	0.58
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.38	0.58
14:M:10:SER:O	14:M:11:ARG:HB3	2.03	0.58
15:N:153:THR:O	15:N:156:ARG:HG3	2.01	0.58
1:A:257:G:O2'	1:A:258:G:H5'	2.04	0.58
1:A:514:G:H2'	1:A:514:G:P	2.42	0.58
1:A:970:U:H2'	39:A:5791:HOH:O	2.04	0.58
1:A:1175:G:H8	39:A:6854:HOH:O	1.86	0.58
1:A:1973:A:P	39:A:6350:HOH:O	2.61	0.58
1:A:2650:U:O2'	1:A:2651:C:H5'	2.02	0.58
39:A:6030:HOH:O	25:X:154:ARG:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:77:THR:OG1	8:G:78:GLU:N	2.36	0.58
8:G:97:VAL:C	39:G:4191:HOH:O	2.41	0.58
11:J:55:GLN:HE21	11:J:124:ARG:NE	1.99	0.58
39:L:1387:HOH:O	23:V:20:MET:HE3	2.04	0.58
17:P:96:VAL:HG12	17:P:97:SER:O	2.02	0.58
21:T:57:THR:HG22	21:T:59:ASP:HB2	1.85	0.58
1:A:797:A:H4'	28:1:10:ARG:N	2.19	0.58
1:A:1747:A:H1'	39:A:3597:HOH:O	2.02	0.58
1:A:1891:G:N7	39:A:7259:HOH:O	2.32	0.58
1:A:2768:A:O2'	1:A:2769:C:H5'	2.04	0.58
2:B:3023:U:H3'	2:B:3024:U:H5"	1.84	0.58
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.33	0.58
11:J:53:PRO:HA	11:J:125:VAL:O	2.03	0.58
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.68	0.58
1:A:158:A:O2'	1:A:159:G:H5'	2.04	0.58
1:A:281:U:H3'	39:A:6674:HOH:O	2.02	0.58
1:A:458:G:H2'	1:A:459:A:C8	2.38	0.58
1:A:1014:A:H2'	1:A:1015:C:H5'	1.86	0.58
1:A:1636:G:O2'	1:A:1637:A:H5'	2.03	0.58
1:A:2276:U:H5'	39:A:8606:HOH:O	2.03	0.58
1:A:2908:A:H2'	1:A:2909:G:O4'	2.02	0.58
4:C:86:ALA:O	39:C:8615:HOH:O	2.16	0.58
5:D:62:ARG:HG2	5:D:65:MET:HE3	1.85	0.58
7:F:92:GLU:O	7:F:93:LEU:O	2.21	0.58
15:N:184:ARG:HB2	15:N:184:ARG:CZ	2.32	0.58
18:Q:37:ARG:O	18:Q:41:ARG:HG3	2.02	0.58
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.24	0.58
24:W:16:ARG:NH1	24:W:65:ASP:O	2.36	0.58
27:Z:144:ARG:CZ	39:Z:8613:HOH:O	2.50	0.58
28:1:17:ARG:HG2	39:1:4874:HOH:O	2.03	0.58
1:A:801:U:H2'	1:A:802:G:C8	2.39	0.58
1:A:844:A:C6	1:A:882:A:C6	2.91	0.58
1:A:1205:U:H2'	1:A:1206:U:H5'	1.83	0.58
1:A:2044:G:OP1	26:Y:23:HIS:HE1	1.86	0.58
1:A:2050:G:OP1	39:A:3535:HOH:O	2.17	0.58
1:A:2253:G:N2	39:A:5010:HOH:O	2.25	0.58
2:B:3036:C:C5	2:B:3037:C:C5	2.92	0.58
4:C:200:PRO:HD3	39:C:8521:HOH:O	2.04	0.58
7:F:97:GLN:HG2	7:F:97:GLN:O	2.04	0.58
16:O:154:LEU:HD12	16:O:156:GLU:O	2.02	0.58
1:A:73:C:O2'	1:A:74:A:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:U:O4	1:A:627:G:C6	2.57	0.58
1:A:1552:G:H2'	1:A:1553:C:C6	2.38	0.58
1:A:2035:C:O2'	1:A:2036:C:H5'	2.03	0.58
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.34	0.58
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.03	0.58
21:T:43:GLU:HB3	39:T:8345:HOH:O	2.02	0.58
25:X:122:ARG:CZ	39:X:5817:HOH:O	2.52	0.58
1:A:68:U:OP1	39:A:9505:HOH:O	2.17	0.58
1:A:121:U:OP2	30:3:10:ARG:NH2	2.37	0.58
1:A:2621:U:H2'	1:A:2622:A:O4'	2.04	0.58
5:D:249:SER:OG	12:K:66:ASP:OD1	2.22	0.58
5:D:337:GLY:C	39:D:8557:HOH:O	2.42	0.58
7:F:95:THR:C	7:F:97:GLN:H	2.07	0.58
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.86	0.58
16:O:143:ARG:NH1	16:O:173:ASP:OD2	2.33	0.58
20:S:33:ARG:NH1	39:S:8545:HOH:O	2.35	0.58
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.86	0.58
1:A:283:U:H5	1:A:284:C:H42	1.52	0.58
1:A:1666:C:H2'	1:A:1667:A:C5'	2.33	0.58
2:B:3003:A:N6	2:B:3022:G:H1'	2.19	0.58
6:E:236:THR:H	6:E:239:ALA:HB3	1.69	0.58
8:G:127:ASP:HB3	39:G:6772:HOH:O	2.04	0.58
1:A:847:C:O2'	1:A:848:C:H5'	2.04	0.57
1:A:2745:C:H5	39:A:5361:HOH:O	1.87	0.57
5:D:102:THR:CG2	5:D:182:VAL:HG12	2.34	0.57
5:D:175:LEU:C	5:D:175:LEU:CD2	2.72	0.57
11:J:4:ALA:HB3	39:J:8365:HOH:O	2.02	0.57
11:J:27:LYS:H	11:J:58:HIS:CD2	2.15	0.57
11:J:71:TYR:C	11:J:73:GLN:N	2.56	0.57
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.69	0.57
1:A:244:C:O5'	1:A:244:C:H6	1.85	0.57
1:A:282:C:H1'	1:A:368:C:H42	1.66	0.57
1:A:299:U:C5'	39:A:6800:HOH:O	2.51	0.57
1:A:2421:G:H3'	1:A:2422:U:H5"	1.85	0.57
39:A:4048:HOH:O	15:N:86:MET:SD	2.56	0.57
4:C:213:LYS:HB2	39:C:8512:HOH:O	2.04	0.57
9:H:28:ALA:HB3	9:H:99:THR:O	2.04	0.57
12:K:70:PHE:N	39:K:6807:HOH:O	2.36	0.57
1:A:1743:G:N3	39:A:4368:HOH:O	2.32	0.57
1:A:2505:G:H8	39:A:5116:HOH:O	1.86	0.57
5:D:51:VAL:HG23	5:D:329:TYR:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:162:MET:HE3	5:D:308:LEU:CD2	2.29	0.57
20:S:119:VAL:O	20:S:119:VAL:HG12	2.03	0.57
23:V:8:TYR:O	23:V:46:ALA:CB	2.51	0.57
25:X:6:GLN:HB2	25:X:26:ILE:HD11	1.86	0.57
1:A:41:G:OP1	39:A:3436:HOH:O	2.17	0.57
1:A:825:U:H5"	1:A:826:U:OP1	2.04	0.57
1:A:952:G:H4'	39:A:3517:HOH:O	2.03	0.57
1:A:1215:A:O3'	1:A:1216:G:H4'	2.04	0.57
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.33	0.57
11:J:112:ARG:O	11:J:113:ALA:C	2.42	0.57
14:M:148:GLU:CG	39:M:8429:HOH:O	2.52	0.57
23:V:6:CYS:HB2	23:V:32:CYS:HB3	1.86	0.57
1:A:154:C:C2	1:A:155:C:C5	2.92	0.57
1:A:512:G:O3'	1:A:513:A:H8	1.87	0.57
1:A:792:G:O2'	1:A:793:A:H5'	2.04	0.57
1:A:1908:G:N1	1:A:1930:A:OP2	2.34	0.57
2:B:3049:G:H5"	39:B:8469:HOH:O	2.03	0.57
4:C:120:ARG:NH2	39:C:8584:HOH:O	2.36	0.57
18:Q:89:ASN:OD1	18:Q:89:ASN:O	2.21	0.57
1:A:569:A:OP2	39:A:8842:HOH:O	2.17	0.57
1:A:694:A:H2'	1:A:695:C:H5'	1.84	0.57
1:A:812:A:N3	39:A:3448:HOH:O	2.32	0.57
1:A:1163:G:H3'	1:A:1164:U:H2'	1.85	0.57
1:A:1299:G:O6	14:M:6:ARG:HD3	2.04	0.57
1:A:1512:G:N2	1:A:1513:C:H1'	2.19	0.57
1:A:2112:A:H2'	1:A:2113:G:C8	2.39	0.57
1:A:2860:G:N2	1:A:2898:G:C4	2.73	0.57
1:A:2864:U:OP1	23:V:35:LYS:HD2	2.05	0.57
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.51	0.57
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.86	0.57
11:J:151:MET:CE	11:J:151:MET:HA	2.35	0.57
12:K:52:GLN:HG2	39:K:5290:HOH:O	2.03	0.57
16:O:163:PHE:HA	39:O:8563:HOH:O	2.04	0.57
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.87	0.57
28:1:29:VAL:O	28:1:33:HIS:HB2	2.04	0.57
1:A:1456:C:H2'	1:A:1457:U:C6	2.39	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
1:A:1762:C:H4'	39:A:4130:HOH:O	2.05	0.57
1:A:1829:A:H5"	39:A:9585:HOH:O	2.04	0.57
1:A:2109:U:OP1	39:A:8642:HOH:O	2.17	0.57
1:A:2316:G:H4'	39:A:5562:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2453:G:O3'	14:M:50:GLY:HA2	2.05	0.57
1:A:2769:C:H2'	1:A:2770:G:O4'	2.04	0.57
39:A:4313:HOH:O	12:K:47:THR:HB	2.04	0.57
2:B:3013:A:O2'	2:B:3014:G:H5"	2.04	0.57
5:D:175:LEU:O	5:D:178:ALA:HB3	2.04	0.57
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.85	0.57
13:L:22:ASP:HB2	39:L:5264:HOH:O	2.05	0.57
16:O:151:ASP:OD1	16:O:151:ASP:O	2.21	0.57
1:A:245:C:H2'	1:A:246:G:H5'	1.87	0.57
1:A:532:A:N6	1:A:2661:U:H4'	2.19	0.57
1:A:534:C:OP2	39:A:6911:HOH:O	2.17	0.57
1:A:536:A:HO2'	1:A:2061:C:HO2'	1.45	0.57
1:A:781:C:H4'	1:A:873:G:OP1	2.05	0.57
1:A:1314:U:C2	1:A:1316:G:N2	2.73	0.57
1:A:2301:A:H5"	1:A:2302:A:H5'	1.87	0.57
1:A:2382:A:OP1	31:4:80:ARG:HG2	2.04	0.57
1:A:2613:G:H2'	1:A:2614:C:H6	1.70	0.57
1:A:2769:C:O2'	1:A:2770:G:H5'	2.04	0.57
1:A:2862:G:H4'	5:D:336:GLN:O	2.04	0.57
6:E:21:VAL:C	6:E:23:GLU:H	2.08	0.57
6:E:233:THR:CG2	6:E:234:VAL:N	2.68	0.57
12:K:74:ARG:HH11	12:K:74:ARG:CB	2.16	0.57
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.87	0.57
14:M:148:GLU:HB2	39:M:8467:HOH:O	2.03	0.57
27:Z:143:TRP:CE2	27:Z:164:VAL:HG23	2.40	0.57
1:A:21:G:H4'	20:S:2:ILE:HG22	1.85	0.57
1:A:422:G:O2'	1:A:423:A:H5'	2.04	0.57
1:A:960:G:N3	1:A:960:G:C2'	2.67	0.57
1:A:1667:A:H2'	1:A:1668:U:C6	2.40	0.57
1:A:1973:A:H5'	1:A:1973:A:H8	1.67	0.57
2:B:3055:U:H4'	2:B:3056:A:C8	2.40	0.57
6:E:15:GLU:HG3	39:E:8340:HOH:O	2.03	0.57
8:G:57:LYS:O	8:G:60:SER:HB2	2.04	0.57
10:I:64:ASN:HD22	10:I:64:ASN:H	1.53	0.57
14:M:73:VAL:HG23	14:M:74:THR:N	2.20	0.57
1:A:200:U:H2'	39:A:9937:HOH:O	2.04	0.57
1:A:1193:A:O2'	39:A:6854:HOH:O	2.17	0.57
1:A:1654:U:H5"	39:A:6881:HOH:O	2.03	0.57
1:A:1696:U:H5"	39:A:4987:HOH:O	2.05	0.57
1:A:2135:A:O2'	1:A:2136:G:H5'	2.05	0.57
1:A:2729:C:H2'	1:A:2730:G:C8	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:120:ASP:HB3	6:E:123:LEU:HB2	1.87	0.57
7:F:49:PRO:HG3	39:F:5828:HOH:O	2.05	0.57
9:H:19:ALA:O	9:H:22:VAL:HG22	2.05	0.57
15:N:157:LEU:HD23	39:N:8628:HOH:O	2.04	0.57
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.87	0.57
23:V:52:THR:HG22	23:V:54:THR:HB	1.87	0.57
31:4:55:VAL:HB	31:4:56:PRO:HD2	1.87	0.57
1:A:506:G:C5'	39:A:5408:HOH:O	2.53	0.56
1:A:1164:U:O5'	1:A:1164:U:H6	1.88	0.56
1:A:2897:C:H2'	1:A:2898:G:H8	1.70	0.56
5:D:41:PHE:HB3	5:D:190:MET:HE1	1.87	0.56
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.86	0.56
16:O:139:TRP:HH2	16:O:176:ARG:HH11	1.53	0.56
16:O:151:ASP:OD1	16:O:154:LEU:HD13	2.05	0.56
16:O:154:LEU:HD11	16:O:157:PRO:HA	1.87	0.56
30:3:19:SER:O	30:3:36:ASN:ND2	2.38	0.56
31:4:15:ASN:ND2	39:4:8547:HOH:O	2.37	0.56
1:A:347:A:O2'	1:A:348:C:H5'	2.06	0.56
1:A:638:C:OP1	27:Z:138:ARG:HG2	2.05	0.56
1:A:1169:U:C5	1:A:1170:U:C4	2.93	0.56
1:A:1377:C:H5'	1:A:1377:C:C6	2.36	0.56
1:A:2715:G:H5'	5:D:13:PHE:CE1	2.40	0.56
2:B:3031:C:O2'	2:B:3032:G:H5'	2.04	0.56
14:M:143:THR:HG22	14:M:145:LEU:H	1.69	0.56
15:N:67:ILE:CG2	15:N:97:ILE:HG23	2.35	0.56
1:A:559:U:H2'	1:A:560:C:O4'	2.05	0.56
1:A:695:C:H2'	1:A:696:C:C6	2.40	0.56
1:A:1393:A:H2'	1:A:1394:C:C6	2.40	0.56
1:A:1728:G:H1'	39:A:9205:HOH:O	2.04	0.56
1:A:2053:G:H4'	20:S:136:TRP:CE2	2.41	0.56
1:A:2436:U:OP1	31:4:68:LYS:NZ	2.37	0.56
1:A:2890:A:H1'	23:V:56:ARG:HH21	1.68	0.56
4:C:88:ILE:HG22	4:C:88:ILE:O	2.04	0.56
5:D:7:ARG:HG2	5:D:7:ARG:NH1	2.18	0.56
5:D:7:ARG:NH2	39:D:8538:HOH:O	2.35	0.56
11:J:28:ILE:HA	11:J:62:GLU:OE1	2.04	0.56
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.15	0.56
28:1:30:GLU:HA	28:1:33:HIS:CB	2.35	0.56
28:1:34:LYS:NZ	39:1:7354:HOH:O	2.27	0.56
1:A:2812:A:H1'	39:A:5262:HOH:O	2.05	0.56
39:A:5675:HOH:O	5:D:2:GLN:CD	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:76:DA:H2"	36:5:77:PO4:O1	2.05	0.56
8:G:132:THR:O	8:G:132:THR:HG23	2.06	0.56
25:X:122:ARG:NH1	25:X:152:ALA:O	2.39	0.56
29:2:28:HIS:HD2	29:2:30:LYS:H	1.54	0.56
1:A:29:C:O2'	1:A:30:U:H5'	2.05	0.56
1:A:1370:G:OP1	20:S:64:SER:OG	2.18	0.56
1:A:1439:C:OP1	30:3:41:HIS:HE1	1.89	0.56
1:A:1462:C:O2'	1:A:1463:A:H5'	2.05	0.56
1:A:1632:A:O5'	1:A:1632:A:H8	1.89	0.56
1:A:1916:C:O2'	1:A:1917:G:H5'	2.05	0.56
1:A:2400:G:H4'	39:A:4620:HOH:O	2.06	0.56
1:A:2785:C:H4'	1:A:2786:G:OP2	2.06	0.56
15:N:28:MET:HA	15:N:31:TRP:HB2	1.88	0.56
19:R:29:ALA:HB1	39:R:1295:HOH:O	2.05	0.56
23:V:44:ARG:HB3	39:V:3805:HOH:O	2.06	0.56
23:V:52:THR:HG22	23:V:54:THR:H	1.69	0.56
1:A:474:C:O3'	6:E:73:LEU:HD21	2.06	0.56
1:A:613:C:H5'	39:A:3428:HOH:O	2.06	0.56
1:A:668:C:H2'	1:A:669:G:C8	2.41	0.56
1:A:734:U:O2'	1:A:737:A:N6	2.39	0.56
1:A:1787:C:H4'	1:A:2883:A:O4'	2.06	0.56
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.36	0.56
5:D:146:THR:O	5:D:159:PRO:HB3	2.05	0.56
13:L:101:ASN:O	13:L:102:GLU:HB2	2.04	0.56
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.56
1:A:1666:C:C2'	1:A:1667:A:C5'	2.84	0.56
1:A:1923:G:H4'	31:4:31:THR:O	2.06	0.56
1:A:2346:C:O3'	7:F:52:THR:CG2	2.54	0.56
4:C:4:ILE:HB	39:C:8516:HOH:O	2.05	0.56
6:E:78:ARG:HG3	6:E:78:ARG:NH1	1.95	0.56
7:F:93:LEU:HG	39:F:3862:HOH:O	2.05	0.56
12:K:93:ARG:HB3	12:K:93:ARG:NH1	2.20	0.56
12:K:107:ASN:HD22	12:K:109:TYR:H	1.52	0.56
18:Q:120:ARG:NH2	18:Q:123:TYR:CD2	2.74	0.56
19:R:26:PRO:HA	39:R:2847:HOH:O	2.04	0.56
20:S:99:ALA:CB	20:S:109:MET:CE	2.80	0.56
1:A:42:C:H1'	39:A:4151:HOH:O	2.04	0.56
1:A:1162:G:N3	1:A:1162:G:H2'	2.20	0.56
1:A:1772:C:H5'	1:A:1773:G:C5	2.40	0.56
1:A:1886:A:H4'	39:1:395:HOH:O	2.05	0.56
1:A:2058:G:N7	39:A:9333:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:6853:HOH:O	27:Z:133:HIS:HE1	1.88	0.56
39:A:8718:HOH:O	27:Z:125:LYS:HD3	2.05	0.56
4:C:101:GLU:HG2	4:C:131:HIS:ND1	2.21	0.56
7:F:50:VAL:O	7:F:71:ALA:HA	2.06	0.56
12:K:63:ILE:HG22	12:K:64:GLY:N	2.20	0.56
17:P:25:VAL:HG23	17:P:26:TRP:H	1.71	0.56
24:W:39:ALA:O	24:W:41:GLU:N	2.39	0.56
1:A:120:A:H2'	1:A:120:A:N3	2.21	0.56
1:A:236:A:H8	1:A:236:A:OP1	1.89	0.56
1:A:668:C:H2'	1:A:669:G:H8	1.71	0.56
1:A:710:G:O2'	1:A:711:G:H5'	2.06	0.56
1:A:800:G:H4'	39:A:6524:HOH:O	2.05	0.56
1:A:1236:A:H2'	1:A:1237:U:O4'	2.06	0.56
5:D:41:PHE:CE1	5:D:79:MET:HG3	2.41	0.56
5:D:87:TYR:O	5:D:138:GLY:N	2.31	0.56
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.54	0.56
7:F:67:ASP:O	7:F:69:ILE:HG13	2.06	0.56
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.87	0.56
15:N:60:ILE:HG12	15:N:134:ILE:HD12	1.87	0.56
1:A:31:C:OP2	22:U:8:ARG:HD2	2.05	0.56
1:A:84:G:O2'	1:A:85:C:H5'	2.06	0.56
1:A:251:C:H1'	15:N:58:GLN:HE22	1.71	0.56
1:A:1329:A:C2	39:A:4159:HOH:O	2.53	0.56
39:A:4723:HOH:O	15:N:29:GLN:HA	2.05	0.56
2:B:3037:C:H4'	16:O:110:THR:CG2	2.35	0.56
4:C:188:ASN:HA	39:C:8562:HOH:O	2.05	0.56
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.88	0.56
7:F:86:THR:O	7:F:90:LEU:HG	2.06	0.56
9:H:33:THR:O	9:H:33:THR:HG22	2.05	0.56
13:L:101:ASN:HA	39:L:6456:HOH:O	2.06	0.56
15:N:77:PHE:HD2	39:N:8525:HOH:O	1.89	0.56
25:X:63:GLU:HG2	25:X:93:ILE:HG22	1.87	0.56
25:X:72:PRO:CG	25:X:77:ALA:HB3	2.34	0.56
1:A:1186:C:C4	1:A:1187:U:C4	2.93	0.55
1:A:1701:A:H4'	1:A:1702:U:H5"	1.88	0.55
1:A:1878:G:H1'	39:A:5591:HOH:O	2.06	0.55
1:A:2241:C:O2'	1:A:2242:U:H5'	2.06	0.55
4:C:217:ARG:HH11	4:C:217:ARG:CG	2.19	0.55
7:F:93:LEU:HB3	7:F:97:GLN:OE1	2.07	0.55
7:F:146:LYS:HE2	16:O:107:ASN:ND2	2.21	0.55
7:F:156:ARG:NH1	39:F:5234:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:81:GLU:HB3	39:G:4761:HOH:O	2.05	0.55
11:J:44:ALA:HA	11:J:163:PRO:O	2.06	0.55
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.35	0.55
16:O:37:ARG:HD3	35:O:8507:CL:CL	2.43	0.55
19:R:10:THR:HB	19:R:14:LEU:HG	1.88	0.55
1:A:113:A:OP2	1:A:114:A:H5"	2.06	0.55
1:A:1592:G:C5	1:A:1593:C:C4	2.94	0.55
1:A:1878:G:O2'	1:A:1879:U:C6	2.58	0.55
1:A:2613:G:H2'	1:A:2614:C:C6	2.41	0.55
5:D:129:ARG:O	5:D:133:GLU:HG3	2.07	0.55
8:G:11:VAL:CG1	8:G:12:ASP:N	2.69	0.55
11:J:26:LYS:CD	11:J:28:ILE:HB	2.36	0.55
11:J:86:ARG:NH1	11:J:130:HIS:CD2	2.75	0.55
18:Q:38:GLU:CA	18:Q:41:ARG:NH1	2.68	0.55
20:S:39:THR:HB	20:S:42:GLU:HG3	1.87	0.55
1:A:51:G:N2	1:A:111:C:C2	2.74	0.55
1:A:522:U:O2'	1:A:1366:C:H5'	2.05	0.55
1:A:797:A:O4'	28:1:10:ARG:N	2.39	0.55
1:A:849:C:C2'	1:A:850:U:H5'	2.36	0.55
1:A:1305:C:O2'	1:A:1306:U:H5'	2.06	0.55
1:A:2477:C:O2'	1:A:2478:U:H5'	2.06	0.55
2:B:3001:U:O3'	2:B:3003:A:H5"	2.07	0.55
2:B:3076:G:C3'	2:B:3077:A:H5"	2.35	0.55
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.12	0.55
6:E:107:ARG:CB	6:E:107:ARG:HH11	2.19	0.55
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.75	0.55
15:N:79:LYS:NZ	39:N:8554:HOH:O	2.38	0.55
16:O:154:LEU:O	16:O:155:GLU:HB3	2.06	0.55
19:R:26:PRO:O	19:R:27:GLN:C	2.44	0.55
22:U:20:HIS:CE1	22:U:67:LEU:HD11	2.41	0.55
1:A:790:A:H1'	1:A:1710:A:C2'	2.36	0.55
1:A:1425:G:O2'	1:A:1426:C:H5'	2.06	0.55
1:A:2594:C:H2'	1:A:2595:U:H5'	1.86	0.55
6:E:54:LEU:HD23	6:E:79:ARG:HG3	1.87	0.55
6:E:115:LEU:CD1	6:E:223:LEU:HD21	2.34	0.55
9:H:91:VAL:CG1	39:H:985:HOH:O	2.54	0.55
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.53	0.55
13:L:109:LEU:HD13	13:L:113:ILE:HD11	1.89	0.55
15:N:36:ALA:HB1	39:N:8548:HOH:O	2.07	0.55
25:X:81:ASP:OD1	25:X:92:ASP:HB2	2.06	0.55
1:A:154:C:N3	1:A:155:C:C5	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:A:H2'	6:E:150:THR:OG1	2.06	0.55
1:A:1477:C:H5'	1:A:1868:G:H5'	1.89	0.55
1:A:1593:C:OP1	18:Q:117:SER:HB3	2.07	0.55
1:A:1631:A:O2'	1:A:1632:A:H5'	2.07	0.55
1:A:1869:A:OP2	39:A:4447:HOH:O	2.17	0.55
7:F:63:ILE:C	39:F:5728:HOH:O	2.45	0.55
7:F:153:THR:HG22	39:F:5234:HOH:O	2.05	0.55
7:F:154:LYS:HD3	39:F:1796:HOH:O	2.06	0.55
16:O:48:VAL:HG12	39:O:8552:HOH:O	2.06	0.55
17:P:59:VAL:HG23	17:P:111:VAL:HG23	1.87	0.55
30:3:40:ARG:HG2	30:3:40:ARG:NH1	2.20	0.55
1:A:877:G:H1'	39:A:8677:HOH:O	2.06	0.55
1:A:1166:A:H61	1:A:1180:U:H3	1.52	0.55
1:A:2032:U:H5'	39:A:3988:HOH:O	2.05	0.55
1:A:2419:U:H5"	1:A:2420:G:H5'	1.89	0.55
1:A:2900:G:H2'	1:A:2901:C:O4'	2.07	0.55
2:B:3023:U:H5"	2:B:3023:U:C6	2.42	0.55
5:D:241:PRO:HD2	39:D:8658:HOH:O	2.06	0.55
15:N:164:THR:CG2	15:N:165:SER:N	2.67	0.55
16:O:32:PRO:HD2	16:O:99:GLU:O	2.06	0.55
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.42	0.55
1:A:820:G:H5'	1:A:821:U:H5'	1.87	0.55
1:A:1851:G:O2'	1:A:1852:A:H5'	2.05	0.55
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.71	0.55
2:B:3037:C:H4'	16:O:110:THR:HG23	1.88	0.55
5:D:41:PHE:HB3	5:D:190:MET:CE	2.37	0.55
9:H:101:ALA:HB2	9:H:108:LEU:CD2	2.37	0.55
11:J:150:LYS:O	11:J:150:LYS:HG2	2.03	0.55
11:J:163:PRO:O	11:J:164:ALA:HB2	2.06	0.55
17:P:33:LEU:HA	17:P:40:HIS:CE1	2.42	0.55
17:P:88:LYS:O	39:P:4826:HOH:O	2.18	0.55
18:Q:8:ARG:HG3	39:Q:5725:HOH:O	2.06	0.55
18:Q:59:ARG:HG2	18:Q:59:ARG:HH11	1.72	0.55
26:Y:25:ARG:HG2	39:Y:5356:HOH:O	2.05	0.55
1:A:285:A:H2'	1:A:286:U:O4'	2.06	0.55
1:A:656:G:OP2	17:P:37:ARG:HD2	2.07	0.55
1:A:849:C:H2'	1:A:850:U:H5'	1.89	0.55
1:A:1652:C:O2	4:C:164:ARG:HD2	2.06	0.55
39:A:9971:HOH:O	6:E:98:ARG:HB3	2.07	0.55
6:E:29:ASP:OD1	17:P:5:PRO:CD	2.55	0.55
7:F:23:VAL:HG12	7:F:130:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:57:ARG:HG3	11:J:57:ARG:HH11	1.71	0.55
11:J:112:ARG:C	11:J:114:PRO:HD3	2.27	0.55
15:N:39:ARG:HA	15:N:63:VAL:HG22	1.88	0.55
23:V:37:GLU:OE2	39:V:408:HOH:O	2.18	0.55
29:2:10:LYS:HB2	39:2:2979:HOH:O	2.05	0.55
1:A:212:A:H8	1:A:212:A:OP1	1.90	0.55
1:A:329:A:C5	1:A:347:A:C2	2.95	0.55
1:A:1930:A:H2'	1:A:1931:A:C8	2.41	0.55
1:A:2896:A:H5"	39:A:5569:HOH:O	2.06	0.55
2:B:3011:A:OP2	39:B:8536:HOH:O	2.18	0.55
14:M:73:VAL:HG23	14:M:74:THR:H	1.72	0.55
14:M:145:LEU:O	14:M:148:GLU:HG3	2.06	0.55
16:O:114:LYS:O	16:O:117:ALA:HB3	2.07	0.55
19:R:43:ILE:O	19:R:45:PRO:HD3	2.06	0.55
26:Y:71:ARG:HB2	39:Y:6590:HOH:O	2.07	0.55
28:1:31:ILE:HG23	28:1:32:LYS:H	1.70	0.55
1:A:78:G:N1	1:A:98:A:OP2	2.39	0.55
1:A:80:A:H5"	22:U:41:ARG:CZ	2.37	0.55
1:A:447:A:O2'	1:A:448:G:H5'	2.07	0.55
1:A:797:A:H5'	28:1:10:ARG:HG2	1.89	0.55
1:A:1016:U:O2'	1:A:2303:A:N7	2.26	0.55
1:A:1316:G:O6	39:A:6027:HOH:O	2.18	0.55
1:A:1810:C:N3	1:A:1811:A:C5	2.75	0.55
1:A:1871:U:P	39:A:4642:HOH:O	2.65	0.55
1:A:2626:C:H2'	1:A:2627:G:C8	2.42	0.55
2:B:3092:G:C6	2:B:3093:A:C6	2.95	0.55
4:C:97:ALA:HB2	4:C:150:PRO:HB2	1.89	0.55
11:J:139:ASP:N	11:J:140:PRO:CD	2.66	0.55
15:N:69:LYS:CG	15:N:127:LYS:HG3	2.37	0.55
24:W:4:HIS:HB3	39:W:6622:HOH:O	2.07	0.55
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.54
1:A:1215:A:O3'	1:A:1216:G:C4'	2.55	0.54
1:A:1590:A:H1'	1:A:1606:A:C2	2.42	0.54
1:A:2632:G:O2'	39:A:9389:HOH:O	2.18	0.54
7:F:62:ASP:HA	39:F:4233:HOH:O	2.07	0.54
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.88	0.54
10:I:27:ILE:HD12	10:I:70:ALA:HB1	1.89	0.54
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.72	0.54
11:J:117:LYS:O	11:J:119:VAL:HG13	2.08	0.54
26:Y:71:ARG:HD3	39:Y:2171:HOH:O	2.06	0.54
1:A:169:A:HO2'	1:A:170:U:H6	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:N3	1:A:644:G:H5'	2.22	0.54
1:A:1292:G:H5'	39:A:9882:HOH:O	2.05	0.54
1:A:1593:C:OP1	18:Q:117:SER:CB	2.55	0.54
1:A:1827:G:C6	1:A:1828:G:C6	2.95	0.54
1:A:2104:C:O2	1:A:2485:A:N1	2.41	0.54
1:A:2526:C:C2'	1:A:2527:U:H5'	2.38	0.54
2:B:3056:A:C3'	2:B:3057:A:H5"	2.37	0.54
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.42	0.54
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.89	0.54
8:G:23:GLU:HG2	8:G:28:SER:CB	2.37	0.54
13:L:115:ARG:O	13:L:118:ALA:N	2.37	0.54
14:M:134:GLU:HG3	39:M:8435:HOH:O	2.07	0.54
18:Q:13:VAL:HG11	18:Q:40:VAL:CG1	2.37	0.54
28:1:31:ILE:CG2	28:1:32:LYS:H	2.20	0.54
1:A:234:A:O2'	1:A:436:A:N3	2.37	0.54
1:A:255:A:H2'	1:A:256:C:H6	1.70	0.54
1:A:585:C:H2'	1:A:586:C:C6	2.42	0.54
1:A:1188:A:C5	1:A:1189:A:C2	2.95	0.54
1:A:1669:A:C2	39:A:3196:HOH:O	2.52	0.54
1:A:1979:G:OP1	39:A:5778:HOH:O	2.18	0.54
1:A:2387:U:O2	1:A:2402:A:C2	2.60	0.54
1:A:2727:A:C2'	1:A:2728:C:H5'	2.37	0.54
1:A:2729:C:O2'	1:A:2730:G:H5'	2.07	0.54
6:E:103:ASN:O	6:E:104:ASP:C	2.45	0.54
9:H:28:ALA:CB	9:H:99:THR:HG23	2.37	0.54
12:K:93:ARG:HH11	12:K:93:ARG:CB	2.20	0.54
15:N:87:MET:CG	31:4:46:ILE:HG21	2.30	0.54
16:O:71:TRP:N	39:O:8538:HOH:O	2.40	0.54
17:P:32:ARG:CB	39:P:4656:HOH:O	2.49	0.54
24:W:27:LEU:HA	24:W:49:LEU:HD13	1.88	0.54
1:A:933:C:O2'	1:A:934:C:H5'	2.07	0.54
1:A:1118:A:H8	1:A:1119:G:H5"	1.71	0.54
1:A:1286:A:H2'	39:A:3321:HOH:O	2.06	0.54
1:A:1330:A:H5"	1:A:1331:A:OP2	2.07	0.54
1:A:1625:U:H5'	39:A:4142:HOH:O	2.07	0.54
1:A:2361:A:O2'	39:A:8578:HOH:O	2.18	0.54
1:A:2501:G:N7	39:A:9281:HOH:O	2.33	0.54
1:A:2819:C:O2	5:D:85:ARG:NH2	2.40	0.54
39:A:5314:HOH:O	13:L:79:PRO:HG2	2.07	0.54
39:B:8479:HOH:O	16:O:23:ARG:NH1	2.39	0.54
6:E:78:ARG:CG	6:E:78:ARG:NH1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:99:ASP:HB2	7:F:103:ASN:H	1.73	0.54
11:J:62:GLU:O	11:J:66:VAL:HG23	2.08	0.54
11:J:74:ASN:HD22	11:J:141:ASN:CG	2.11	0.54
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.07	0.54
28:1:73:THR:O	28:1:76:GLY:N	2.40	0.54
1:A:61:G:O2'	1:A:62:C:H5'	2.08	0.54
1:A:426:G:H2'	1:A:427:C:O4'	2.08	0.54
1:A:1352:A:N1	6:E:48:SER:HB3	2.22	0.54
1:A:2338:G:OP1	7:F:97:GLN:HG3	2.07	0.54
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.72	0.54
2:B:3026:C:OP2	39:B:8443:HOH:O	2.19	0.54
9:H:22:VAL:CG2	9:H:104:ALA:HB2	2.38	0.54
13:L:118:ALA:O	13:L:120:ARG:N	2.41	0.54
22:U:23:VAL:HG23	22:U:41:ARG:HG3	1.89	0.54
25:X:122:ARG:NH2	39:X:4276:HOH:O	2.38	0.54
26:Y:18:ARG:NH1	39:Y:4132:HOH:O	2.32	0.54
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	1.87	0.54
1:A:2050:G:H5"	20:S:80:TYR:O	2.08	0.54
4:C:211:LYS:HB2	39:C:8619:HOH:O	2.06	0.54
5:D:36:PRO:CA	5:D:168:GLY:HA3	2.38	0.54
5:D:139:ASP:O	39:D:8584:HOH:O	2.18	0.54
14:M:35:ARG:C	14:M:35:ARG:HD3	2.28	0.54
17:P:49:GLU:HG2	39:P:5191:HOH:O	2.06	0.54
18:Q:31:ILE:HG12	18:Q:43:LEU:HD13	1.89	0.54
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	2.05	0.54
19:R:24:SER:N	39:R:4792:HOH:O	2.35	0.54
20:S:132:ARG:NH2	39:S:8587:HOH:O	2.41	0.54
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.08	0.54
1:A:241:A:N1	1:A:378:A:H4'	2.22	0.54
1:A:2533:C:H5'	1:A:2533:C:C6	2.38	0.54
1:A:2849:U:OP1	39:A:6680:HOH:O	2.18	0.54
39:B:8531:HOH:O	16:O:107:ASN:HB3	2.07	0.54
10:I:12:ILE:N	10:I:13:PRO:CD	2.71	0.54
11:J:5:MET:HG3	39:J:8365:HOH:O	2.07	0.54
18:Q:143:ALA:N	39:Q:5521:HOH:O	2.40	0.54
1:A:152:A:C2	1:A:153:C:C2	2.96	0.54
1:A:1815:A:N1	39:A:9069:HOH:O	2.34	0.54
1:A:2064:U:H5'	1:A:2652:U:H4'	1.89	0.54
1:A:2281:C:H2'	1:A:2282:U:H5'	1.89	0.54
1:A:2716:G:H1'	39:D:8545:HOH:O	2.07	0.54
1:A:2878:U:H2'	1:A:2879:A:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3039:U:H1'	2:B:3044:A:H61	1.72	0.54
7:F:25:MET:HE1	7:F:37:ALA:O	2.08	0.54
11:J:48:LEU:HD11	11:J:157:ILE:HG21	1.90	0.54
13:L:122:GLY:O	13:L:125:ALA:N	2.41	0.54
16:O:159:TYR:CE2	16:O:163:PHE:HE2	2.26	0.54
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.20	0.54
27:Z:134:HIS:CD2	27:Z:134:HIS:H	2.25	0.54
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.89	0.54
1:A:274:G:N2	1:A:377:C:C2	2.76	0.54
1:A:1116:U:HO2'	1:A:1118:A:H2	0.70	0.54
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.54
1:A:1204:C:H1'	39:A:4219:HOH:O	2.07	0.54
1:A:1874:U:C2'	4:C:120:ARG:HG3	2.35	0.54
1:A:1974:G:OP1	39:A:6324:HOH:O	2.18	0.54
1:A:2114:C:OP1	4:C:1:GLY:HA2	2.08	0.54
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.54
1:A:2779:G:O2'	1:A:2780:C:H5'	2.08	0.54
2:B:3047:A:C2	2:B:3048:C:C2	2.95	0.54
2:B:3055:U:H4'	2:B:3056:A:H8	1.72	0.54
4:C:194:MET:CE	4:C:199:HIS:HB2	2.37	0.54
6:E:201:SER:HB3	6:E:204:ALA:HB3	1.89	0.54
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.37	0.54
16:O:151:ASP:O	16:O:154:LEU:HB2	2.08	0.54
18:Q:7:LYS:HD3	18:Q:21:VAL:HG21	1.90	0.54
22:U:4:PRO:CB	39:U:2331:HOH:O	2.55	0.54
26:Y:15:ARG:HB3	26:Y:15:ARG:HH11	1.72	0.54
29:2:22:CYS:HB2	39:2:1159:HOH:O	2.08	0.54
1:A:119:A:H2'	1:A:120:A:C5'	2.38	0.54
1:A:136:C:H2'	1:A:137:U:O4'	2.07	0.54
1:A:645:U:OP2	14:M:4:LYS:CE	2.54	0.54
1:A:1189:A:H1'	1:A:1209:C:O4'	2.08	0.54
1:A:1473:U:C2	39:A:9250:HOH:O	2.53	0.54
1:A:1473:U:O2'	1:A:1474:C:H5"	2.08	0.54
1:A:2775:A:C6	1:A:2799:A:C8	2.96	0.54
39:A:9734:HOH:O	4:C:221:PRO:HA	2.07	0.54
5:D:55:ASN:HB3	5:D:64:GLY:H	1.73	0.54
7:F:10:PHE:CE1	7:F:11:HIS:HB3	2.43	0.54
10:I:23:ILE:HG22	10:I:70:ALA:CB	2.38	0.54
11:J:59:ASN:N	11:J:59:ASN:ND2	2.46	0.54
15:N:24:MET:HE3	15:N:28:MET:HE3	1.90	0.54
15:N:84:LYS:HE2	39:N:8574:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:16:VAL:CG1	18:Q:17:GLY:H	2.19	0.54
29:2:1:THR:HB	39:2:6858:HOH:O	2.07	0.54
1:A:799:C:O2	39:A:8533:HOH:O	2.18	0.53
1:A:839:C:P	39:A:9043:HOH:O	2.66	0.53
1:A:1509:C:O2'	1:A:1510:G:H5'	2.09	0.53
1:A:1741:U:O3'	1:A:1742:A:H8	1.90	0.53
1:A:1815:A:H5'	39:A:3650:HOH:O	2.07	0.53
1:A:2039:A:H2'	1:A:2040:C:C6	2.43	0.53
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.41	0.53
4:C:48:ASP:HB3	39:C:8608:HOH:O	2.06	0.53
5:D:162:MET:HE2	5:D:310:ARG:HD3	1.91	0.53
6:E:246:ARG:NH2	39:E:8431:HOH:O	2.40	0.53
7:F:154:LYS:H	7:F:154:LYS:CD	2.15	0.53
8:G:54:ASP:OD1	8:G:54:ASP:N	2.40	0.53
11:J:136:VAL:HG23	39:J:8342:HOH:O	2.08	0.53
1:A:363:A:O5'	1:A:363:A:H8	1.91	0.53
1:A:1625:U:C5'	39:A:4142:HOH:O	2.57	0.53
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.90	0.53
5:D:54:VAL:HB	39:D:8615:HOH:O	2.07	0.53
5:D:82:VAL:HG12	5:D:101:TRP:CZ3	2.43	0.53
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.43	0.53
13:L:49:LEU:HD12	13:L:80:ILE:HD13	1.90	0.53
14:M:72:ASN:HB2	39:M:8461:HOH:O	2.09	0.53
15:N:186:SER:O	15:N:189:VAL:HG12	2.08	0.53
17:P:70:LEU:O	17:P:92:VAL:HG21	2.08	0.53
20:S:80:TYR:N	20:S:81:PRO:HD3	2.24	0.53
28:1:31:ILE:CG2	28:1:32:LYS:N	2.71	0.53
1:A:755:G:O2'	1:A:756:A:H5'	2.08	0.53
1:A:1269:G:H2'	1:A:1270:U:C6	2.42	0.53
1:A:1400:C:H1'	39:A:3622:HOH:O	2.08	0.53
1:A:1853:C:H5'	4:C:228:ILE:O	2.08	0.53
1:A:2269:C:H2'	1:A:2270:G:C5'	2.39	0.53
1:A:2309:C:H5"	39:A:9513:HOH:O	2.07	0.53
39:A:5759:HOH:O	7:F:99:ASP:HA	2.08	0.53
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.38	0.53
5:D:16:ARG:NE	39:D:8558:HOH:O	2.26	0.53
6:E:20:ASP:O	6:E:23:GLU:HB2	2.08	0.53
6:E:98:ARG:NH1	39:E:8362:HOH:O	2.35	0.53
6:E:152:GLU:OE1	39:E:8421:HOH:O	2.19	0.53
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.38	0.53
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:G:H5'	39:A:5408:HOH:O	2.07	0.53
1:A:793:A:H5"	18:Q:83:LYS:HG2	1.91	0.53
1:A:1181:A:H2'	1:A:1182:C:O4'	2.07	0.53
1:A:1405:U:O2'	39:A:5751:HOH:O	2.19	0.53
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.74	0.53
1:A:2782:G:O6	1:A:2790:C:H5"	2.08	0.53
4:C:94:LEU:N	4:C:94:LEU:HD23	2.23	0.53
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.90	0.53
6:E:5:ILE:CG2	39:E:8438:HOH:O	2.55	0.53
7:F:10:PHE:O	7:F:11:HIS:O	2.26	0.53
14:M:143:THR:CG2	14:M:144:ASP:H	2.21	0.53
1:A:106:A:H1'	39:A:9003:HOH:O	2.07	0.53
1:A:247:A:C6	1:A:262:A:C2	2.96	0.53
1:A:399:C:OP2	39:A:3398:HOH:O	2.18	0.53
1:A:542:A:H2'	1:A:543:G:O4'	2.08	0.53
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.08	0.53
1:A:2819:C:H2'	1:A:2820:A:H8	1.72	0.53
4:C:55:VAL:CG1	4:C:67:LEU:HD22	2.37	0.53
4:C:84:VAL:O	4:C:98:GLU:HG3	2.07	0.53
4:C:94:LEU:HD21	4:C:156:ILE:HD11	1.90	0.53
4:C:114:ASP:HB2	4:C:117:LYS:HE2	1.91	0.53
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.08	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.57	0.53
13:L:30:LYS:O	13:L:55:VAL:HG13	2.08	0.53
14:M:143:THR:CG2	14:M:144:ASP:N	2.71	0.53
17:P:32:ARG:CG	39:P:3240:HOH:O	2.56	0.53
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.06	0.53
1:A:860:U:H2'	1:A:861:A:C8	2.43	0.53
1:A:1795:G:OP2	39:A:3003:HOH:O	2.18	0.53
1:A:2240:U:H5"	39:A:5844:HOH:O	2.09	0.53
1:A:2413:A:N6	16:O:109:PRO:HG3	2.24	0.53
1:A:2754:G:H2'	1:A:2755:G:O4'	2.08	0.53
1:A:2815:G:C8	39:A:5194:HOH:O	2.53	0.53
39:B:8479:HOH:O	16:O:23:ARG:HD3	2.09	0.53
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.91	0.53
6:E:76:ARG:HD3	39:E:8372:HOH:O	2.09	0.53
6:E:127:ARG:HH21	6:E:225:PRO:HG2	1.64	0.53
11:J:46:VAL:HG13	11:J:160:ASP:O	2.09	0.53
15:N:3:SER:OG	15:N:5:TYR:HB2	2.08	0.53
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.43	0.53
28:1:47:LEU:HA	28:1:56:MET:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:1:MET:N	31:4:87:ARG:O	2.38	0.53
1:A:660:A:H4'	1:A:661:G:O5'	2.09	0.53
1:A:1345:A:C6	1:A:1346:U:O4	2.62	0.53
1:A:1972:U:H2'	1:A:1973:A:H5'	1.91	0.53
39:A:9059:HOH:O	25:X:119:HIS:HE1	1.92	0.53
2:B:3078:G:O2'	2:B:3079:U:P	2.67	0.53
9:H:107:VAL:O	9:H:111:ILE:HG13	2.08	0.53
11:J:35:ASN:ND2	11:J:79:ALA:O	2.42	0.53
14:M:98:GLU:O	14:M:99:GLU:CB	2.57	0.53
1:A:1096:U:O2	1:A:1261:A:C2	2.62	0.53
1:A:1306:U:OP1	6:E:184:ARG:HD2	2.08	0.53
1:A:1615:A:H5'	39:A:3670:HOH:O	2.08	0.53
4:C:1:GLY:HA2	4:C:197:VAL:HG23	1.91	0.53
5:D:294:TYR:CD1	5:D:294:TYR:C	2.83	0.53
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.91	0.53
13:L:79:PRO:HB2	39:L:782:HOH:O	2.09	0.53
16:O:58:LEU:N	16:O:58:LEU:CD1	2.72	0.53
22:U:37:GLN:OE1	22:U:118:SER:HA	2.08	0.53
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.39	0.53
24:W:64:GLY:O	24:W:65:ASP:HB2	2.09	0.53
25:X:88:THR:CG2	25:X:89:ASP:H	2.17	0.53
1:A:28:G:H5"	1:A:1343:C:OP1	2.09	0.53
1:A:45:A:C5	1:A:147:G:C6	2.96	0.53
1:A:1084:C:O5'	1:A:1084:C:H6	1.91	0.53
1:A:1157:C:C4	1:A:1158:G:N7	2.77	0.53
1:A:2038:A:O2'	1:A:2039:A:H5'	2.09	0.53
1:A:2349:G:OP1	7:F:20:LYS:NZ	2.41	0.53
1:A:2437:A:H2'	1:A:2438:G:C8	2.44	0.53
39:A:5952:HOH:O	15:N:189:VAL:HA	2.09	0.53
5:D:72:THR:HB	39:D:8608:HOH:O	2.08	0.53
5:D:185:GLY:HA2	39:D:8635:HOH:O	2.09	0.53
8:G:31:ARG:HH12	8:G:68:HIS:CE1	2.27	0.53
14:M:7:GLN:NE2	39:M:8464:HOH:O	2.41	0.53
15:N:61:ILE:HA	39:N:8623:HOH:O	2.07	0.53
16:O:167:ASP:O	16:O:168:LEU:HD23	2.08	0.53
20:S:65:GLY:C	39:S:8514:HOH:O	2.47	0.53
27:Z:189:ASN:HD22	27:Z:191:ASP:N	2.07	0.53
29:2:29:THR:O	29:2:32:LYS:CE	2.53	0.53
1:A:514:G:O5'	1:A:514:G:C2'	2.57	0.53
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.53
1:A:1535:G:C2	1:A:1536:C:C2	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:C:H4'	11:J:151:MET:HG2	1.91	0.53
1:A:2672:C:P	5:D:25:ARG:HH11	2.32	0.53
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.41	0.53
6:E:42:ARG:HG2	6:E:42:ARG:HH11	1.74	0.53
13:L:40:THR:O	13:L:41:LYS:C	2.47	0.53
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.91	0.53
16:O:44:ARG:HG3	16:O:45:ALA:N	2.24	0.53
16:O:80:SER:HB2	39:O:8535:HOH:O	2.09	0.53
18:Q:131:PHE:O	39:Q:1865:HOH:O	2.19	0.53
22:U:71:VAL:HG11	22:U:90:PRO:CB	2.32	0.53
26:Y:12:ILE:HG23	26:Y:36:HIS:CG	2.44	0.53
26:Y:27:ASP:OD2	26:Y:27:ASP:N	2.42	0.53
1:A:875:A:N7	4:C:189:VAL:HG21	2.24	0.52
1:A:1306:U:H5'	6:E:184:ARG:NH1	2.23	0.52
1:A:1375:A:H2'	1:A:1376:G:H5'	1.90	0.52
1:A:2010:A:H2'	39:A:5432:HOH:O	2.08	0.52
1:A:2389:U:OP1	19:R:82:LYS:NZ	2.35	0.52
1:A:2445:U:H2'	1:A:2446:G:C8	2.44	0.52
1:A:2911:C:H3'	39:A:5028:HOH:O	2.09	0.52
4:C:85:ASP:C	39:C:8615:HOH:O	2.47	0.52
8:G:11:VAL:HG12	8:G:12:ASP:H	1.72	0.52
8:G:118:ILE:HG23	8:G:144:THR:CG2	2.38	0.52
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.39	0.52
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.39	0.52
1:A:155:C:OP1	15:N:186:SER:OG	2.21	0.52
1:A:243:A:C2	1:A:275:G:O4'	2.62	0.52
1:A:558:C:H2'	1:A:559:U:C5'	2.39	0.52
1:A:1565:C:O2'	1:A:1566:C:H5'	2.09	0.52
1:A:1942:A:O2'	1:A:1943:C:H5'	2.09	0.52
7:F:27:ILE:HG22	7:F:28:GLY:N	2.19	0.52
15:N:138:HIS:C	15:N:139:PRO:O	2.45	0.52
18:Q:55:LYS:HG3	18:Q:56:GLY:N	2.24	0.52
22:U:2:LYS:HE2	39:U:7214:HOH:O	2.08	0.52
27:Z:107:PRO:HD3	27:Z:182:PHE:CD1	2.43	0.52
1:A:246:G:OP2	39:A:6456:HOH:O	2.19	0.52
1:A:1015:C:H2'	1:A:1016:U:C6	2.44	0.52
1:A:1865:A:H2'	1:A:1866:A:C8	2.44	0.52
1:A:2291:A:C8	1:A:2309:C:H5'	2.45	0.52
5:D:14:GLY:HA2	5:D:15:PRO:C	2.28	0.52
5:D:204:GLY:HA3	39:D:8656:HOH:O	2.10	0.52
7:F:146:LYS:CE	16:O:107:ASN:ND2	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:166:ILE:HD12	39:F:6326:HOH:O	2.08	0.52
19:R:26:PRO:CA	39:R:2847:HOH:O	2.57	0.52
1:A:280:C:H2'	1:A:281:U:O4'	2.09	0.52
1:A:819:A:H5"	39:1:4400:HOH:O	2.10	0.52
1:A:1181:A:N1	1:A:1192:A:O2'	2.42	0.52
1:A:2497:A:OP2	39:A:3480:HOH:O	2.19	0.52
1:A:2830:U:C4	1:A:2831:C:C5	2.98	0.52
7:F:94:ALA:HB3	7:F:174:VAL:HA	1.91	0.52
7:F:174:VAL:CG1	39:F:2195:HOH:O	2.41	0.52
9:H:105:ALA:HB2	39:H:5522:HOH:O	2.08	0.52
11:J:152:LYS:NZ	39:J:8358:HOH:O	2.41	0.52
13:L:101:ASN:O	13:L:102:GLU:CB	2.57	0.52
14:M:130:ARG:O	14:M:131:GLU:C	2.48	0.52
19:R:40:HIS:CE1	19:R:94:GLN:HA	2.44	0.52
20:S:13:THR:O	20:S:13:THR:HG22	2.09	0.52
1:A:204:A:C2'	1:A:205:U:H5'	2.40	0.52
1:A:2346:C:H4'	7:F:52:THR:CG2	2.38	0.52
1:A:2415:A:C2	16:O:25:ARG:HB3	2.45	0.52
1:A:2601:A:N1	13:L:38:SER:HB2	2.24	0.52
5:D:7:ARG:NH1	5:D:11:LEU:HD21	2.24	0.52
7:F:11:HIS:C	7:F:13:MET:H	2.12	0.52
10:I:64:ASN:O	10:I:68:GLU:HG3	2.09	0.52
11:J:26:LYS:HD2	11:J:28:ILE:CB	2.39	0.52
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.74	0.52
11:J:114:PRO:O	11:J:115:PHE:C	2.46	0.52
15:N:137:ASP:HA	15:N:142:LYS:HE3	1.92	0.52
16:O:143:ARG:HA	16:O:172:PHE:CE2	2.44	0.52
20:S:29:LYS:HD3	39:S:8532:HOH:O	2.10	0.52
29:2:45:ARG:NH1	39:2:3370:HOH:O	2.41	0.52
1:A:151:A:H2'	1:A:152:A:O4'	2.09	0.52
1:A:321:A:H1'	39:A:6499:HOH:O	2.10	0.52
1:A:626:U:C4	1:A:627:G:C6	2.97	0.52
1:A:1134:G:C5'	11:J:151:MET:HE3	2.39	0.52
1:A:1314:U:C2	1:A:1316:G:C2	2.97	0.52
1:A:1317:A:N3	1:A:1342:C:O2'	2.41	0.52
1:A:1764:C:N4	1:A:1765:G:C6	2.78	0.52
1:A:2361:A:H5"	39:A:8523:HOH:O	2.09	0.52
6:E:138:VAL:O	6:E:234:VAL:HA	2.09	0.52
11:J:75:SER:C	11:J:79:ALA:HB2	2.30	0.52
17:P:21:SER:OG	17:P:106:PRO:HB2	2.10	0.52
25:X:4:LEU:O	25:X:32:CYS:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:85:VAL:HG12	26:Y:86:GLU:H	1.75	0.52
29:2:45:ARG:NH2	39:2:2086:HOH:O	2.26	0.52
1:A:450:C:OP1	6:E:184:ARG:NH2	2.37	0.52
1:A:475:G:OP1	6:E:73:LEU:HD22	2.09	0.52
1:A:593:A:C8	39:A:3881:HOH:O	2.54	0.52
1:A:1085:C:N4	1:A:1086:A:C6	2.77	0.52
1:A:1194:A:N7	39:A:4952:HOH:O	2.43	0.52
1:A:1497:G:OP2	39:A:6011:HOH:O	2.19	0.52
1:A:1750:C:N4	1:A:1751:G:C6	2.78	0.52
1:A:2355:G:C2'	39:A:5113:HOH:O	2.58	0.52
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.44	0.52
2:B:3023:U:C3'	2:B:3024:U:H5"	2.40	0.52
2:B:3026:C:P	39:B:8443:HOH:O	2.68	0.52
5:D:54:VAL:O	5:D:55:ASN:C	2.46	0.52
5:D:223:ARG:O	5:D:228:ALA:HB2	2.10	0.52
7:F:59:GLY:O	7:F:61:PHE:N	2.34	0.52
8:G:26:ASN:ND2	39:G:7046:HOH:O	2.42	0.52
12:K:19:MET:CE	12:K:79:PHE:HA	2.36	0.52
18:Q:27:ARG:CD	39:Q:5262:HOH:O	2.58	0.52
22:U:4:PRO:HB3	39:U:2331:HOH:O	2.09	0.52
25:X:122:ARG:HH22	25:X:154:ARG:C	2.12	0.52
26:Y:62:GLY:HA2	39:Y:2724:HOH:O	2.10	0.52
29:2:46:ARG:O	39:2:4074:HOH:O	2.19	0.52
1:A:316:A:H1'	1:A:336:G:N3	2.24	0.52
1:A:515:C:H3'	39:A:5123:HOH:O	2.09	0.52
1:A:920:C:H5'	1:A:921:G:C4	2.45	0.52
1:A:1471:A:H2'	1:A:1472:C:C6	2.44	0.52
1:A:1583:U:H1'	39:A:9481:HOH:O	2.09	0.52
1:A:2019:A:H5'	39:A:4014:HOH:O	2.10	0.52
1:A:2506:A:O2'	1:A:2507:G:C8	2.60	0.52
11:J:44:ALA:HB3	11:J:136:VAL:O	2.09	0.52
13:L:74:VAL:HG21	13:L:96:VAL:HG23	1.91	0.52
15:N:12:TRP:HB2	39:N:8599:HOH:O	2.09	0.52
18:Q:41:ARG:O	18:Q:44:VAL:HB	2.10	0.52
24:W:64:GLY:O	24:W:65:ASP:CB	2.57	0.52
27:Z:213:LYS:O	27:Z:217:ILE:HG13	2.09	0.52
1:A:707:C:O2'	1:A:708:A:H5'	2.10	0.52
4:C:36:ASP:O	4:C:38:ILE:N	2.43	0.52
6:E:35:VAL:HG11	6:E:227:GLY:N	2.25	0.52
6:E:180:SER:N	39:E:8379:HOH:O	2.42	0.52
6:E:219:ASN:O	6:E:222:ASP:OD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:154:LYS:HD2	7:F:154:LYS:N	2.18	0.52
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.74	0.52
11:J:154:THR:HB	11:J:155:PRO:CD	2.40	0.52
13:L:99:ASP:OD1	13:L:101:ASN:N	2.42	0.52
25:X:7:LEU:CD1	25:X:53:ALA:HB2	2.40	0.52
1:A:92:G:H4'	24:W:44:GLY:HA3	1.92	0.52
1:A:871:G:P	4:C:8:ARG:HE	2.32	0.52
1:A:1772:C:O4'	1:A:1773:G:C2	2.63	0.52
1:A:2084:C:H2'	1:A:2085:A:H8	1.75	0.52
1:A:2685:C:O2'	1:A:2686:C:H5'	2.10	0.52
2:B:3097:U:H2'	2:B:3098:C:H6	1.75	0.52
5:D:234:ARG:NH1	39:D:8622:HOH:O	2.42	0.52
6:E:16:VAL:HG12	6:E:17:ASP:H	1.73	0.52
17:P:22:GLY:CA	39:P:2823:HOH:O	2.58	0.52
18:Q:7:LYS:CD	18:Q:21:VAL:CG2	2.88	0.52
18:Q:22:TRP:O	18:Q:23:PHE:HD1	1.92	0.52
31:4:84:ARG:HD3	39:4:8550:HOH:O	2.10	0.52
1:A:245:C:C2'	1:A:246:G:H5'	2.40	0.51
1:A:295:C:O2'	1:A:296:G:H5'	2.10	0.51
1:A:764:C:O2'	1:A:765:G:H5'	2.10	0.51
1:A:1050:G:C6	1:A:1051:C:C4	2.99	0.51
1:A:1370:G:N3	39:A:9638:HOH:O	2.42	0.51
1:A:2239:C:H6	39:A:6137:HOH:O	1.93	0.51
1:A:2365:G:H4'	19:R:45:PRO:O	2.10	0.51
1:A:2613:G:H1'	39:A:8662:HOH:O	2.10	0.51
2:B:3008:G:O6	16:O:11:ARG:NH1	2.43	0.51
4:C:73:GLY:N	28:1:65:ALA:O	2.34	0.51
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.91	0.51
6:E:72:LYS:O	39:E:8334:HOH:O	2.19	0.51
11:J:26:LYS:HG2	11:J:28:ILE:N	2.20	0.51
11:J:53:PRO:HG3	11:J:127:GLY:H	1.74	0.51
15:N:96:ASN:ND2	39:N:8536:HOH:O	2.34	0.51
25:X:90:TYR:N	25:X:90:TYR:CD1	2.78	0.51
25:X:142:ASP:HB3	25:X:145:GLY:H	1.75	0.51
28:1:46:LYS:O	28:1:57:CYS:HA	2.10	0.51
1:A:25:A:C2'	1:A:26:U:H5'	2.40	0.51
1:A:229:G:H2'	1:A:230:C:H6	1.75	0.51
1:A:559:U:H5'	1:A:559:U:C6	2.32	0.51
1:A:1116:U:O2'	1:A:1118:A:C2	2.39	0.51
1:A:1262:C:O2'	25:X:120:PRO:HD3	2.10	0.51
1:A:1666:C:C2'	1:A:1667:A:H5"	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2241:C:H2'	1:A:2242:U:C6	2.44	0.51
1:A:2549:C:H5"	39:A:9941:HOH:O	2.10	0.51
2:B:3097:U:H2'	2:B:3098:C:C6	2.45	0.51
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.74	0.51
7:F:65:GLU:HA	39:F:6752:HOH:O	2.10	0.51
7:F:94:ALA:HB3	7:F:174:VAL:CA	2.39	0.51
11:J:47:GLU:CB	11:J:133:ILE:CD1	2.86	0.51
11:J:62:GLU:OE2	11:J:66:VAL:CG2	2.58	0.51
11:J:140:PRO:HA	11:J:142:VAL:HG12	1.91	0.51
13:L:75:ARG:HD3	13:L:112:PRO:O	2.10	0.51
16:O:72:GLU:H	16:O:171:HIS:CE1	2.28	0.51
19:R:32:GLU:HA	19:R:71:TYR:OH	2.10	0.51
23:V:47:ARG:HG2	39:V:4381:HOH:O	2.10	0.51
1:A:245:C:H2'	39:A:5046:HOH:O	2.10	0.51
1:A:516:A:P	39:A:5123:HOH:O	2.66	0.51
5:D:217:ARG:HE	5:D:257:THR:HG22	1.75	0.51
5:D:254:GLN:HB3	39:D:8537:HOH:O	2.09	0.51
6:E:140:VAL:C	39:E:8459:HOH:O	2.47	0.51
8:G:133:VAL:HG12	8:G:141:VAL:HG13	1.92	0.51
10:I:71:LEU:C	10:I:73:ASP:H	2.14	0.51
15:N:14:ARG:HB3	15:N:17:GLU:HG3	1.92	0.51
15:N:87:MET:CB	31:4:46:ILE:HD13	2.33	0.51
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.41	0.51
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.25	0.51
22:U:20:HIS:ND1	22:U:41:ARG:NE	2.50	0.51
1:A:222:A:H2'	1:A:223:G:O4'	2.10	0.51
1:A:1311:G:C2	1:A:1312:G:C8	2.98	0.51
5:D:301:VAL:HG13	5:D:302:PRO:HD2	1.91	0.51
7:F:170:TYR:O	7:F:171:ASP:HB3	2.10	0.51
17:P:10:LEU:HD12	17:P:10:LEU:O	2.10	0.51
18:Q:13:VAL:HG11	18:Q:40:VAL:HG12	1.92	0.51
20:S:111:ILE:O	20:S:111:ILE:CG2	2.55	0.51
25:X:38:THR:HG22	25:X:39:ASP:H	1.75	0.51
1:A:146:U:O2'	1:A:147:G:H5'	2.11	0.51
1:A:2791:U:H1'	1:A:2792:A:H5"	1.92	0.51
2:B:3002:U:H4'	39:B:8484:HOH:O	2.10	0.51
5:D:138:GLY:O	5:D:139:ASP:O	2.27	0.51
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.93	0.51
6:E:22:PHE:HA	6:E:116:ALA:HA	1.93	0.51
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.40	0.51
16:O:67:ALA:HA	16:O:71:TRP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:87:LEU:CD1	16:O:186:LEU:HD21	2.37	0.51
21:T:75:GLN:HG3	39:T:8321:HOH:O	2.10	0.51
22:U:69:LYS:O	22:U:71:VAL:HG23	2.10	0.51
27:Z:117:LEU:HA	27:Z:174:VAL:HG11	1.91	0.51
29:2:15:THR:O	29:2:28:HIS:HA	2.09	0.51
29:2:30:LYS:HD3	39:2:3205:HOH:O	2.11	0.51
1:A:88:G:N3	30:3:24:TRP:HB2	2.26	0.51
1:A:815:U:OP1	39:A:9168:HOH:O	2.19	0.51
1:A:1003:U:H5"	39:A:9140:HOH:O	2.09	0.51
1:A:1589:G:C2	1:A:1605:G:N3	2.78	0.51
1:A:2420:G:O2'	1:A:2421:G:H5'	2.10	0.51
1:A:2642:G:H2'	1:A:2643:G:O4'	2.10	0.51
2:B:3096:C:H2'	2:B:3097:U:C6	2.45	0.51
5:D:125:GLU:O	5:D:129:ARG:HG3	2.10	0.51
7:F:84:LEU:C	7:F:86:THR:H	2.14	0.51
7:F:91:ALA:HB1	39:F:5198:HOH:O	2.10	0.51
8:G:15:GLN:NE2	8:G:40:VAL:O	2.44	0.51
13:L:51:ASP:OD2	39:L:5632:HOH:O	2.19	0.51
15:N:169:ARG:HB3	39:N:8587:HOH:O	2.09	0.51
16:O:74:PRO:HD3	16:O:159:TYR:CE2	2.46	0.51
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.10	0.51
22:U:9:LYS:CD	39:U:2196:HOH:O	2.58	0.51
24:W:27:LEU:CA	24:W:49:LEU:HD13	2.40	0.51
1:A:475:G:H5'	6:E:73:LEU:HD23	1.91	0.51
1:A:1278:A:H4'	1:A:1279:U:C4	2.45	0.51
2:B:3025:G:H2'	39:B:8465:HOH:O	2.10	0.51
12:K:77:GLY:O	12:K:78:ILE:C	2.47	0.51
15:N:154:ARG:NH1	39:N:8639:HOH:O	2.42	0.51
15:N:156:ARG:O	15:N:161:ARG:NH2	2.42	0.51
21:T:23:LYS:HD3	21:T:65:VAL:HG12	1.93	0.51
27:Z:96:GLU:O	27:Z:235:GLU:HA	2.11	0.51
1:A:158:A:C2'	1:A:159:G:H5'	2.41	0.51
1:A:202:U:H2'	1:A:203:G:O4'	2.11	0.51
1:A:1372:A:H3'	39:A:6657:HOH:O	2.09	0.51
1:A:1505:U:H5'	1:A:1505:U:C6	2.43	0.51
1:A:1890:U:H4'	1:A:2010:A:C6	2.46	0.51
1:A:2274:A:H3'	39:A:9620:HOH:O	2.10	0.51
1:A:2415:A:H2'	1:A:2416:G:H5'	1.92	0.51
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.92	0.51
5:D:41:PHE:CG	5:D:190:MET:HE3	2.46	0.51
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.25	0.51
11:J:48:LEU:CD1	11:J:157:ILE:CG2	2.89	0.51
11:J:53:PRO:O	11:J:54:VAL:HG13	2.11	0.51
15:N:37:VAL:HG21	15:N:108:LYS:HG2	1.92	0.51
19:R:46:SER:O	39:R:3488:HOH:O	2.19	0.51
24:W:1:THR:HG23	24:W:2:VAL:N	2.15	0.51
25:X:11:VAL:O	25:X:12:ASN:HB2	2.10	0.51
26:Y:29:ALA:O	26:Y:32:LEU:N	2.44	0.51
28:1:25:ARG:HD2	39:1:2448:HOH:O	2.10	0.51
1:A:551:A:C6	1:A:552:A:N1	2.79	0.51
1:A:1552:G:C6	1:A:1553:C:C4	2.98	0.51
39:A:3265:HOH:O	22:U:52:ARG:HD2	2.10	0.51
6:E:56:THR:O	39:E:8317:HOH:O	2.20	0.51
9:H:26:THR:HB	9:H:102:GLY:O	2.11	0.51
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.41	0.51
13:L:118:ALA:HA	13:L:125:ALA:HB2	1.93	0.51
22:U:92:ASP:O	22:U:94:SER:N	2.44	0.51
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.92	0.51
39:A:3476:HOH:O	22:U:82:THR:HG23	2.10	0.51
6:E:84:VAL:O	6:E:85:LYS:HB2	2.11	0.51
7:F:57:THR:HG23	7:F:63:ILE:CB	2.41	0.51
7:F:155:HIS:NE2	39:F:7597:HOH:O	2.23	0.51
12:K:19:MET:HE3	12:K:78:ILE:HG22	1.93	0.51
15:N:69:LYS:HG2	15:N:127:LYS:HG3	1.91	0.51
16:O:42:HIS:CG	16:O:62:HIS:HE1	2.29	0.51
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.93	0.51
16:O:152:GLU:C	16:O:154:LEU:H	2.13	0.51
19:R:32:GLU:O	19:R:93:ARG:NH2	2.44	0.51
22:U:24:ARG:HH21	22:U:39:ASN:ND2	2.09	0.51
23:V:37:GLU:HB3	39:V:408:HOH:O	2.10	0.51
1:A:1150:A:O3'	10:I:16:LYS:NZ	2.44	0.50
1:A:1350:U:H4'	39:A:4599:HOH:O	2.11	0.50
4:C:194:MET:HE1	4:C:199:HIS:HB2	1.92	0.50
7:F:58:VAL:HG12	7:F:59:GLY:N	2.26	0.50
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.76	0.50
19:R:93:ARG:HG3	19:R:93:ARG:NH1	2.21	0.50
1:A:212:A:H5'	1:A:214:U:O4'	2.10	0.50
1:A:703:G:O2'	1:A:704:C:H5'	2.11	0.50
1:A:1197:G:N2	39:A:5699:HOH:O	2.43	0.50
2:B:3057:A:C8	7:F:141:VAL:HG21	2.46	0.50
5:D:102:THR:HG23	5:D:182:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:224:ALA:O	6:E:225:PRO:C	2.49	0.50
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.37	0.50
15:N:97:ILE:HA	15:N:100:ILE:HD12	1.91	0.50
22:U:9:LYS:HD2	39:U:2196:HOH:O	2.11	0.50
25:X:38:THR:HG22	39:X:3580:HOH:O	2.10	0.50
30:3:9:LYS:O	30:3:12:ALA:HB3	2.11	0.50
1:A:244:C:OP2	9:H:38:LYS:HE3	2.11	0.50
1:A:332:G:O2'	1:A:333:G:H5'	2.11	0.50
1:A:542:A:C8	1:A:542:A:C5'	2.89	0.50
1:A:830:G:O2'	1:A:831:U:H5'	2.11	0.50
1:A:841:A:C8	1:A:843:A:C8	3.00	0.50
1:A:1210:G:O2'	1:A:1211:G:H5'	2.11	0.50
1:A:1525:G:H5'	1:A:1526:A:OP2	2.12	0.50
1:A:1763:C:O2'	1:A:1764:C:H5'	2.11	0.50
1:A:1823:G:C2	1:A:2027:U:C2	3.00	0.50
1:A:1864:C:OP1	15:N:75:THR:HG23	2.11	0.50
1:A:2276:U:H2'	1:A:2277:U:H6	1.75	0.50
1:A:2499:U:O2'	1:A:2500:C:H5'	2.11	0.50
1:A:2687:G:O4'	13:L:1:MET:HA	2.12	0.50
11:J:144:GLU:OE1	11:J:144:GLU:HA	2.11	0.50
11:J:154:THR:HB	11:J:155:PRO:HD3	1.92	0.50
15:N:57:LYS:HE2	15:N:140:ALA:O	2.12	0.50
19:R:93:ARG:HH11	19:R:93:ARG:CG	2.22	0.50
20:S:40:ALA:O	20:S:44:VAL:HG23	2.10	0.50
28:1:46:LYS:HB3	39:1:7239:HOH:O	2.10	0.50
1:A:154:C:C2	1:A:155:C:C6	2.99	0.50
1:A:154:C:O2	1:A:155:C:C6	2.64	0.50
1:A:218:C:C5	1:A:220:C:C4	2.99	0.50
1:A:832:U:H2'	1:A:833:G:C8	2.47	0.50
1:A:1007:A:OP1	39:A:5567:HOH:O	2.19	0.50
1:A:1161:A:O5'	1:A:1161:A:C8	2.62	0.50
1:A:1746:A:O4'	1:A:1747:A:C2	2.64	0.50
5:D:128:ILE:O	5:D:131:ALA:HB3	2.11	0.50
8:G:21:THR:HG23	8:G:30:THR:OG1	2.12	0.50
8:G:69:ILE:HA	8:G:72:MET:CE	2.41	0.50
8:G:158:ASP:HA	39:G:2712:HOH:O	2.12	0.50
26:Y:76:ARG:NH1	26:Y:76:ARG:CG	2.67	0.50
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.92	0.50
1:A:485:A:N3	1:A:487:G:H5"	2.26	0.50
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.47	0.50
1:A:1204:C:H6	1:A:1204:C:O5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:G:H3'	1:A:1261:A:N7	2.27	0.50
1:A:1308:A:O4'	6:E:226:GLY:HA3	2.12	0.50
1:A:1730:G:H5'	1:A:1731:C:C6	2.47	0.50
1:A:1920:C:H2'	1:A:1921:A:C5'	2.41	0.50
1:A:2344:G:H8	39:A:6126:HOH:O	1.94	0.50
1:A:2889:U:O2'	39:A:8764:HOH:O	2.17	0.50
5:D:82:VAL:O	5:D:82:VAL:CG1	2.59	0.50
5:D:162:MET:CE	5:D:310:ARG:HD3	2.41	0.50
9:H:100:ASP:O	9:H:101:ALA:O	2.30	0.50
12:K:48:GLY:CA	12:K:53:ILE:HD11	2.40	0.50
15:N:65:VAL:HG11	15:N:101:ALA:HA	1.94	0.50
16:O:77:ASN:O	16:O:80:SER:HB3	2.12	0.50
19:R:48:PRO:HG3	39:R:3488:HOH:O	2.12	0.50
26:Y:15:ARG:HB3	26:Y:15:ARG:NH1	2.26	0.50
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.95	0.50
1:A:738:G:H8	1:A:738:G:O5'	1.95	0.50
1:A:1021:G:O2'	1:A:1022:A:H5'	2.12	0.50
1:A:1194:A:C5	39:A:4952:HOH:O	2.55	0.50
1:A:2511:A:N7	39:A:5958:HOH:O	2.44	0.50
39:A:3217:HOH:O	15:N:157:LEU:CD1	2.37	0.50
2:B:3056:A:N1	7:F:13:MET:HE3	2.27	0.50
4:C:130:THR:C	39:C:8575:HOH:O	2.49	0.50
6:E:166:ILE:CD1	6:E:207:LEU:HD13	2.41	0.50
8:G:7:ILE:CG2	8:G:45:ASP:O	2.59	0.50
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.93	0.50
15:N:138:HIS:ND1	15:N:139:PRO:O	2.38	0.50
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.93	0.50
16:O:139:TRP:CH2	16:O:176:ARG:NH1	2.79	0.50
17:P:77:ALA:HB1	17:P:98:LEU:HD12	1.93	0.50
1:A:233:U:H5'	1:A:667:C:O2'	2.12	0.50
1:A:949:U:O2'	19:R:40:HIS:HE1	1.94	0.50
1:A:2274:A:N3	15:N:86:MET:CE	2.75	0.50
1:A:2314:G:H2'	1:A:2315:C:H5'	1.92	0.50
1:A:2649:A:H5'	1:A:2649:A:H8	1.77	0.50
1:A:2815:G:OP2	12:K:99:GLU:HG2	2.12	0.50
5:D:82:VAL:O	5:D:83:ALA:CB	2.54	0.50
15:N:40:ILE:HD11	15:N:130:GLU:HG2	1.93	0.50
24:W:39:ALA:N	24:W:40:PRO:CD	2.73	0.50
25:X:38:THR:HB	39:X:5390:HOH:O	2.11	0.50
1:A:120:A:OP1	29:2:32:LYS:NZ	2.37	0.50
1:A:161:A:OP1	15:N:81:ARG:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:C:H2'	1:A:1024:G:O4'	2.11	0.50
1:A:1139:U:H2'	1:A:1140:C:C6	2.47	0.50
1:A:1166:A:C6	1:A:1167:G:C5	2.99	0.50
1:A:1469:C:N3	1:A:1472:C:OP2	2.45	0.50
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.76	0.50
1:A:2004:U:H5"	1:A:2005:G:C8	2.46	0.50
1:A:2332:A:C2	1:A:2355:G:C5	3.00	0.50
1:A:2719:A:C2	5:D:70:PRO:HG3	2.47	0.50
1:A:2780:C:C1'	8:G:143:GLN:HE21	2.21	0.50
6:E:39:GLN:O	6:E:43:LYS:CD	2.60	0.50
8:G:22:VAL:O	8:G:28:SER:HA	2.11	0.50
11:J:68:ALA:HB2	11:J:149:ALA:HB2	1.92	0.50
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.76	0.50
26:Y:26:ALA:HB1	26:Y:59:TRP:CE2	2.46	0.50
28:1:38:LYS:CG	28:1:45:LYS:HG2	2.42	0.50
29:2:37:CYS:SG	29:2:39:PHE:HB2	2.51	0.50
1:A:469:G:N2	1:A:472:A:OP2	2.33	0.50
1:A:1327:G:N2	1:A:1331:A:C4	2.80	0.50
1:A:1380:U:OP2	1:A:2747:C:N4	2.45	0.50
1:A:1522:A:H2'	1:A:1523:G:H5'	1.93	0.50
1:A:1771:U:H4'	1:A:1772:C:OP2	2.12	0.50
1:A:2355:G:OP2	39:A:6282:HOH:O	2.19	0.50
1:A:2362:A:H2'	1:A:2363:G:C8	2.47	0.50
1:A:2379:G:H4'	1:A:2380:A:H5"	1.92	0.50
1:A:2472:C:O2'	1:A:2634:G:H4'	2.12	0.50
1:A:2635:A:C4	1:A:2636:C:C5	2.99	0.50
4:C:109:GLU:OE2	4:C:153:ARG:NH1	2.45	0.50
5:D:36:PRO:HA	5:D:167:GLY:O	2.12	0.50
5:D:79:MET:HE1	39:D:8628:HOH:O	2.10	0.50
6:E:162:VAL:HG12	6:E:192:ILE:CD1	2.37	0.50
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.77	0.50
7:F:102:GLY:O	7:F:134:LEU:HD12	2.12	0.50
7:F:128:LEU:N	39:F:6007:HOH:O	2.44	0.50
8:G:31:ARG:HH12	8:G:68:HIS:CD2	2.30	0.50
8:G:145:ALA:O	8:G:148:ILE:HB	2.12	0.50
8:G:156:ASP:OD2	8:G:157:LYS:NZ	2.32	0.50
9:H:58:GLU:HA	9:H:61:MET:HG3	1.92	0.50
16:O:64:SER:C	16:O:66:LEU:H	2.16	0.50
16:O:113:SER:C	39:O:8556:HOH:O	2.50	0.50
39:O:8541:HOH:O	19:R:19:ARG:HD3	2.12	0.50
20:S:39:THR:HB	20:S:42:GLU:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:16:ASN:O	21:T:20:PHE:HB2	2.11	0.50
22:U:48:VAL:CG1	22:U:96:VAL:HG13	2.41	0.50
23:V:52:THR:HG21	23:V:54:THR:HB	1.94	0.50
25:X:19:ASP:O	25:X:23:MET:HG3	2.12	0.50
25:X:125:HIS:HD2	25:X:127:GLY:H	1.60	0.50
30:3:24:TRP:NE1	39:3:6863:HOH:O	2.45	0.50
31:4:48:ASN:ND2	31:4:50:GLY:H	2.10	0.50
1:A:795:G:N3	1:A:817:G:C2	2.80	0.49
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.47	0.49
1:A:1783:A:C2'	1:A:1784:U:H5'	2.42	0.49
1:A:1856:C:O2	39:A:9710:HOH:O	2.17	0.49
1:A:2290:U:H4'	1:A:2291:A:OP1	2.12	0.49
1:A:2421:G:H3'	1:A:2422:U:C5'	2.41	0.49
1:A:2467:A:O2'	1:A:2468:A:H2'	2.11	0.49
1:A:2573:G:N3	39:A:6765:HOH:O	2.34	0.49
6:E:46:TYR:CE1	6:E:92:PRO:HB3	2.46	0.49
11:J:48:LEU:CG	11:J:157:ILE:HG21	2.42	0.49
15:N:98:GLN:NE2	15:N:117:SER:OG	2.42	0.49
17:P:17:ALA:O	17:P:21:SER:HB2	2.12	0.49
22:U:41:ARG:NH1	22:U:42:VAL:O	2.45	0.49
24:W:4:HIS:O	24:W:8:ILE:HG13	2.11	0.49
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.77	0.49
26:Y:66:THR:CG2	26:Y:67:PRO:HD2	2.37	0.49
1:A:269:G:C2	1:A:270:U:O4	2.65	0.49
1:A:283:U:C5	1:A:284:C:N4	2.75	0.49
1:A:327:A:H4'	1:A:329:A:C8	2.47	0.49
1:A:945:U:O2'	1:A:946:C:H5'	2.12	0.49
1:A:1213:C:N4	1:A:1214:G:H1	2.09	0.49
1:A:1375:A:C2'	1:A:1376:G:H5'	2.42	0.49
1:A:2254:G:C1'	39:A:5010:HOH:O	2.60	0.49
1:A:2735:U:H2'	1:A:2736:U:C6	2.47	0.49
39:A:4882:HOH:O	4:C:164:ARG:NE	2.44	0.49
39:A:9373:HOH:O	29:2:1:THR:HG21	2.11	0.49
2:B:3039:U:H3'	2:B:3040:C:H5"	1.95	0.49
4:C:223:ARG:NE	39:C:8574:HOH:O	2.44	0.49
5:D:30:PRO:HG2	5:D:313:PRO:HD2	1.92	0.49
7:F:52:THR:O	7:F:52:THR:HG22	2.12	0.49
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.41	0.49
17:P:42:GLU:HB2	39:P:2176:HOH:O	2.11	0.49
21:T:57:THR:CG2	21:T:59:ASP:HB2	2.41	0.49
25:X:7:LEU:HD12	25:X:53:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:G:O2'	1:A:526:U:H5'	2.12	0.49
1:A:1125:U:H3'	1:A:1126:C:C6	2.48	0.49
1:A:1603:A:C5'	1:A:1605:G:H5'	2.43	0.49
1:A:2406:U:C4	1:A:2407:G:N7	2.80	0.49
1:A:2668:G:H2'	1:A:2669:U:C6	2.47	0.49
4:C:88:ILE:CD1	4:C:100:PRO:HD3	2.41	0.49
11:J:111:MET:O	11:J:114:PRO:HD3	2.13	0.49
12:K:131:THR:HG22	12:K:134:GLU:N	2.09	0.49
16:O:182:GLY:N	39:O:8567:HOH:O	2.45	0.49
17:P:32:ARG:HG2	39:P:3240:HOH:O	2.11	0.49
31:4:38:ARG:O	31:4:42:ARG:HB2	2.13	0.49
1:A:952:G:OP1	19:R:42:LYS:HE2	2.13	0.49
1:A:2793:A:H2'	39:A:3970:HOH:O	2.11	0.49
5:D:307:ARG:HD3	39:D:8524:HOH:O	2.13	0.49
6:E:42:ARG:HG2	6:E:42:ARG:NH1	2.25	0.49
6:E:193:LEU:HD12	6:E:211:ASP:O	2.13	0.49
7:F:95:THR:OG1	7:F:174:VAL:HG22	2.12	0.49
10:I:18:GLU:O	10:I:21:ASP:HB2	2.12	0.49
11:J:162:SER:CA	39:J:8341:HOH:O	2.60	0.49
15:N:189:VAL:O	15:N:189:VAL:HG22	2.11	0.49
17:P:99:GLU:CG	39:P:6044:HOH:O	2.57	0.49
25:X:6:GLN:HA	25:X:52:VAL:HG23	1.93	0.49
27:Z:129:ASN:OD1	27:Z:141:THR:OG1	2.30	0.49
1:A:342:C:OP1	39:A:5852:HOH:O	2.19	0.49
1:A:533:U:O2	12:K:95:ARG:NH2	2.45	0.49
1:A:1016:U:H1'	39:A:3153:HOH:O	2.11	0.49
1:A:1250:C:O2'	1:A:1251:C:H5'	2.12	0.49
1:A:1280:A:N6	1:A:1281:C:C4	2.81	0.49
1:A:1649:G:C2'	39:A:5009:HOH:O	2.60	0.49
1:A:1667:A:O2'	1:A:1668:U:H5'	2.13	0.49
1:A:1866:A:H8	1:A:1866:A:O5'	1.96	0.49
1:A:2242:U:O2'	39:A:4394:HOH:O	2.14	0.49
1:A:2334:C:O2'	1:A:2335:C:H5'	2.12	0.49
1:A:2499:U:H2'	1:A:2500:C:H6	1.76	0.49
1:A:2660:G:P	39:A:3878:HOH:O	2.69	0.49
39:A:9054:HOH:O	31:4:46:ILE:HB	2.12	0.49
2:B:3029:C:C2'	2:B:3030:C:H5'	2.42	0.49
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.42	0.49
6:E:168:ARG:NH2	6:E:190:ALA:O	2.46	0.49
7:F:10:PHE:N	39:F:7345:HOH:O	2.45	0.49
7:F:147:ALA:HA	16:O:15:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:91:VAL:HG13	39:H:985:HOH:O	2.12	0.49
14:M:98:GLU:O	14:M:99:GLU:HB2	2.11	0.49
16:O:78:MET:CB	16:O:79:PRO:HD3	2.36	0.49
26:Y:71:ARG:CD	39:Y:2171:HOH:O	2.61	0.49
1:A:23:G:C6	1:A:24:G:N1	2.81	0.49
1:A:169:A:H5"	39:A:9115:HOH:O	2.09	0.49
1:A:392:U:O2'	15:N:182:LYS:HE2	2.13	0.49
1:A:486:A:H1'	39:A:6238:HOH:O	2.13	0.49
1:A:1256:C:H5"	39:A:6621:HOH:O	2.12	0.49
1:A:1323:G:C2	1:A:1324:G:C8	3.00	0.49
1:A:1552:G:H2'	1:A:1553:C:H6	1.75	0.49
1:A:1574:C:H4'	39:A:3284:HOH:O	2.11	0.49
1:A:2896:A:H2'	1:A:2896:A:N3	2.27	0.49
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.13	0.49
16:O:35:VAL:HB	16:O:46:GLN:HB2	1.95	0.49
17:P:32:ARG:CZ	39:P:3360:HOH:O	2.59	0.49
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.46	0.49
22:U:27:LEU:HD21	22:U:40:VAL:CG1	2.43	0.49
25:X:13:MET:CE	25:X:17:ILE:CG2	2.90	0.49
31:4:18:GLN:O	31:4:20:HIS:ND1	2.45	0.49
31:4:71:CYS:HG	38:4:8404:CD:CD	1.47	0.49
1:A:622:G:P	27:Z:148:GLY:HA3	2.52	0.49
1:A:1073:A:H4'	27:Z:155:ARG:O	2.12	0.49
1:A:1666:C:H2'	1:A:1667:A:H8	1.78	0.49
1:A:1683:G:H1'	1:A:1723:G:HO2'	1.77	0.49
1:A:1724:U:OP2	39:A:3710:HOH:O	2.18	0.49
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.11	0.49
2:B:3002:U:C4'	39:B:8484:HOH:O	2.61	0.49
6:E:204:ALA:O	6:E:207:LEU:HB2	2.13	0.49
7:F:103:ASN:ND2	7:F:134:LEU:H	2.11	0.49
8:G:167:TYR:N	8:G:167:TYR:CD1	2.81	0.49
11:J:50:VAL:HG21	11:J:125:VAL:HG11	1.95	0.49
13:L:74:VAL:HG13	13:L:113:ILE:HG12	1.93	0.49
18:Q:27:ARG:HD3	39:Q:5262:HOH:O	2.12	0.49
23:V:47:ARG:CG	39:V:4381:HOH:O	2.60	0.49
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.46	0.49
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.36	0.49
1:A:134:U:C2	1:A:145:A:C2	3.01	0.49
1:A:736:A:N1	39:A:6169:HOH:O	2.34	0.49
1:A:1450:C:O2'	1:A:1494:A:H5'	2.13	0.49
1:A:2773:G:H22	1:A:2801:A:H2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:7141:HOH:O	15:N:154:ARG:HB2	2.13	0.49
5:D:16:ARG:NH1	39:D:8620:HOH:O	2.46	0.49
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.43	0.49
9:H:26:THR:HG21	9:H:103:ALA:CB	2.43	0.49
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.42	0.49
11:J:162:SER:HB3	39:J:8341:HOH:O	2.11	0.49
18:Q:7:LYS:CD	18:Q:21:VAL:HG21	2.42	0.49
20:S:39:THR:O	20:S:40:ALA:C	2.50	0.49
1:A:95:A:H5"	1:A:97:G:O4'	2.13	0.49
1:A:518:G:H4'	39:A:5532:HOH:O	2.13	0.49
1:A:627:G:H2'	1:A:2071:C:C5	2.48	0.49
1:A:779:U:H5'	1:A:1836:A:C2	2.48	0.49
1:A:1497:G:C2'	1:A:1498:G:H5'	2.43	0.49
2:B:3056:A:P	39:B:8525:HOH:O	2.71	0.49
4:C:179:MET:HG2	4:C:186:TRP:CB	2.42	0.49
5:D:132:HIS:CE1	5:D:171:VAL:CG2	2.95	0.49
5:D:177:HIS:O	5:D:181:ILE:HG13	2.13	0.49
5:D:201:ASP:HB2	5:D:312:ARG:CD	2.39	0.49
11:J:139:ASP:HB2	39:J:8346:HOH:O	2.12	0.49
16:O:73:ALA:HB1	16:O:74:PRO:HD2	1.94	0.49
18:Q:111:GLU:OE2	18:Q:113:THR:OG1	2.24	0.49
1:A:319:A:H4'	1:A:338:C:C5	2.47	0.49
1:A:370:G:O2'	1:A:371:U:H5'	2.13	0.49
1:A:677:C:O2'	1:A:678:G:H5'	2.13	0.49
1:A:834:G:H5"	1:A:835:U:O5'	2.13	0.49
1:A:1087:G:H8	25:X:10:GLU:OE2	1.96	0.49
1:A:1304:U:O2	39:A:9967:HOH:O	2.18	0.49
1:A:1461:U:H4'	39:A:3039:HOH:O	2.13	0.49
1:A:1565:C:O4'	1:A:2738:G:H1'	2.13	0.49
1:A:2112:A:H2'	1:A:2113:G:H8	1.77	0.49
1:A:2780:C:C4	1:A:2781:U:C4	3.01	0.49
6:E:164:ALA:O	6:E:167:ASP:HB2	2.13	0.49
10:I:23:ILE:HD13	10:I:67:LEU:CD2	2.27	0.49
11:J:149:ALA:C	11:J:151:MET:H	2.16	0.49
15:N:14:ARG:HB3	15:N:17:GLU:CG	2.42	0.49
15:N:113:ARG:HH21	15:N:156:ARG:HG2	1.78	0.49
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.59	0.49
1:A:251:C:O2'	1:A:252:C:H5'	2.13	0.48
1:A:272:A:H3'	39:A:6993:HOH:O	2.13	0.48
1:A:282:C:H2'	1:A:283:U:O4'	2.12	0.48
1:A:1307:A:H2'	1:A:1308:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1888:C:N4	1:A:1889:C:C4	2.81	0.48
1:A:1996:U:C5	1:A:2592:G:N2	2.80	0.48
1:A:2249:G:C2	1:A:2253:G:C6	3.01	0.48
1:A:2324:G:H4'	1:A:2418:G:O2'	2.13	0.48
1:A:2385:G:H2'	1:A:2386:U:C6	2.48	0.48
1:A:2547:C:H2'	1:A:2548:C:C6	2.45	0.48
1:A:2707:C:O2	1:A:2707:C:H2'	2.13	0.48
1:A:2781:U:O2'	1:A:2782:G:H5'	2.13	0.48
4:C:46:GLU:O	4:C:55:VAL:N	2.39	0.48
6:E:12:THR:HB	39:E:8449:HOH:O	2.13	0.48
9:H:63:ILE:CB	9:H:64:PRO:HD3	2.42	0.48
21:T:80:ARG:NH1	39:T:8346:HOH:O	2.45	0.48
22:U:61:GLU:HG3	39:U:3851:HOH:O	2.11	0.48
25:X:122:ARG:CG	25:X:122:ARG:NH1	2.73	0.48
1:A:314:G:N2	1:A:316:A:H3'	2.27	0.48
1:A:1125:U:H3'	1:A:1126:C:H6	1.78	0.48
1:A:1162:G:C2	1:A:1163:G:C8	3.02	0.48
1:A:1295:G:OP1	14:M:16:GLY:N	2.43	0.48
1:A:1407:A:O2'	1:A:1408:U:H3'	2.13	0.48
1:A:1559:A:C1'	39:A:5341:HOH:O	2.39	0.48
1:A:1804:A:H2'	1:A:1805:G:C8	2.47	0.48
1:A:1821:A:N6	1:A:2029:C:H42	2.11	0.48
1:A:1947:G:H2'	1:A:1948:G:H8	1.78	0.48
1:A:1996:U:H5	1:A:2592:G:N2	2.10	0.48
1:A:2355:G:H2'	39:A:5113:HOH:O	2.13	0.48
1:A:2453:G:H4'	14:M:50:GLY:C	2.33	0.48
1:A:2831:C:H2'	1:A:2832:C:C5'	2.41	0.48
2:B:3030:C:OP1	7:F:137:PRO:O	2.31	0.48
6:E:221:GLU:O	6:E:225:PRO:N	2.46	0.48
8:G:45:ASP:OD2	8:G:46:THR:HG23	2.13	0.48
8:G:152:THR:HG21	8:G:165:GLY:HA2	1.93	0.48
13:L:87:ARG:CB	39:V:1102:HOH:O	2.61	0.48
20:S:39:THR:HB	20:S:42:GLU:CD	2.33	0.48
22:U:113:GLU:O	22:U:114:SER:O	2.31	0.48
25:X:61:THR:HG22	25:X:61:THR:O	2.13	0.48
25:X:65:VAL:HA	25:X:68:THR:HG22	1.95	0.48
25:X:122:ARG:NE	39:X:5817:HOH:O	2.46	0.48
1:A:585:C:H2'	1:A:586:C:H6	1.79	0.48
1:A:658:C:N4	39:A:9607:HOH:O	2.47	0.48
1:A:870:G:C3'	1:A:871:G:H5"	2.42	0.48
1:A:1310:U:C2'	1:A:1311:G:O5'	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2266:A:OP2	15:N:90:ARG:NH2	2.47	0.48
1:A:2911:C:H2'	1:A:2912:C:C6	2.49	0.48
2:B:3049:G:H2'	2:B:3050:G:O4'	2.14	0.48
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.42	0.48
4:C:125:ASN:CB	4:C:158:VAL:HG12	2.42	0.48
5:D:215:VAL:HB	5:D:234:ARG:HH12	1.77	0.48
6:E:27:ARG:HD2	6:E:29:ASP:OD1	2.13	0.48
6:E:214:THR:CB	39:E:8327:HOH:O	2.56	0.48
7:F:53:LYS:HA	7:F:67:ASP:O	2.14	0.48
8:G:98:GLU:N	39:G:4191:HOH:O	2.46	0.48
11:J:140:PRO:HA	11:J:142:VAL:CG1	2.43	0.48
19:R:18:PRO:O	19:R:21:ARG:HB2	2.14	0.48
1:A:60:A:OP2	39:A:3580:HOH:O	2.20	0.48
1:A:393:G:O6	15:N:181:GLU:HG2	2.14	0.48
1:A:920:C:C4	1:A:2467:A:C5	3.02	0.48
1:A:948:G:N7	39:A:5325:HOH:O	2.35	0.48
1:A:1114:A:H2'	1:A:1115:U:H6	1.77	0.48
1:A:1182:C:H1'	1:A:1192:A:C8	2.46	0.48
1:A:1248:A:OP1	39:A:8876:HOH:O	2.20	0.48
1:A:1732:A:O5'	1:A:1732:A:H8	1.96	0.48
1:A:2413:A:H2'	1:A:2414:A:O4'	2.13	0.48
2:B:3074:G:C6	2:B:3075:G:N7	2.81	0.48
5:D:23:THR:HA	5:D:24:PRO:HD3	1.54	0.48
5:D:37:GLY:N	5:D:167:GLY:O	2.45	0.48
8:G:38:ILE:HG21	8:G:65:PHE:CE1	2.48	0.48
9:H:38:LYS:O	9:H:42:ARG:HD2	2.14	0.48
10:I:63:ARG:O	10:I:67:LEU:HG	2.12	0.48
13:L:75:ARG:NH1	39:L:6493:HOH:O	2.27	0.48
13:L:125:ALA:C	13:L:127:ALA:H	2.16	0.48
15:N:154:ARG:CZ	39:N:8639:HOH:O	2.61	0.48
16:O:115:VAL:HG23	39:O:8556:HOH:O	2.12	0.48
18:Q:89:ASN:OD1	18:Q:89:ASN:C	2.51	0.48
20:S:114:VAL:O	20:S:114:VAL:HG13	2.13	0.48
24:W:55:ARG:NH2	39:W:2551:HOH:O	2.36	0.48
25:X:13:MET:O	25:X:14:HIS:O	2.32	0.48
26:Y:51:ASP:OD2	26:Y:52:PRO:HD2	2.13	0.48
26:Y:72:VAL:O	26:Y:72:VAL:CG1	2.60	0.48
1:A:227:A:O2'	39:A:8978:HOH:O	2.14	0.48
1:A:292:G:H2'	1:A:358:G:N2	2.29	0.48
1:A:558:C:H2'	1:A:559:U:H5"	1.96	0.48
1:A:793:A:OP2	39:A:4345:HOH:O	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:U:O5'	1:A:825:U:H6	1.95	0.48
1:A:1420:C:C2	1:A:1445:G:N2	2.80	0.48
1:A:2029:C:O2'	1:A:2030:A:H5'	2.13	0.48
1:A:2387:U:C2	1:A:2402:A:C2	3.02	0.48
1:A:2832:C:H5'	39:A:6212:HOH:O	2.13	0.48
2:B:3008:G:C6	2:B:3009:C:C4	3.02	0.48
8:G:11:VAL:CG1	8:G:12:ASP:H	2.27	0.48
10:I:12:ILE:CB	39:I:4714:HOH:O	2.48	0.48
10:I:12:ILE:HA	39:I:4499:HOH:O	2.13	0.48
11:J:26:LYS:CG	11:J:28:ILE:H	2.19	0.48
11:J:72:VAL:CG1	11:J:81:TYR:CZ	2.97	0.48
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.43	0.48
14:M:65:ASP:O	14:M:66:VAL:C	2.52	0.48
14:M:144:ASP:HA	14:M:147:GLU:HG3	1.96	0.48
1:A:175:G:H2'	15:N:192:ALA:HB3	1.95	0.48
1:A:204:A:H2'	1:A:205:U:C5'	2.44	0.48
1:A:259:G:O2'	1:A:260:C:H5'	2.14	0.48
1:A:1766:U:O2	1:A:1778:A:H5'	2.13	0.48
1:A:2445:U:H2'	1:A:2446:G:H8	1.78	0.48
1:A:2542:C:H5	39:A:8579:HOH:O	1.95	0.48
1:A:2763:G:C5	1:A:2764:C:C5	3.01	0.48
13:L:72:VAL:O	13:L:95:ALA:CB	2.60	0.48
15:N:155:HIS:O	15:N:158:ARG:HG2	2.13	0.48
20:S:56:PRO:HB3	20:S:80:TYR:CE2	2.48	0.48
22:U:20:HIS:HB3	22:U:41:ARG:HD2	1.94	0.48
23:V:35:LYS:HB2	39:V:774:HOH:O	2.13	0.48
25:X:40:ALA:HB3	39:X:5390:HOH:O	2.14	0.48
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.75	0.48
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.14	0.48
1:A:431:G:H5'	39:N:8545:HOH:O	2.11	0.48
1:A:1019:C:P	39:A:3437:HOH:O	2.71	0.48
1:A:1223:G:O2'	1:A:1224:G:H5'	2.13	0.48
1:A:1484:G:H2'	39:A:8621:HOH:O	2.13	0.48
1:A:1886:A:H1'	39:A:4299:HOH:O	2.13	0.48
1:A:1992:U:OP2	13:L:66:ARG:HD2	2.14	0.48
1:A:2001:G:O2'	1:A:2002:C:H5'	2.13	0.48
1:A:2243:C:P	39:A:3245:HOH:O	2.71	0.48
1:A:2505:G:C2'	1:A:2506:A:H5'	2.43	0.48
1:A:2506:A:O2'	1:A:2507:G:O5'	2.32	0.48
1:A:2825:C:H4'	1:A:2826:G:O5'	2.14	0.48
2:B:3104:A:O2'	2:B:3105:A:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:147:ALA:HA	16:O:16:ALA:HB3	1.96	0.48
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.29	0.48
13:L:55:VAL:CG1	13:L:56:SER:H	2.26	0.48
14:M:149:ARG:O	14:M:150:GLN:HB2	2.14	0.48
15:N:35:PRO:CD	15:N:38:VAL:CG2	2.88	0.48
15:N:81:ARG:HG3	15:N:85:ARG:HB2	1.96	0.48
16:O:24:LEU:O	16:O:25:ARG:C	2.49	0.48
17:P:36:PRO:O	17:P:39:THR:OG1	2.32	0.48
22:U:71:VAL:CG1	22:U:72:ILE:N	2.76	0.48
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.12	0.48
31:4:14:CYS:HB3	31:4:16:GLU:HG2	1.96	0.48
31:4:40:ARG:HD2	39:4:8548:HOH:O	2.14	0.48
1:A:25:A:H1'	1:A:519:A:C2	2.49	0.48
1:A:181:G:H5"	1:A:1472:C:H4'	1.96	0.48
1:A:240:C:C4'	15:N:146:GLN:NE2	2.76	0.48
1:A:306:A:O5'	22:U:38:ARG:NH2	2.46	0.48
1:A:347:A:H2'	1:A:348:C:H5'	1.95	0.48
1:A:515:C:H5	39:A:6564:HOH:O	1.97	0.48
1:A:966:U:H4'	11:J:90:PHE:HE2	1.78	0.48
1:A:1015:C:H2'	1:A:1016:U:H6	1.78	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.31	0.48
1:A:1334:C:OP2	39:A:3503:HOH:O	2.20	0.48
1:A:1596:U:H2'	1:A:1598:A:OP2	2.13	0.48
1:A:1692:C:OP2	39:A:9643:HOH:O	2.20	0.48
1:A:1848:G:H4'	39:A:6007:HOH:O	2.14	0.48
1:A:2668:G:N2	1:A:2669:U:C2	2.82	0.48
2:B:3008:G:OP1	39:B:8479:HOH:O	2.20	0.48
2:B:3052:A:H8	2:B:3052:A:O5'	1.97	0.48
6:E:19:PRO:CB	6:E:244:ALA:HB2	2.44	0.48
6:E:123:LEU:HD23	6:E:123:LEU:HA	1.64	0.48
12:K:14:ALA:O	12:K:15:ARG:C	2.50	0.48
13:L:28:GLU:OE2	13:L:58:THR:HG21	2.12	0.48
16:O:176:ARG:O	16:O:180:LEU:HG	2.13	0.48
16:O:180:LEU:O	16:O:181:ASP:HB3	2.14	0.48
25:X:125:HIS:CD2	25:X:127:GLY:H	2.31	0.48
29:2:25:LYS:HD2	30:3:49:GLU:H	1.79	0.48
1:A:67:A:N3	1:A:67:A:H5'	2.29	0.48
1:A:155:C:OP2	15:N:188:ARG:NH1	2.38	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.14	0.48
1:A:721:A:H2'	1:A:722:G:H5'	1.96	0.48
1:A:1173:A:H4'	1:A:1174:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:C:OP2	1:A:1624:A:O2'	2.25	0.48
1:A:2549:C:H1'	5:D:248:ARG:NH2	2.29	0.48
39:A:4831:HOH:O	18:Q:117:SER:HB2	2.13	0.48
4:C:29:HIS:CE1	4:C:107:ASN:ND2	2.82	0.48
8:G:11:VAL:HG11	8:G:22:VAL:CG1	2.44	0.48
8:G:69:ILE:O	8:G:72:MET:N	2.46	0.48
9:H:21:GLU:HA	9:H:24:ARG:HE	1.78	0.48
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.96	0.48
15:N:63:VAL:O	15:N:130:GLU:HA	2.14	0.48
28:1:46:LYS:NZ	39:1:7607:HOH:O	2.46	0.48
1:A:116:G:H5"	1:A:131:A:H5'	1.95	0.48
1:A:343:C:H2'	1:A:344:C:H6	1.78	0.48
1:A:380:A:OP1	1:A:380:A:H3'	2.13	0.48
1:A:517:U:C2'	1:A:518:G:H5'	2.43	0.48
1:A:664:U:O4	1:A:681:G:H5"	2.13	0.48
1:A:1570:C:N4	1:A:1571:G:C6	2.82	0.48
1:A:2039:A:H2'	1:A:2040:C:H6	1.78	0.48
1:A:2100:A:H5'	39:E:8470:HOH:O	2.12	0.48
5:D:36:PRO:CA	5:D:168:GLY:CA	2.88	0.48
6:E:27:ARG:HD2	17:P:5:PRO:HD2	1.96	0.48
6:E:109:LEU:HD12	6:E:109:LEU:O	2.14	0.48
1:A:135:G:H1'	15:N:135:ASP:OD2	2.14	0.47
1:A:1205:U:H2'	1:A:1206:U:C5'	2.43	0.47
1:A:1231:A:H2'	39:A:8804:HOH:O	2.13	0.47
1:A:1697:G:H1'	39:A:6744:HOH:O	2.14	0.47
1:A:1760:G:C8	1:A:1813:U:C2	3.01	0.47
1:A:2595:U:H2'	1:A:2596:A:O4'	2.13	0.47
1:A:2758:G:O2'	1:A:2759:C:H5'	2.13	0.47
39:A:5537:HOH:O	28:1:34:LYS:HE2	2.13	0.47
5:D:251:VAL:O	5:D:251:VAL:HG22	2.14	0.47
9:H:28:ALA:HB3	9:H:99:THR:HG23	1.96	0.47
11:J:161:SER:N	39:J:8362:HOH:O	2.42	0.47
16:O:8:VAL:O	16:O:9:PRO:O	2.32	0.47
18:Q:5:ALA:O	18:Q:8:ARG:HB3	2.13	0.47
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.44	0.47
22:U:32:ARG:NH1	22:U:38:ARG:NH1	2.61	0.47
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.96	0.47
1:A:171:C:O5'	1:A:171:C:H6	1.97	0.47
1:A:696:C:O2'	1:A:731:U:OP1	2.30	0.47
1:A:746:A:P	39:A:4988:HOH:O	2.72	0.47
1:A:1190:G:H5'	1:A:1208:C:O2'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:A:C2	1:A:1481:G:C2	3.02	0.47
1:A:1504:A:H5'	39:A:3896:HOH:O	2.14	0.47
1:A:1730:G:C5'	1:A:1731:C:C6	2.97	0.47
1:A:1857:A:N6	1:A:2247:C:H1'	2.29	0.47
1:A:1979:G:O2'	1:A:1980:U:OP1	2.30	0.47
1:A:2545:U:P	39:A:5675:HOH:O	2.72	0.47
1:A:2909:G:H2'	1:A:2910:A:H8	1.79	0.47
8:G:69:ILE:HA	8:G:72:MET:HE2	1.96	0.47
11:J:26:LYS:CD	11:J:28:ILE:HD12	2.28	0.47
14:M:24:ALA:HB2	14:M:30:ARG:HD2	1.95	0.47
16:O:154:LEU:C	16:O:156:GLU:H	2.16	0.47
16:O:176:ARG:HE	16:O:180:LEU:HD11	1.78	0.47
16:O:182:GLY:O	16:O:183:ASP:O	2.32	0.47
17:P:47:ARG:HG3	17:P:47:ARG:NH1	2.17	0.47
19:R:41:LEU:N	19:R:41:LEU:HD12	2.29	0.47
21:T:37:VAL:O	21:T:41:VAL:HG23	2.14	0.47
25:X:67:ALA:HB2	25:X:93:ILE:HD13	1.95	0.47
27:Z:186:ARG:NH1	27:Z:186:ARG:CG	2.74	0.47
28:1:33:HIS:CE1	28:1:49:ARG:HD2	2.49	0.47
1:A:51:G:C2	1:A:111:C:C2	3.02	0.47
1:A:191:A:N1	1:A:236:A:O2'	2.41	0.47
1:A:491:C:O2'	1:A:492:C:H5'	2.14	0.47
1:A:1500:U:P	18:Q:41:ARG:HH22	2.37	0.47
1:A:1555:G:H4'	1:A:1630:A:H2	1.78	0.47
1:A:1767:A:O2'	1:A:1768:C:H5'	2.14	0.47
1:A:1942:A:H3'	39:A:6809:HOH:O	2.14	0.47
39:A:6336:HOH:O	15:N:178:LYS:HB2	2.14	0.47
4:C:69:LEU:HB3	39:C:8578:HOH:O	2.14	0.47
5:D:275:GLY:O	5:D:291:ASP:HA	2.14	0.47
9:H:21:GLU:O	9:H:25:ASP:OD2	2.31	0.47
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.37	0.47
12:K:42:GLU:OE2	12:K:106:GLY:N	2.48	0.47
15:N:138:HIS:HD1	15:N:140:ALA:HB3	1.80	0.47
18:Q:20:ARG:NH1	18:Q:54:LYS:HD3	2.29	0.47
20:S:100:ASP:C	20:S:102:GLN:H	2.17	0.47
25:X:13:MET:O	25:X:14:HIS:C	2.53	0.47
26:Y:23:HIS:O	26:Y:63:ARG:HG2	2.13	0.47
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.17	0.47
1:A:61:G:C6	1:A:62:C:C4	3.03	0.47
1:A:556:C:OP1	27:Z:121:HIS:HE1	1.97	0.47
1:A:1632:A:O5'	1:A:1632:A:C8	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2748:G:H1'	39:A:7361:HOH:O	2.14	0.47
2:B:3034:A:O5'	2:B:3034:A:H8	1.96	0.47
7:F:128:LEU:HD23	7:F:128:LEU:C	2.34	0.47
9:H:46:GLU:OE1	9:H:100:ASP:HA	2.15	0.47
9:H:75:ILE:HG23	9:H:75:ILE:O	2.13	0.47
11:J:47:GLU:CG	11:J:133:ILE:HD12	2.41	0.47
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.31	0.47
13:L:8:VAL:HG12	13:L:9:THR:N	2.30	0.47
13:L:61:THR:O	13:L:64:MET:N	2.47	0.47
1:A:474:C:O3'	6:E:73:LEU:CD2	2.63	0.47
1:A:677:C:H4'	6:E:246:ARG:NH2	2.29	0.47
1:A:707:C:C2	1:A:708:A:C8	3.02	0.47
1:A:783:C:O2'	1:A:784:A:H5'	2.14	0.47
1:A:1098:A:H2'	1:A:1099:G:O4'	2.15	0.47
1:A:1192:A:H3'	1:A:1193:A:H5'	1.96	0.47
1:A:1269:G:H2'	1:A:1270:U:H6	1.80	0.47
1:A:1406:A:H5'	1:A:1407:A:C8	2.49	0.47
1:A:1701:A:H4'	1:A:1702:U:C5'	2.44	0.47
1:A:1859:A:N7	1:A:1860:U:C5	2.83	0.47
1:A:2080:G:N3	39:A:9993:HOH:O	2.36	0.47
2:B:3039:U:H1'	2:B:3044:A:N6	2.29	0.47
5:D:238:ASN:ND2	5:D:240:GLY:N	2.52	0.47
5:D:243:ASN:HA	5:D:244:PRO:C	2.33	0.47
7:F:55:LYS:C	39:F:4069:HOH:O	2.53	0.47
7:F:67:ASP:N	7:F:67:ASP:OD1	2.47	0.47
7:F:94:ALA:CB	7:F:173:GLU:C	2.83	0.47
7:F:135:VAL:CG2	7:F:136:ARG:N	2.78	0.47
8:G:84:MET:HB2	8:G:131:LEU:HB2	1.97	0.47
16:O:47:LEU:HD13	16:O:97:VAL:HG11	1.95	0.47
16:O:155:GLU:O	16:O:156:GLU:HG3	2.15	0.47
27:Z:189:ASN:ND2	27:Z:192:ASP:N	2.62	0.47
1:A:100:C:P	39:A:3593:HOH:O	2.73	0.47
1:A:477:A:C6	1:A:478:C:C4	3.02	0.47
1:A:840:U:O2	1:A:2055:A:H1'	2.15	0.47
1:A:1191:A:H3'	1:A:1192:A:C5'	2.36	0.47
1:A:1728:G:N2	1:A:2048:C:C2	2.83	0.47
1:A:1892:C:C4	1:A:1893:C:C5	3.03	0.47
1:A:1942:A:C4'	39:A:6809:HOH:O	2.63	0.47
1:A:2379:G:C8	1:A:2381:C:C5	3.02	0.47
1:A:2594:C:H2'	1:A:2595:U:C5'	2.45	0.47
1:A:2598:U:O2	1:A:2600:A:H8	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2871:G:C6	1:A:2872:U:C4	3.02	0.47
39:A:8568:HOH:O	28:1:19:GLY:HA2	2.14	0.47
4:C:170:VAL:HG13	28:1:22:ILE:CG2	2.43	0.47
4:C:192:VAL:CG2	4:C:201:PHE:HB3	2.44	0.47
5:D:258:GLY:N	5:D:260:HIS:CE1	2.70	0.47
6:E:16:VAL:CG1	6:E:17:ASP:N	2.75	0.47
6:E:129:HIS:HE1	6:E:231:ARG:HA	1.78	0.47
6:E:187:ARG:HA	39:E:8393:HOH:O	2.15	0.47
7:F:104:PHE:CE2	7:F:166:ILE:CD1	2.97	0.47
14:M:7:GLN:HB3	14:M:13:HIS:ND1	2.30	0.47
16:O:15:GLU:O	16:O:16:ALA:HB3	2.14	0.47
16:O:157:PRO:HA	39:O:8525:HOH:O	2.15	0.47
39:O:8541:HOH:O	19:R:19:ARG:CD	2.62	0.47
24:W:16:ARG:CZ	24:W:63:GLU:HG3	2.44	0.47
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.27	0.47
1:A:187:A:H3'	1:A:188:C:C6	2.47	0.47
1:A:380:A:H5"	15:N:48:ARG:HH21	1.80	0.47
1:A:461:C:H2'	39:A:3488:HOH:O	2.14	0.47
1:A:758:A:H2'	1:A:759:C:O4'	2.14	0.47
1:A:816:G:C6	1:A:817:G:N1	2.83	0.47
1:A:1102:C:H2'	1:A:1103:C:H6	1.79	0.47
1:A:1246:A:O2'	1:A:1247:A:H3'	2.14	0.47
1:A:1355:A:N3	1:A:1355:A:H2'	2.30	0.47
1:A:2254:G:H1'	39:A:5010:HOH:O	2.14	0.47
1:A:2314:G:O2'	1:A:2361:A:C1'	2.63	0.47
1:A:2587:U:H2'	1:A:2589:U:H5"	1.95	0.47
39:A:4313:HOH:O	12:K:47:THR:CB	2.61	0.47
5:D:102:THR:HG22	39:D:8618:HOH:O	2.15	0.47
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.95	0.47
7:F:11:HIS:O	7:F:12:GLU:HB3	2.14	0.47
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.61	0.47
9:H:104:ALA:O	9:H:108:LEU:HB3	2.14	0.47
11:J:86:ARG:H	11:J:86:ARG:HG2	1.53	0.47
13:L:63:GLU:CG	39:L:6344:HOH:O	2.58	0.47
15:N:8:ILE:O	15:N:9:ARG:C	2.52	0.47
18:Q:27:ARG:HA	39:Q:3969:HOH:O	2.13	0.47
20:S:92:LEU:HD23	20:S:145:LEU:CD2	2.41	0.47
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.45	0.47
25:X:58:SER:O	25:X:59:GLN:C	2.52	0.47
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.45	0.47
31:4:91:GLN:O	31:4:92:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.47
1:A:201:G:N2	1:A:202:U:C2	2.83	0.47
1:A:297:U:H2'	1:A:298:C:H6	1.80	0.47
1:A:794:U:H3	1:A:819:A:H61	1.63	0.47
1:A:1306:U:H5"	6:E:184:ARG:HH11	1.79	0.47
1:A:1635:U:O2'	1:A:1636:G:H5'	2.15	0.47
1:A:1684:A:O2'	1:A:1685:A:H5"	2.15	0.47
1:A:1711:A:C2'	1:A:1712:A:H5'	2.45	0.47
1:A:1748:U:H4'	39:A:6984:HOH:O	2.14	0.47
1:A:1819:G:H2'	1:A:1820:G:C4'	2.44	0.47
1:A:1916:C:C2'	1:A:1917:G:H5'	2.45	0.47
1:A:1929:G:H1'	39:A:4634:HOH:O	2.14	0.47
1:A:2038:A:H5"	5:D:222:LYS:HG3	1.96	0.47
1:A:2514:U:H6	1:A:2514:U:O5'	1.98	0.47
1:A:2656:G:C2'	1:A:2657:G:H5'	2.45	0.47
7:F:23:VAL:O	7:F:23:VAL:CG2	2.60	0.47
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.47
13:L:68:VAL:O	13:L:68:VAL:HG12	2.14	0.47
15:N:24:MET:CE	15:N:28:MET:HE3	2.44	0.47
1:A:151:A:C2	1:A:442:A:C8	3.03	0.47
1:A:1085:C:C4	1:A:1086:A:C5	3.03	0.47
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.44	0.47
1:A:1711:A:O2'	1:A:1712:A:H5'	2.14	0.47
1:A:2311:A:O2'	1:A:2312:G:H5'	2.15	0.47
1:A:2861:G:O4'	5:D:282:GLY:HA2	2.15	0.47
2:B:3107:C:H2'	2:B:3108:C:C6	2.50	0.47
5:D:7:ARG:NH1	5:D:11:LEU:CD2	2.78	0.47
11:J:166:ASN:N	11:J:166:ASN:HD22	2.12	0.47
13:L:10:GLN:NE2	13:L:10:GLN:N	2.48	0.47
13:L:86:THR:HG22	13:L:87:ARG:N	2.29	0.47
14:M:53:ARG:NH2	14:M:57:VAL:CG1	2.77	0.47
14:M:145:LEU:O	14:M:145:LEU:HD23	2.14	0.47
15:N:38:VAL:O	15:N:63:VAL:HG13	2.15	0.47
16:O:86:LEU:HD12	16:O:125:ALA:CB	2.43	0.47
16:O:141:ARG:CA	39:O:8565:HOH:O	2.62	0.47
19:R:42:LYS:NZ	19:R:43:ILE:O	2.41	0.47
20:S:119:VAL:O	20:S:119:VAL:CG1	2.62	0.47
25:X:14:HIS:HA	39:X:2978:HOH:O	2.14	0.47
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.96	0.47
25:X:132:VAL:O	25:X:134:GLU:N	2.48	0.47
28:1:73:THR:O	28:1:75:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:C:O2	39:A:9551:HOH:O	2.18	0.47
1:A:777:U:OP2	1:A:777:U:H4'	2.15	0.47
1:A:840:U:H2'	20:S:128:ARG:NH1	2.30	0.47
1:A:912:A:N6	39:A:4355:HOH:O	2.48	0.47
1:A:1088:A:OP1	39:A:5125:HOH:O	2.20	0.47
1:A:1118:A:C8	1:A:1119:G:H5"	2.49	0.47
1:A:1186:C:N4	1:A:1187:U:O4	2.48	0.47
1:A:2032:U:H2'	1:A:2033:G:C5'	2.45	0.47
1:A:2388:C:O2'	1:A:2389:U:H5'	2.15	0.47
1:A:2732:U:H1'	39:A:4443:HOH:O	2.14	0.47
39:A:5039:HOH:O	5:D:3:PRO:HD2	2.14	0.47
2:B:3012:C:OP2	2:B:3069:U:O2'	2.33	0.47
6:E:112:ARG:O	6:E:115:LEU:HB2	2.15	0.47
6:E:162:VAL:HG12	6:E:162:VAL:O	2.15	0.47
8:G:15:GLN:HG2	8:G:19:ASP:O	2.15	0.47
10:I:67:LEU:O	10:I:71:LEU:HG	2.15	0.47
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.50	0.47
15:N:149:TRP:O	15:N:152:ARG:HG2	2.15	0.47
24:W:6:GLN:HA	39:W:7325:HOH:O	2.13	0.47
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.96	0.47
1:A:123:U:H2'	1:A:124:C:C6	2.50	0.46
1:A:926:A:O4'	14:M:39:GLU:HG2	2.15	0.46
1:A:1285:U:H4'	25:X:74:GLU:OE1	2.15	0.46
1:A:1327:G:C2	1:A:1331:A:C2	3.03	0.46
1:A:1555:G:H4'	1:A:1630:A:C2	2.50	0.46
1:A:2247:C:O2'	1:A:2248:C:H5'	2.14	0.46
1:A:2443:C:H3'	39:A:9966:HOH:O	2.14	0.46
1:A:2501:G:H1'	39:A:4019:HOH:O	2.15	0.46
4:C:75:GLY:HA3	28:1:62:TYR:CZ	2.50	0.46
8:G:7:ILE:HG22	8:G:45:ASP:O	2.15	0.46
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.46	0.46
15:N:45:ARG:HB3	15:N:48:ARG:HB2	1.97	0.46
15:N:123:ASP:C	15:N:123:ASP:OD1	2.54	0.46
20:S:47:LEU:O	20:S:51:ILE:HG13	2.15	0.46
20:S:114:VAL:HA	20:S:144:GLU:O	2.15	0.46
27:Z:103:THR:HG22	27:Z:104:GLU:OE2	2.15	0.46
28:1:55:TRP:O	28:1:63:LYS:HA	2.16	0.46
1:A:645:U:H2'	1:A:646:G:C8	2.51	0.46
1:A:908:A:O2'	1:A:909:U:H5'	2.16	0.46
1:A:920:C:H5"	1:A:921:G:O5'	2.15	0.46
1:A:1947:G:N2	1:A:1966:U:O2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2094:G:H4'	5:D:245:SER:HB3	1.97	0.46
1:A:2833:C:C2	1:A:2848:G:N2	2.84	0.46
4:C:135:VAL:N	39:C:8596:HOH:O	2.47	0.46
5:D:53:LEU:HD21	5:D:270:ILE:HD12	1.97	0.46
6:E:139:VAL:HG21	6:E:240:LEU:HD12	1.97	0.46
9:H:105:ALA:CB	39:H:5522:HOH:O	2.62	0.46
11:J:127:GLY:O	11:J:128:ALA:CB	2.62	0.46
13:L:75:ARG:NH1	39:L:5638:HOH:O	2.48	0.46
22:U:87:VAL:HB	22:U:88:PRO:HD2	1.97	0.46
1:A:324:G:C6	1:A:325:U:C5	3.03	0.46
1:A:444:C:H1'	39:A:3531:HOH:O	2.16	0.46
1:A:561:G:O2'	1:A:562:A:H5'	2.16	0.46
1:A:699:C:C2	1:A:744:G:C2	3.02	0.46
1:A:1042:U:H1'	39:A:3037:HOH:O	2.15	0.46
5:D:52:VAL:O	5:D:53:LEU:HD12	2.15	0.46
6:E:238:SER:HB3	39:E:8386:HOH:O	2.16	0.46
7:F:104:PHE:CE2	7:F:166:ILE:HD13	2.51	0.46
10:I:16:LYS:O	10:I:20:VAL:HG23	2.16	0.46
11:J:150:LYS:HE2	39:J:8378:HOH:O	2.15	0.46
18:Q:16:VAL:CG1	18:Q:20:ARG:HB2	2.45	0.46
20:S:29:LYS:NZ	39:S:8541:HOH:O	2.48	0.46
23:V:44:ARG:CB	39:V:3805:HOH:O	2.62	0.46
26:Y:30:MET:HE3	26:Y:55:ASN:OD1	2.16	0.46
31:4:60:LYS:HG3	31:4:61:PRO:CD	2.32	0.46
1:A:39:G:N2	1:A:444:C:C2	2.84	0.46
1:A:69:A:H5'	1:A:69:A:C8	2.50	0.46
1:A:661:G:C5	1:A:686:A:C2	3.03	0.46
1:A:1191:A:N3	1:A:1207:A:C2	2.83	0.46
1:A:1421:C:C2	1:A:1422:U:C5	3.04	0.46
1:A:2356:A:H5'	39:A:5113:HOH:O	2.16	0.46
4:C:99:ILE:O	4:C:131:HIS:HE1	1.97	0.46
4:C:217:ARG:CG	4:C:217:ARG:NH1	2.76	0.46
5:D:16:ARG:CZ	39:D:8558:HOH:O	2.61	0.46
6:E:83:ALA:O	6:E:86:GLY:N	2.42	0.46
6:E:95:GLU:OE1	6:E:95:GLU:N	2.40	0.46
7:F:84:LEU:HA	7:F:87:ALA:HB3	1.96	0.46
14:M:90:ARG:HH21	14:M:121:ILE:HD11	1.79	0.46
15:N:99:ARG:HD2	15:N:167:GLY:HA2	1.97	0.46
18:Q:102:ARG:HG2	18:Q:123:TYR:CE1	2.50	0.46
19:R:30:VAL:O	19:R:30:VAL:HG12	2.15	0.46
19:R:42:LYS:NZ	19:R:43:ILE:N	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:132:VAL:C	25:X:134:GLU:H	2.19	0.46
1:A:485:A:HO2'	1:A:487:G:H5'	1.80	0.46
1:A:1846:U:H5"	4:C:186:TRP:CZ2	2.51	0.46
1:A:2088:C:H1'	1:A:2841:A:N1	2.30	0.46
1:A:2796:U:C4	1:A:2797:C:C5	3.04	0.46
2:B:3001:U:O3'	2:B:3003:A:C5'	2.64	0.46
2:B:3057:A:N3	2:B:3057:A:H5'	2.31	0.46
4:C:192:VAL:O	4:C:207:GLN:HG2	2.14	0.46
5:D:145:HIS:C	5:D:145:HIS:CD2	2.88	0.46
6:E:96:LYS:HG2	6:E:97:ASP:N	2.30	0.46
9:H:110:GLU:O	9:H:114:LYS:HG3	2.15	0.46
11:J:81:TYR:CD1	11:J:81:TYR:C	2.88	0.46
12:K:88:PRO:C	35:K:8502:CL:CL	2.91	0.46
16:O:10:MET:N	39:O:8550:HOH:O	2.36	0.46
16:O:74:PRO:CD	16:O:159:TYR:CE2	2.99	0.46
16:O:181:ASP:CB	39:O:8567:HOH:O	2.63	0.46
19:R:25:PRO:HB2	39:R:4350:HOH:O	2.14	0.46
1:A:351:G:O2'	1:A:352:A:H5'	2.16	0.46
1:A:593:A:P	39:A:3881:HOH:O	2.70	0.46
1:A:710:G:N2	1:A:719:C:C2	2.84	0.46
1:A:2361:A:H5'	39:A:8694:HOH:O	2.14	0.46
1:A:2543:G:H2'	1:A:2544:G:O4'	2.15	0.46
1:A:2679:G:H2'	1:A:2681:A:OP2	2.15	0.46
1:A:2716:G:P	5:D:262:ARG:HH21	2.39	0.46
1:A:2717:C:H5'	5:D:302:PRO:HA	1.98	0.46
1:A:2719:A:H5"	39:A:3176:HOH:O	2.13	0.46
1:A:2769:C:H2'	1:A:2770:G:C5'	2.45	0.46
1:A:2769:C:H2'	1:A:2770:G:H5'	1.98	0.46
39:A:9283:HOH:O	19:R:48:PRO:HB3	2.14	0.46
4:C:99:ILE:O	4:C:131:HIS:CE1	2.68	0.46
4:C:130:THR:HB	4:C:137:VAL:HB	1.98	0.46
4:C:223:ARG:CZ	39:C:8574:HOH:O	2.63	0.46
6:E:11:ASN:O	6:E:12:THR:C	2.54	0.46
12:K:22:VAL:O	12:K:26:VAL:HG23	2.15	0.46
14:M:113:GLN:HA	39:M:8444:HOH:O	2.16	0.46
17:P:21:SER:HB2	17:P:106:PRO:O	2.13	0.46
22:U:113:GLU:O	22:U:114:SER:C	2.54	0.46
26:Y:23:HIS:HD2	39:Y:1192:HOH:O	1.98	0.46
1:A:107:U:C2'	1:A:108:U:H5'	2.46	0.46
1:A:168:C:H6	1:A:168:C:O5'	1.99	0.46
1:A:327:A:N6	39:A:4350:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:C:O2'	6:E:73:LEU:HD21	2.15	0.46
1:A:657:G:H2'	1:A:658:C:C6	2.51	0.46
1:A:1277:C:N4	1:A:1278:A:C6	2.84	0.46
1:A:1315:G:H1'	27:Z:211:ALA:HB3	1.96	0.46
1:A:1751:G:C3'	1:A:1752:G:H5"	2.45	0.46
1:A:2245:C:OP1	39:A:4723:HOH:O	2.20	0.46
39:A:3677:HOH:O	27:Z:186:ARG:HD2	2.15	0.46
4:C:55:VAL:HG22	4:C:68:ILE:O	2.16	0.46
6:E:165:ASP:O	6:E:168:ARG:HB3	2.16	0.46
7:F:169:THR:O	7:F:169:THR:HG22	2.15	0.46
9:H:48:VAL:HG23	9:H:74:PHE:HB3	1.98	0.46
25:X:65:VAL:HA	25:X:68:THR:CG2	2.45	0.46
28:1:10:ARG:HG3	28:1:11:THR:N	2.31	0.46
31:4:35:TRP:O	31:4:35:TRP:CG	2.68	0.46
1:A:80:A:H4'	1:A:81:G:O5'	2.16	0.46
1:A:670:G:N2	1:A:677:C:C2	2.84	0.46
1:A:1114:A:H2'	1:A:1115:U:C6	2.51	0.46
1:A:2688:U:H2'	1:A:2689:A:H8	1.81	0.46
1:A:2712:G:OP1	13:L:43:ARG:NH1	2.48	0.46
1:A:2763:G:H2'	1:A:2764:C:C6	2.51	0.46
1:A:2795:C:O2'	1:A:2796:U:H5'	2.16	0.46
4:C:19:PRO:HD3	39:C:8603:HOH:O	2.16	0.46
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.43	0.46
4:C:132:ASP:HB3	4:C:135:VAL:H	1.81	0.46
4:C:164:ARG:CB	28:1:68:CYS:SG	2.93	0.46
5:D:62:ARG:CA	5:D:65:MET:HE2	2.30	0.46
5:D:222:LYS:HE2	39:D:8551:HOH:O	2.16	0.46
7:F:136:ARG:CD	7:F:155:HIS:O	2.62	0.46
10:I:27:ILE:HD12	10:I:70:ALA:CB	2.46	0.46
11:J:17:ARG:HD3	11:J:23:ILE:CD1	2.46	0.46
11:J:85:ILE:HG23	11:J:85:ILE:O	2.15	0.46
12:K:53:ILE:O	12:K:57:TYR:HD1	1.99	0.46
13:L:76:GLN:HB2	39:L:1433:HOH:O	2.16	0.46
15:N:76:ARG:HG2	15:N:76:ARG:HH11	1.81	0.46
16:O:93:GLN:CG	39:O:8554:HOH:O	2.64	0.46
21:T:10:VAL:HG13	24:W:35:ALA:O	2.14	0.46
21:T:32:ALA:HA	21:T:36:GLU:OE1	2.16	0.46
22:U:19:ARG:NH1	22:U:68:ASP:O	2.49	0.46
25:X:2:HIS:HD2	25:X:56:GLU:N	2.14	0.46
25:X:38:THR:O	25:X:42:ARG:HB2	2.16	0.46
28:1:30:GLU:O	28:1:33:HIS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:C:C5’	39:A:4691:HOH:O	2.57	0.46
1:A:1079:A:N1	1:A:2068:G:O2’	2.28	0.46
1:A:1174:A:H5’	1:A:1176:C:OP2	2.15	0.46
1:A:1210:G:C2	1:A:1211:G:C8	3.04	0.46
1:A:1327:G:N1	1:A:1331:A:C6	2.83	0.46
1:A:1396:C:H4’	18:Q:2:ASP:OD1	2.15	0.46
1:A:1468:G:O2’	1:A:1865:A:N3	2.42	0.46
1:A:2256:G:C2’	1:A:2257:G:C5’	2.83	0.46
1:A:2299:G:O6	19:R:1:PRO:HA	2.16	0.46
1:A:2397:G:C5	1:A:2465:A:C6	3.04	0.46
1:A:2398:A:O2’	39:A:3319:HOH:O	2.19	0.46
1:A:2441:U:H4’	14:M:53:ARG:HD2	1.97	0.46
1:A:2912:C:H2’	1:A:2913:A:O4’	2.16	0.46
39:A:9015:HOH:O	5:D:18:ARG:HD3	2.15	0.46
4:C:100:PRO:HG2	4:C:103:VAL:CG2	2.44	0.46
5:D:248:ARG:O	5:D:251:VAL:HG12	2.16	0.46
5:D:305:ASP:O	5:D:306:LYS:CB	2.63	0.46
5:D:316:ARG:N	5:D:317:PRO:HD3	2.31	0.46
6:E:33:LYS:HD2	39:E:8466:HOH:O	2.16	0.46
6:E:95:GLU:H	6:E:95:GLU:CD	2.13	0.46
8:G:107:PHE:CZ	8:G:108:LEU:HD13	2.46	0.46
14:M:1:THR:HA	39:M:8396:HOH:O	2.15	0.46
16:O:93:GLN:HG2	39:O:8554:HOH:O	2.16	0.46
1:A:407:A:H3’	39:A:3937:HOH:O	2.17	0.46
1:A:686:A:O2’	1:A:747:G:H4’	2.16	0.46
1:A:924:G:P	39:A:3173:HOH:O	2.73	0.46
1:A:1097:A:N3	1:A:1259:A:C6	2.84	0.46
1:A:1136:U:H4’	39:A:3454:HOH:O	2.15	0.46
1:A:1874:U:P	4:C:51:ARG:HD2	2.56	0.46
1:A:2274:A:H1’	15:N:86:MET:SD	2.56	0.46
1:A:2388:C:H2’	1:A:2389:U:O4’	2.16	0.46
1:A:2642:G:H5’	39:A:7206:HOH:O	2.16	0.46
39:A:4732:HOH:O	6:E:73:LEU:HD11	2.16	0.46
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.97	0.46
6:E:219:ASN:O	6:E:223:LEU:HB2	2.15	0.46
6:E:223:LEU:HD12	6:E:223:LEU:HA	1.68	0.46
7:F:55:LYS:HA	39:F:6752:HOH:O	2.16	0.46
7:F:57:THR:CG2	7:F:63:ILE:HG22	2.44	0.46
7:F:81:GLU:O	7:F:83:PHE:N	2.49	0.46
11:J:110:GLY:N	39:J:8394:HOH:O	2.49	0.46
15:N:85:ARG:HA	15:N:87:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:37:ARG:NE	39:O:8533:HOH:O	2.49	0.46
16:O:104:ILE:O	16:O:105:GLY:C	2.54	0.46
17:P:113:VAL:O	17:P:114:ILE:HD13	2.15	0.46
31:4:69:TYR:CB	31:4:78:HIS:CE1	2.99	0.46
1:A:196:G:O2'	14:M:56:LYS:NZ	2.50	0.45
1:A:746:A:H5'	39:A:4988:HOH:O	2.17	0.45
1:A:1086:A:C6	25:X:11:VAL:HG11	2.50	0.45
1:A:1112:G:C2	1:A:1252:A:C2	3.04	0.45
1:A:1189:A:O2'	1:A:1208:C:H2'	2.15	0.45
1:A:1707:G:N2	1:A:1710:A:OP2	2.47	0.45
1:A:1821:A:N6	1:A:2029:C:N4	2.64	0.45
1:A:2055:A:H4'	39:S:8587:HOH:O	2.16	0.45
1:A:2338:G:P	7:F:97:GLN:HG3	2.55	0.45
1:A:2365:G:N3	1:A:2370:A:C2	2.84	0.45
1:A:2715:G:O2'	5:D:262:ARG:HD2	2.16	0.45
1:A:2884:G:O2'	1:A:2885:A:H5'	2.16	0.45
2:B:3057:A:N6	39:B:8446:HOH:O	2.37	0.45
2:B:3118:C:O2'	2:B:3119:C:H5'	2.16	0.45
7:F:140:ARG:O	7:F:140:ARG:HG2	2.16	0.45
9:H:99:THR:O	9:H:100:ASP:HB2	2.15	0.45
13:L:4:LEU:HD22	13:L:116:GLU:HB3	1.97	0.45
16:O:142:THR:HG22	16:O:142:THR:O	2.16	0.45
20:S:29:LYS:HD3	39:S:8541:HOH:O	2.14	0.45
24:W:20:LEU:HD11	24:W:53:ILE:HG23	1.98	0.45
1:A:150:G:N2	1:A:185:G:O6	2.49	0.45
1:A:1167:G:O2'	1:A:1168:C:H5'	2.17	0.45
1:A:1189:A:N3	39:A:7142:HOH:O	2.48	0.45
1:A:1213:C:C2'	1:A:1214:G:H5'	2.46	0.45
1:A:1592:G:O2'	1:A:1593:C:O4'	2.32	0.45
1:A:1734:C:N3	1:A:1735:C:C5	2.84	0.45
1:A:1964:U:C6	39:A:4034:HOH:O	2.56	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.15	0.45
1:A:2508:C:P	39:A:4017:HOH:O	2.73	0.45
1:A:2668:G:C2	1:A:2669:U:C2	3.04	0.45
5:D:74:ILE:HG22	5:D:76:THR:CG2	2.44	0.45
7:F:29:HIS:C	39:F:5858:HOH:O	2.55	0.45
7:F:64:ARG:HB3	7:F:67:ASP:OD2	2.16	0.45
8:G:11:VAL:HG13	8:G:23:GLU:O	2.15	0.45
14:M:7:GLN:HB3	14:M:13:HIS:CE1	2.52	0.45
19:R:53:HIS:ND1	19:R:54:PRO:HD2	2.31	0.45
25:X:31:HIS:C	39:X:5420:HOH:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:G:C6	1:A:119:A:C5	3.04	0.45
1:A:184:G:H5"	15:N:153:THR:HG22	1.98	0.45
1:A:241:A:N1	1:A:378:A:O2'	2.44	0.45
1:A:378:A:OP1	15:N:9:ARG:NH2	2.33	0.45
1:A:401:C:P	39:A:5265:HOH:O	2.74	0.45
1:A:472:A:O4'	1:A:774:C:H4'	2.16	0.45
1:A:484:A:C6	1:A:486:A:C6	3.05	0.45
1:A:731:U:H2'	1:A:732:C:C6	2.51	0.45
1:A:832:U:H2'	1:A:833:G:H8	1.81	0.45
1:A:853:C:H2'	1:A:854:G:O4'	2.15	0.45
1:A:877:G:C2	1:A:885:G:O4'	2.69	0.45
1:A:903:U:OP2	14:M:11:ARG:NH1	2.43	0.45
1:A:1874:U:OP1	4:C:51:ARG:HD2	2.16	0.45
1:A:1887:U:OP1	28:1:21:LYS:HG3	2.16	0.45
1:A:2379:G:N7	1:A:2408:A:N1	2.65	0.45
1:A:2502:C:C4'	11:J:151:MET:HG2	2.46	0.45
1:A:2673:U:C2	1:A:2817:G:C2	3.04	0.45
1:A:2863:G:C2	1:A:2894:C:O2	2.69	0.45
5:D:55:ASN:HB3	5:D:64:GLY:N	2.31	0.45
5:D:233:ARG:HG2	5:D:233:ARG:HH11	1.81	0.45
6:E:5:ILE:HD13	39:E:8438:HOH:O	2.15	0.45
7:F:58:VAL:CG1	7:F:59:GLY:N	2.78	0.45
8:G:108:LEU:HD11	8:G:164:ASP:HB2	1.99	0.45
15:N:154:ARG:HG3	39:N:8610:HOH:O	2.15	0.45
17:P:53:GLN:HG3	17:P:53:GLN:O	2.16	0.45
18:Q:103:THR:HB	39:Q:4563:HOH:O	2.16	0.45
22:U:30:ASP:O	22:U:33:GLU:HB3	2.17	0.45
31:4:39:GLN:O	31:4:39:GLN:HG2	2.16	0.45
1:A:318:C:H5'	1:A:339:A:C4	2.50	0.45
1:A:652:G:N2	1:A:653:C:H1'	2.31	0.45
1:A:714:U:H3'	39:A:6405:HOH:O	2.16	0.45
1:A:1389:G:H1'	1:A:1435:U:O2	2.16	0.45
1:A:2067:A:C2'	39:A:4460:HOH:O	2.63	0.45
1:A:2363:G:C6	1:A:2364:A:C5	3.04	0.45
1:A:2364:A:OP1	19:R:11:ARG:NH1	2.49	0.45
1:A:2763:G:C6	1:A:2764:C:C4	3.05	0.45
2:B:3097:U:O5'	2:B:3097:U:H6	2.00	0.45
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.45	0.45
9:H:117:GLU:C	9:H:119:ARG:H	2.20	0.45
11:J:84:ARG:NH2	11:J:135:TRP:CH2	2.83	0.45
12:K:107:ASN:HD22	12:K:107:ASN:C	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:28:HIS:CD2	29:2:31:LYS:HG3	2.50	0.45
1:A:533:U:C5	1:A:2084:C:H5'	2.52	0.45
1:A:760:G:H2'	1:A:761:A:N7	2.32	0.45
1:A:844:A:C6	1:A:882:A:C5	3.04	0.45
1:A:1134:G:C4'	11:J:151:MET:HE1	2.29	0.45
1:A:1592:G:C2	1:A:1593:C:C2	3.05	0.45
1:A:1862:C:N4	1:A:1868:G:C6	2.84	0.45
1:A:2346:C:H4'	7:F:52:THR:HG22	1.98	0.45
1:A:2505:G:N2	39:A:5526:HOH:O	2.49	0.45
39:A:9546:HOH:O	29:2:54:ALA:HA	2.15	0.45
2:B:3093:A:C5	2:B:3094:G:H1'	2.52	0.45
5:D:279:THR:CG2	5:D:280:VAL:N	2.79	0.45
13:L:37:TYR:HD2	39:L:7169:HOH:O	2.00	0.45
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.51	0.45
16:O:163:PHE:O	16:O:164:ASP:OD1	2.34	0.45
1:A:111:C:O2'	29:2:20:ARG:HG2	2.17	0.45
1:A:187:A:OP1	15:N:154:ARG:NE	2.49	0.45
1:A:229:G:H2'	1:A:230:C:C6	2.51	0.45
1:A:458:G:H2'	1:A:459:A:H8	1.80	0.45
1:A:907:A:H4'	1:A:1328:A:C2	2.52	0.45
1:A:1104:C:H4'	12:K:88:PRO:HD3	1.99	0.45
1:A:1184:C:O2'	1:A:1185:U:OP2	2.31	0.45
1:A:1252:A:H4'	39:A:9431:HOH:O	2.17	0.45
1:A:1527:A:H1'	1:A:1528:A:C8	2.51	0.45
1:A:1642:A:O2'	39:A:6443:HOH:O	2.21	0.45
1:A:1878:G:C1'	39:A:5591:HOH:O	2.64	0.45
1:A:2544:G:H2'	1:A:2545:U:O4'	2.16	0.45
1:A:2557:U:C2	1:A:2800:A:N7	2.85	0.45
4:C:110:SER:N	4:C:114:ASP:OD2	2.49	0.45
5:D:7:ARG:NH1	5:D:7:ARG:CG	2.73	0.45
5:D:7:ARG:CD	5:D:9:GLY:O	2.64	0.45
6:E:25:PRO:HG2	39:E:8325:HOH:O	2.17	0.45
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.16	0.45
8:G:145:ALA:HB1	8:G:168:ILE:HD12	1.98	0.45
11:J:48:LEU:HD11	11:J:157:ILE:CG2	2.46	0.45
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.97	0.45
13:L:55:VAL:CG1	13:L:56:SER:N	2.75	0.45
13:L:115:ARG:CG	13:L:116:GLU:N	2.77	0.45
15:N:186:SER:OG	15:N:189:VAL:HG12	2.16	0.45
27:Z:130:ARG:HA	39:Z:8532:HOH:O	2.15	0.45
31:4:70:ARG:HG2	31:4:70:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:C:OP2	15:N:188:ARG:HD3	2.16	0.45
1:A:158:A:H2'	1:A:159:G:O4'	2.17	0.45
1:A:240:C:C5'	15:N:146:GLN:HE21	2.28	0.45
1:A:462:A:H2'	39:A:4360:HOH:O	2.16	0.45
1:A:676:C:H4'	39:E:8422:HOH:O	2.16	0.45
1:A:1125:U:C2'	1:A:1126:C:H5'	2.46	0.45
1:A:1434:A:H2'	1:A:1436:C:C4	2.51	0.45
1:A:2118:A:O2'	1:A:2119:C:H5'	2.17	0.45
1:A:2572:G:N2	39:A:5170:HOH:O	2.48	0.45
1:A:2638:G:O2'	1:A:2639:G:H5'	2.17	0.45
8:G:24:GLY:HA3	8:G:76:VAL:HB	1.99	0.45
9:H:79:GLN:HB2	9:H:82:ASP:CG	2.37	0.45
14:M:21:ARG:N	39:M:8406:HOH:O	2.48	0.45
15:N:63:VAL:HG21	15:N:109:PHE:CE1	2.52	0.45
18:Q:16:VAL:HG12	18:Q:17:GLY:H	1.77	0.45
19:R:53:HIS:HA	19:R:54:PRO:HD3	1.79	0.45
23:V:6:CYS:C	23:V:8:TYR:H	2.20	0.45
27:Z:130:ARG:HB2	27:Z:142:SER:O	2.16	0.45
28:1:73:THR:O	28:1:74:VAL:C	2.55	0.45
1:A:55:U:H4'	1:A:69:A:C5	2.51	0.45
1:A:159:G:H5"	15:N:74:ARG:HH22	1.82	0.45
1:A:221:G:H2'	1:A:222:A:C8	2.51	0.45
1:A:403:C:OP1	15:N:69:LYS:HB3	2.17	0.45
1:A:629:A:C2	1:A:2074:A:C2	3.05	0.45
1:A:769:C:OP1	39:A:8686:HOH:O	2.20	0.45
1:A:821:U:H2'	1:A:822:C:H6	1.82	0.45
1:A:867:A:H2	1:A:880:C:O2	1.99	0.45
1:A:929:A:C6	1:A:930:C:N3	2.85	0.45
1:A:1102:C:H2'	1:A:1103:C:C6	2.51	0.45
1:A:1463:A:H8	1:A:1463:A:O5'	2.00	0.45
1:A:1535:G:N2	1:A:1536:C:C2	2.85	0.45
1:A:1761:U:H2'	1:A:1762:C:C6	2.51	0.45
1:A:1764:C:C4	1:A:1765:G:C5	3.05	0.45
1:A:2032:U:P	39:A:3988:HOH:O	2.74	0.45
1:A:2673:U:C2	1:A:2817:G:N2	2.85	0.45
2:B:3011:A:O2'	2:B:3013:A:OP2	2.34	0.45
2:B:3038:A:H2	2:B:3043:G:H5"	1.81	0.45
2:B:3041:C:H4'	7:F:48:MET:HB2	1.99	0.45
13:L:71:ALA:HB2	13:L:97:ILE:HA	1.99	0.45
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.47	0.45
14:M:105:TYR:CD2	39:M:8442:HOH:O	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:74:PRO:O	39:O:8535:HOH:O	2.20	0.45
16:O:139:TRP:O	16:O:142:THR:HB	2.16	0.45
20:S:20:GLU:HG3	39:S:8546:HOH:O	2.17	0.45
25:X:35:VAL:CG2	25:X:41:TYR:CD2	2.99	0.45
1:A:192:A:C4'	15:N:176:GLN:HE22	2.30	0.45
1:A:331:A:C6	1:A:332:G:C4	3.04	0.45
1:A:342:C:O5'	1:A:342:C:H6	1.99	0.45
1:A:721:A:C2'	1:A:722:G:H5'	2.46	0.45
1:A:1334:C:H2'	1:A:1335:C:H6	1.82	0.45
1:A:1862:C:H5"	39:C:8514:HOH:O	2.17	0.45
1:A:1985:U:C2	1:A:1996:U:O4'	2.70	0.45
1:A:2518:C:H2'	1:A:2519:C:O4'	2.16	0.45
1:A:2821:C:O5'	1:A:2821:C:H6	2.00	0.45
39:A:6921:HOH:O	6:E:188:ARG:HD3	2.08	0.45
4:C:67:LEU:HD23	4:C:67:LEU:HA	1.75	0.45
5:D:55:ASN:ND2	5:D:67:GLU:OE2	2.50	0.45
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.81	0.45
6:E:59:GLU:C	6:E:71:PRO:HA	2.37	0.45
11:J:150:LYS:CE	39:J:8382:HOH:O	2.48	0.45
15:N:14:ARG:CB	15:N:17:GLU:HG3	2.47	0.45
16:O:125:ALA:C	39:O:8554:HOH:O	2.54	0.45
24:W:16:ARG:HH22	24:W:63:GLU:HG3	1.80	0.45
1:A:577:G:N2	1:A:580:A:OP2	2.32	0.45
1:A:581:G:H4'	1:A:1254:C:O2'	2.17	0.45
1:A:830:G:H2'	1:A:831:U:C6	2.52	0.45
1:A:847:C:H2'	1:A:848:C:C6	2.51	0.45
1:A:1165:G:H4'	1:A:1174:A:O2'	2.17	0.45
1:A:1213:C:C4	1:A:1214:G:N1	2.85	0.45
1:A:1295:G:H5"	14:M:14:GLY:O	2.17	0.45
1:A:1402:G:N2	1:A:1721:C:C2	2.85	0.45
1:A:1730:G:C5'	1:A:1731:C:H6	2.30	0.45
1:A:1832:G:C2	1:A:1833:U:C6	3.05	0.45
1:A:2296:C:H5	39:A:5995:HOH:O	1.98	0.45
1:A:2609:G:C6	1:A:2610:U:N3	2.84	0.45
4:C:179:MET:O	39:C:8523:HOH:O	2.20	0.45
5:D:57:GLU:HA	5:D:58:PRO:HD2	1.87	0.45
5:D:105:PHE:CD1	5:D:115:VAL:HG11	2.52	0.45
5:D:215:VAL:HA	5:D:220:VAL:HG22	1.98	0.45
6:E:57:PRO:HG2	6:E:73:LEU:CD1	2.47	0.45
6:E:115:LEU:O	6:E:118:THR:HB	2.17	0.45
7:F:51:ARG:HD3	39:F:7636:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:95:THR:HG21	7:F:174:VAL:HG22	1.98	0.45
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.82	0.45
15:N:63:VAL:HG12	15:N:64:ARG:N	2.32	0.45
20:S:27:HIS:O	20:S:31:ILE:HG13	2.17	0.45
23:V:14:GLU:OE1	23:V:15:PRO:CG	2.65	0.45
27:Z:189:ASN:ND2	27:Z:191:ASP:N	2.64	0.45
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.14	0.45
30:3:31:GLU:O	39:3:2890:HOH:O	2.20	0.45
1:A:56:G:H5"	24:W:50:ARG:NH1	2.31	0.44
1:A:168:C:H5'	1:A:2277:U:OP1	2.17	0.44
1:A:565:A:OP2	1:A:592:G:N1	2.46	0.44
1:A:1153:C:C4	1:A:1154:A:N7	2.85	0.44
1:A:1687:C:H2'	1:A:1688:G:O4'	2.17	0.44
1:A:1859:A:C5	1:A:1860:U:C5	3.05	0.44
1:A:2001:G:C2'	1:A:2002:C:H5'	2.47	0.44
1:A:2718:C:H6	1:A:2718:C:H5'	1.81	0.44
1:A:2909:G:O2'	1:A:2910:A:H5'	2.17	0.44
2:B:3025:G:OP1	2:B:3026:C:C5	2.70	0.44
2:B:3053:G:O2'	2:B:3054:A:H5'	2.16	0.44
5:D:321:PRO:HG3	39:D:8625:HOH:O	2.17	0.44
7:F:16:PRO:HB2	7:F:165:PHE:CD1	2.52	0.44
7:F:49:PRO:HA	7:F:73:VAL:HG22	1.99	0.44
8:G:3:VAL:CG2	8:G:49:ILE:HB	2.46	0.44
8:G:34:TRP:O	12:K:127:ILE:HD11	2.17	0.44
8:G:125:GLU:O	8:G:132:THR:HG22	2.17	0.44
10:I:64:ASN:ND2	10:I:64:ASN:H	2.11	0.44
11:J:143:GLU:N	39:J:8380:HOH:O	2.50	0.44
14:M:128:GLY:O	14:M:132:LYS:HG3	2.17	0.44
18:Q:13:VAL:CG2	18:Q:41:ARG:HG2	2.45	0.44
23:V:39:ASN:ND2	23:V:44:ARG:NH1	2.58	0.44
25:X:83:TRP:CZ3	25:X:112:LEU:HD21	2.52	0.44
28:1:81:LYS:O	28:1:82:ALA:C	2.55	0.44
1:A:142:G:O2'	1:A:143:C:H5'	2.17	0.44
1:A:473:A:OP1	29:2:51:GLN:NE2	2.50	0.44
1:A:559:U:H6	1:A:559:U:C5'	2.20	0.44
1:A:709:G:O2'	17:P:25:VAL:HG12	2.18	0.44
1:A:1161:A:C6	1:A:1162:G:N7	2.85	0.44
1:A:1183:C:N4	39:A:3882:HOH:O	2.49	0.44
1:A:1206:U:H5'	1:A:1206:U:H6	1.82	0.44
1:A:1884:G:O6	4:C:190:ARG:HD2	2.16	0.44
1:A:2410:G:H2'	1:A:2411:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2497:A:H2'	1:A:2498:C:H6	1.82	0.44
1:A:2531:U:O2'	1:A:2532:A:H5'	2.17	0.44
1:A:2859:C:H6	1:A:2859:C:C5'	2.30	0.44
39:A:5003:HOH:O	15:N:58:GLN:HG3	2.17	0.44
39:A:9185:HOH:O	27:Z:163:THR:HG23	2.17	0.44
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.98	0.44
6:E:26:VAL:HB	39:E:8472:HOH:O	2.16	0.44
7:F:146:LYS:HZ1	16:O:107:ASN:ND2	2.12	0.44
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.35	0.44
8:G:81:GLU:CB	39:G:4761:HOH:O	2.65	0.44
15:N:137:ASP:O	15:N:142:LYS:CE	2.64	0.44
16:O:144:GLY:HA2	16:O:146:HIS:CE1	2.52	0.44
27:Z:116:LEU:HD13	39:Z:8545:HOH:O	2.17	0.44
28:1:58:GLY:N	39:1:7239:HOH:O	2.48	0.44
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.99	0.44
1:A:192:A:N6	1:A:194:A:C2	2.86	0.44
1:A:345:G:N2	1:A:346:U:H1'	2.31	0.44
1:A:380:A:OP2	15:N:9:ARG:HD2	2.17	0.44
1:A:792:G:HO2'	1:A:793:A:H5'	1.81	0.44
1:A:1050:G:C5	1:A:1051:C:C5	3.05	0.44
1:A:1055:G:N7	39:A:3335:HOH:O	2.35	0.44
1:A:1254:C:O2'	1:A:1255:A:H5'	2.17	0.44
1:A:1260:G:H3'	1:A:1261:A:C8	2.53	0.44
1:A:1306:U:C5'	6:E:184:ARG:HH11	2.30	0.44
1:A:1427:A:H61	1:A:1440:U:H1'	1.83	0.44
1:A:1566:C:O2'	1:A:1567:A:H5'	2.17	0.44
1:A:1815:A:H4'	1:A:2751:C:O4'	2.17	0.44
1:A:1885:A:H8	1:A:1885:A:O5'	2.01	0.44
1:A:2079:G:H2'	1:A:2080:G:O4'	2.18	0.44
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.81	0.44
4:C:8:ARG:HG2	39:C:8557:HOH:O	2.18	0.44
4:C:103:VAL:HA	4:C:104:PRO:HD3	1.79	0.44
5:D:329:TYR:CD2	23:V:15:PRO:HG3	2.52	0.44
7:F:16:PRO:HB2	7:F:165:PHE:CG	2.52	0.44
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.47	0.44
8:G:107:PHE:O	8:G:110:GLU:HB2	2.18	0.44
9:H:49:PHE:CE1	9:H:98:VAL:HG23	2.51	0.44
11:J:56:ILE:HG21	11:J:61:LEU:CD1	2.47	0.44
13:L:34:VAL:HB	39:L:7169:HOH:O	2.17	0.44
20:S:79:ARG:O	20:S:81:PRO:HD3	2.17	0.44
22:U:80:GLU:OE2	22:U:84:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:8:TYR:OH	39:V:3805:HOH:O	2.20	0.44
25:X:125:HIS:CD2	25:X:125:HIS:C	2.91	0.44
30:3:31:GLU:O	39:3:5416:HOH:O	2.20	0.44
1:A:88:G:C2	30:3:24:TRP:HB2	2.53	0.44
1:A:322:G:O2'	1:A:323:C:H5'	2.17	0.44
1:A:517:U:H2'	1:A:518:G:H5'	1.98	0.44
1:A:894:A:N1	6:E:87:ARG:NH2	2.66	0.44
1:A:1822:A:O2'	1:A:1823:G:H5'	2.17	0.44
1:A:1855:G:O6	4:C:142:SER:HB3	2.18	0.44
1:A:1942:A:O3'	4:C:213:LYS:HE2	2.18	0.44
1:A:2090:G:N2	1:A:2655:U:C2	2.86	0.44
39:A:8568:HOH:O	28:1:19:GLY:N	2.50	0.44
6:E:95:GLU:HG3	39:E:8481:HOH:O	2.16	0.44
7:F:81:GLU:O	7:F:84:LEU:N	2.50	0.44
8:G:157:LYS:HD2	8:G:162:PHE:CZ	2.52	0.44
9:H:38:LYS:NZ	15:N:3:SER:HA	2.33	0.44
12:K:39:VAL:O	12:K:40:ASN:HB2	2.18	0.44
14:M:98:GLU:C	14:M:99:GLU:HG3	2.38	0.44
15:N:38:VAL:C	15:N:63:VAL:HG13	2.38	0.44
1:A:111:C:C2'	1:A:112:G:H5'	2.47	0.44
1:A:317:A:OP1	22:U:52:ARG:O	2.35	0.44
1:A:665:A:C6	1:A:666:A:C6	3.05	0.44
1:A:844:A:N6	1:A:882:A:N6	2.66	0.44
1:A:1718:G:O2'	1:A:1719:G:H5'	2.17	0.44
1:A:1733:A:H4'	5:D:212:GLN:HA	1.98	0.44
1:A:1755:A:O5'	1:A:1755:A:H8	2.00	0.44
1:A:2244:A:H5"	15:N:29:GLN:OE1	2.17	0.44
1:A:2619:U:H5	39:A:5327:HOH:O	1.99	0.44
7:F:59:GLY:C	7:F:61:PHE:H	2.17	0.44
11:J:14:TYR:H	11:J:91:HIS:CE1	2.35	0.44
11:J:136:VAL:O	11:J:136:VAL:HG13	2.17	0.44
16:O:101:VAL:HG12	39:O:8529:HOH:O	2.17	0.44
1:A:10:U:HO2'	1:A:11:A:P	2.40	0.44
1:A:115:U:O4'	1:A:131:A:C8	2.71	0.44
1:A:184:G:O5'	1:A:184:G:H8	2.00	0.44
1:A:195:C:C2'	1:A:196:G:H5'	2.47	0.44
1:A:671:A:O2'	1:A:672:G:H2'	2.17	0.44
1:A:1023:C:C2'	1:A:1024:G:H5'	2.47	0.44
1:A:1338:U:O2'	1:A:1339:G:H5'	2.18	0.44
1:A:1564:C:O2'	1:A:1565:C:H5'	2.16	0.44
1:A:1625:U:C4'	39:A:4142:HOH:O	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1667:A:C8	1:A:1667:A:C5'	2.89	0.44
1:A:2104:C:O2	1:A:2486:A:C2	2.71	0.44
1:A:2362:A:H4'	39:A:4654:HOH:O	2.16	0.44
1:A:2834:G:OP1	26:Y:39:LYS:HE2	2.17	0.44
1:A:2859:C:H5"	1:A:2859:C:C6	2.48	0.44
39:A:8786:HOH:O	15:N:181:GLU:HB3	2.17	0.44
2:B:3041:C:H2'	2:B:3042:C:H6	1.81	0.44
4:C:232:ARG:NE	39:C:8582:HOH:O	2.47	0.44
5:D:57:GLU:OE1	5:D:60:SER:HB2	2.18	0.44
7:F:168:SER:O	7:F:168:SER:OG	2.28	0.44
16:O:141:ARG:HB3	39:O:8565:HOH:O	2.18	0.44
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.53	0.44
19:R:42:LYS:HZ3	19:R:43:ILE:H	1.64	0.44
21:T:39:ASP:O	21:T:43:GLU:HG3	2.18	0.44
21:T:49:VAL:O	21:T:49:VAL:HG12	2.17	0.44
31:4:60:LYS:CD	31:4:61:PRO:HD2	2.48	0.44
1:A:273:G:H2'	1:A:274:G:O4'	2.17	0.44
1:A:537:G:C6	1:A:2060:A:N3	2.85	0.44
1:A:830:G:H2'	1:A:831:U:H6	1.83	0.44
1:A:1163:G:N2	39:A:5517:HOH:O	2.39	0.44
1:A:1736:A:OP1	5:D:231:GLY:HA2	2.17	0.44
1:A:1771:U:O2'	1:A:1773:G:N7	2.44	0.44
1:A:1777:G:H2'	39:A:4109:HOH:O	2.18	0.44
1:A:1789:G:O6	18:Q:73:HIS:HE1	2.01	0.44
1:A:2100:A:C5'	39:E:8470:HOH:O	2.66	0.44
1:A:2408:A:H2	39:4:8515:HOH:O	2.00	0.44
1:A:2489:G:C4	1:A:2490:A:C8	3.06	0.44
1:A:2626:C:H2'	1:A:2627:G:H8	1.82	0.44
1:A:2754:G:O2'	1:A:2755:G:H5'	2.18	0.44
2:B:3082:U:H2'	2:B:3083:G:C8	2.53	0.44
5:D:74:ILE:HG13	39:D:8608:HOH:O	2.18	0.44
5:D:182:VAL:O	5:D:183:GLU:C	2.55	0.44
6:E:218:VAL:CG1	39:E:8431:HOH:O	2.65	0.44
11:J:46:VAL:HA	11:J:161:SER:HA	2.00	0.44
13:L:111:GLY:C	39:L:4172:HOH:O	2.55	0.44
16:O:39:SER:HB3	16:O:42:HIS:H	1.81	0.44
16:O:96:GLY:O	39:O:8510:HOH:O	2.21	0.44
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.82	0.44
19:R:22:GLY:O	19:R:23:THR:C	2.55	0.44
25:X:5:VAL:HG11	25:X:153:MET:HE3	2.00	0.44
28:1:39:CYS:HB2	28:1:57:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:C:H6	1:A:40:C:O5'	2.01	0.44
1:A:41:G:H8	1:A:41:G:O5'	2.01	0.44
1:A:74:A:H5'	24:W:9:ARG:HH22	1.81	0.44
1:A:297:U:H2'	1:A:298:C:C6	2.53	0.44
1:A:620:A:N3	39:A:9006:HOH:O	2.36	0.44
1:A:1052:G:N3	1:A:1052:G:H2'	2.32	0.44
1:A:1125:U:H2'	1:A:1126:C:H5'	2.00	0.44
1:A:1141:U:H2'	1:A:1142:C:H6	1.82	0.44
1:A:1262:C:H4'	25:X:29:VAL:O	2.17	0.44
1:A:1829:A:C8	1:A:1885:A:C8	3.06	0.44
1:A:1831:U:H2'	1:A:1832:G:H5'	1.99	0.44
1:A:1843:A:C8	1:A:1843:A:O5'	2.71	0.44
1:A:1893:C:C2	1:A:1940:C:N4	2.85	0.44
1:A:2467:A:H1'	39:A:4207:HOH:O	2.18	0.44
1:A:2735:U:P	39:A:4139:HOH:O	2.75	0.44
2:B:3031:C:C2	2:B:3050:G:N2	2.85	0.44
4:C:132:ASP:OD1	4:C:133:ARG:N	2.50	0.44
15:N:37:VAL:HB	15:N:108:LYS:HG3	2.00	0.44
15:N:173:LEU:CD2	15:N:183:VAL:HG12	2.48	0.44
22:U:15:PRO:O	22:U:16:LEU:C	2.56	0.44
25:X:92:ASP:OD1	25:X:92:ASP:N	2.51	0.44
1:A:114:A:H3'	39:A:9934:HOH:O	2.18	0.44
1:A:368:C:H2'	1:A:369:G:H5'	2.00	0.44
1:A:380:A:O2'	39:A:3123:HOH:O	2.09	0.44
1:A:652:G:H8	39:A:9514:HOH:O	2.00	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
1:A:1087:G:OP2	25:X:9:GLY:HA3	2.18	0.44
1:A:1313:A:H5'	27:Z:208:LYS:O	2.17	0.44
1:A:1550:A:C2	1:A:1636:G:C2	3.05	0.44
1:A:1641:A:H2'	1:A:1642:A:C5'	2.46	0.44
1:A:1785:G:OP1	18:Q:76:GLY:HA3	2.17	0.44
1:A:1879:U:H5'	39:A:5591:HOH:O	2.18	0.44
1:A:1947:G:P	39:A:3161:HOH:O	2.75	0.44
1:A:2505:G:O2'	1:A:2506:A:H5'	2.18	0.44
1:A:2673:U:C2'	1:A:2674:G:H5'	2.48	0.44
1:A:2768:A:C2'	1:A:2769:C:O4'	2.60	0.44
1:A:2813:A:P	39:A:3765:HOH:O	2.74	0.44
6:E:149:LYS:HA	6:E:149:LYS:HD2	1.88	0.44
11:J:84:ARG:HH21	11:J:135:TRP:HH2	1.65	0.44
15:N:46:LEU:HD22	15:N:50:ARG:CD	2.48	0.44
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:69:TYR:HE2	16:O:183:ASP:OD2	2.01	0.44
16:O:82:TYR:HD2	16:O:83:LEU:N	2.15	0.44
16:O:138:ASP:O	16:O:139:TRP:HB3	2.18	0.44
22:U:45:GLY:HA3	22:U:102:ASP:CB	2.47	0.44
24:W:42:ASN:N	24:W:43:PRO:HD3	2.33	0.44
26:Y:25:ARG:NH1	39:Y:3861:HOH:O	2.50	0.44
1:A:308:U:H5'	22:U:97:ARG:NH2	2.33	0.43
1:A:380:A:H1'	39:A:3123:HOH:O	2.17	0.43
1:A:593:A:N7	39:A:3881:HOH:O	2.51	0.43
1:A:849:C:H2'	1:A:850:U:C5'	2.47	0.43
1:A:1157:C:H3'	1:A:1157:C:C6	2.53	0.43
1:A:1296:A:O2'	1:A:1297:U:H5'	2.17	0.43
1:A:1477:C:C5'	1:A:1868:G:H5"	2.47	0.43
1:A:1500:U:H2'	1:A:1502:A:OP2	2.18	0.43
1:A:1832:G:O2'	39:A:8683:HOH:O	2.06	0.43
1:A:1973:A:H5'	1:A:1973:A:C8	2.51	0.43
1:A:2404:G:H4'	19:R:68:GLY:CA	2.47	0.43
1:A:2433:A:H1'	39:A:6759:HOH:O	2.18	0.43
1:A:2505:G:H2'	1:A:2506:A:H5'	2.00	0.43
39:A:6190:HOH:O	19:R:2:SER:HA	2.17	0.43
5:D:203:ALA:HA	5:D:263:THR:HA	1.99	0.43
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.48	0.43
12:K:45:VAL:CG2	12:K:46:ILE:N	2.81	0.43
12:K:63:ILE:CG2	12:K:64:GLY:N	2.81	0.43
12:K:122:ASP:OD1	12:K:124:LEU:HB2	2.18	0.43
15:N:169:ARG:CB	39:N:8587:HOH:O	2.66	0.43
22:U:53:GLY:HA3	39:U:6384:HOH:O	2.18	0.43
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.99	0.43
26:Y:85:VAL:CG1	26:Y:86:GLU:N	2.80	0.43
27:Z:152:LYS:NZ	39:Z:8558:HOH:O	2.51	0.43
28:1:55:TRP:HZ2	28:1:70:GLN:N	2.16	0.43
1:A:111:C:H2'	1:A:112:G:C5'	2.49	0.43
1:A:449:A:N7	6:E:43:LYS:HG2	2.32	0.43
1:A:694:A:C2'	1:A:695:C:H5'	2.48	0.43
1:A:822:C:C2	1:A:823:U:C5	3.07	0.43
1:A:844:A:N6	1:A:882:A:C6	2.86	0.43
1:A:869:G:OP1	15:N:79:LYS:HE2	2.17	0.43
1:A:1195:G:C2	1:A:1205:U:C2	3.06	0.43
1:A:1524:U:H4'	1:A:1524:U:OP1	2.19	0.43
1:A:1735:C:C2'	1:A:1736:A:H5'	2.48	0.43
1:A:1835:U:C4	1:A:1839:A:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1920:C:O2'	1:A:1921:A:H5'	2.18	0.43
1:A:2038:A:C5'	5:D:222:LYS:HG3	2.48	0.43
1:A:2296:C:P	19:R:5:GLY:HA3	2.57	0.43
1:A:2403:C:H2'	1:A:2404:G:O5'	2.18	0.43
1:A:2732:U:O2	39:A:4443:HOH:O	2.21	0.43
1:A:2763:G:C4	1:A:2764:C:C5	3.06	0.43
2:B:3024:U:H6	39:B:8490:HOH:O	1.90	0.43
4:C:66:ARG:HB2	4:C:66:ARG:NH1	2.33	0.43
5:D:208:GLY:HA2	5:D:258:GLY:HA3	2.00	0.43
6:E:5:ILE:HG23	39:E:8438:HOH:O	2.16	0.43
6:E:21:VAL:C	6:E:23:GLU:N	2.71	0.43
6:E:61:PHE:HD1	39:E:8383:HOH:O	2.00	0.43
8:G:22:VAL:O	8:G:76:VAL:HG11	2.19	0.43
9:H:58:GLU:HB3	15:N:8:ILE:HG23	2.00	0.43
12:K:79:PHE:HB3	12:K:103:VAL:HG11	2.00	0.43
12:K:107:ASN:HD22	12:K:108:PRO:N	2.17	0.43
16:O:71:TRP:CE3	16:O:175:LEU:CD2	2.98	0.43
16:O:154:LEU:HG	16:O:155:GLU:N	2.32	0.43
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.52	0.43
19:R:93:ARG:NH1	19:R:93:ARG:CG	2.78	0.43
1:A:306:A:P	22:U:38:ARG:NH2	2.89	0.43
1:A:932:U:H2'	1:A:933:C:C6	2.54	0.43
1:A:941:G:O2'	1:A:942:U:H5'	2.18	0.43
1:A:1112:G:C6	1:A:1252:A:N1	2.86	0.43
1:A:1134:G:C5'	11:J:151:MET:CE	2.96	0.43
1:A:1157:C:C2	1:A:1158:G:C8	3.06	0.43
1:A:1336:U:C2	1:A:1337:A:C8	3.06	0.43
1:A:1456:C:H2'	1:A:1457:U:O4'	2.18	0.43
1:A:1496:G:C2	1:A:1510:G:C2	3.07	0.43
1:A:1860:U:H2'	1:A:1861:C:O4'	2.18	0.43
1:A:1886:A:C2'	39:A:4299:HOH:O	2.65	0.43
1:A:1979:G:P	39:A:5778:HOH:O	2.77	0.43
1:A:2251:G:H2'	1:A:2252:A:C8	2.52	0.43
1:A:2455:A:H2'	1:A:2456:A:O4'	2.18	0.43
1:A:2691:A:H8	1:A:2691:A:OP1	2.00	0.43
4:C:81:GLN:H	4:C:92:ASN:ND2	2.16	0.43
4:C:186:TRP:HA	4:C:187:PRO:HA	1.71	0.43
6:E:35:VAL:HG11	6:E:227:GLY:H	1.82	0.43
6:E:47:GLY:HA2	6:E:92:PRO:HB2	2.00	0.43
10:I:23:ILE:CG2	10:I:70:ALA:CB	2.97	0.43
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:19:MET:CE	12:K:78:ILE:HG22	2.48	0.43
17:P:59:VAL:CG2	17:P:111:VAL:HG23	2.48	0.43
20:S:29:LYS:CD	39:S:8541:HOH:O	2.66	0.43
1:A:25:A:H2'	1:A:26:U:H5'	1.99	0.43
1:A:521:A:N1	1:A:1364:G:O2'	2.43	0.43
1:A:724:G:O2'	1:A:725:C:H5'	2.18	0.43
1:A:1029:U:O2'	1:A:1273:C:OP1	2.31	0.43
1:A:1099:G:OP1	25:X:129:LYS:HE3	2.17	0.43
1:A:1117:A:C2	1:A:1244:U:C2	3.07	0.43
1:A:1310:U:H2'	1:A:1311:G:O5'	2.18	0.43
1:A:1436:C:C2	1:A:1437:A:C8	3.07	0.43
1:A:1861:C:H4'	4:C:6:GLY:O	2.18	0.43
1:A:1880:C:C4	1:A:1881:A:N7	2.87	0.43
1:A:2072:G:C6	1:A:2533:C:H1'	2.54	0.43
1:A:2578:G:H5'	1:A:2578:G:H8	1.83	0.43
1:A:2607:U:O5'	1:A:2609:G:H4'	2.18	0.43
1:A:2649:A:H5'	1:A:2649:A:C8	2.54	0.43
39:A:6044:HOH:O	2:B:3083:G:H4'	2.18	0.43
2:B:3024:U:C1'	39:B:8438:HOH:O	2.63	0.43
2:B:3031:C:H2'	2:B:3032:G:O4'	2.18	0.43
4:C:53:ALA:HB1	4:C:54:PRO:HD2	2.00	0.43
7:F:169:THR:C	7:F:170:TYR:HD1	2.22	0.43
8:G:84:MET:HE1	8:G:133:VAL:HG21	2.00	0.43
11:J:73:GLN:OE1	11:J:73:GLN:CA	2.66	0.43
11:J:114:PRO:O	11:J:116:GLY:N	2.52	0.43
25:X:73:LEU:CD1	25:X:112:LEU:O	2.66	0.43
25:X:125:HIS:HB2	25:X:137:GLN:OE1	2.18	0.43
30:3:18:ASN:HD21	30:3:40:ARG:H	1.66	0.43
1:A:10:U:H3'	39:A:9830:HOH:O	2.17	0.43
1:A:256:C:H2'	1:A:257:G:O4'	2.17	0.43
1:A:764:C:H2'	1:A:765:G:O4'	2.18	0.43
1:A:936:C:C2'	1:A:937:C:H5'	2.48	0.43
1:A:1264:U:H2'	1:A:1265:G:H8	1.84	0.43
1:A:1745:G:O6	39:A:5421:HOH:O	2.20	0.43
1:A:1762:C:C2	1:A:1783:A:C2	3.07	0.43
1:A:1991:A:O5'	1:A:1991:A:H8	2.02	0.43
1:A:2808:U:OP1	5:D:261:GLN:HG2	2.17	0.43
2:B:3024:U:H5"	39:B:8485:HOH:O	2.19	0.43
2:B:3044:A:O4'	7:F:76:ARG:NE	2.51	0.43
6:E:200:PRO:HB3	6:E:212:VAL:HG23	2.01	0.43
6:E:218:VAL:HG13	39:E:8431:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:238:SER:C	39:E:8386:HOH:O	2.56	0.43
18:Q:27:ARG:HD2	39:Q:5262:HOH:O	2.18	0.43
25:X:21:LEU:HD23	25:X:21:LEU:HA	1.70	0.43
27:Z:100:ARG:HE	27:Z:234:VAL:HG21	1.84	0.43
30:3:13:LYS:O	30:3:17:GLN:HG3	2.19	0.43
31:4:6:ARG:O	31:4:7:PHE:HB3	2.19	0.43
1:A:383:A:OP1	15:N:174:ARG:NH1	2.49	0.43
1:A:533:U:C6	1:A:2084:C:H5'	2.54	0.43
1:A:602:A:O2'	1:A:605:C:H4'	2.18	0.43
1:A:1070:A:H2'	1:A:1071:G:C8	2.54	0.43
1:A:1162:G:C2	1:A:1163:G:N7	2.87	0.43
1:A:1367:A:H2'	1:A:1368:U:H5'	1.99	0.43
1:A:1461:U:H2'	1:A:1462:C:H6	1.84	0.43
1:A:1766:U:H2'	1:A:1776:A:N6	2.34	0.43
1:A:1902:G:H2'	1:A:1903:U:O4'	2.19	0.43
1:A:2613:G:C1'	39:A:8662:HOH:O	2.66	0.43
1:A:2614:C:O2'	1:A:2615:U:H5'	2.18	0.43
1:A:2629:C:H5	39:A:8726:HOH:O	2.00	0.43
1:A:2858:U:C2	1:A:2900:G:N2	2.86	0.43
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.29	0.43
4:C:65:ARG:C	4:C:66:ARG:HG3	2.39	0.43
4:C:178:LYS:HD3	35:C:8509:CL:CL	2.56	0.43
5:D:43:GLY:HA3	5:D:76:THR:HG22	2.00	0.43
5:D:232:TRP:CD1	5:D:235:ARG:HD2	2.53	0.43
6:E:14:GLY:O	6:E:15:GLU:HB3	2.19	0.43
7:F:101:THR:CG2	39:F:7400:HOH:O	2.57	0.43
11:J:83:PHE:HE1	11:J:146:TRP:CZ2	2.36	0.43
15:N:37:VAL:CB	15:N:108:LYS:HG3	2.48	0.43
15:N:134:ILE:O	15:N:136:PRO:HD3	2.19	0.43
15:N:152:ARG:HG3	39:N:8553:HOH:O	2.18	0.43
18:Q:138:GLU:O	18:Q:141:ILE:HB	2.18	0.43
20:S:72:VAL:CG1	20:S:75:TRP:HB3	2.48	0.43
22:U:48:VAL:CG2	22:U:96:VAL:HG13	2.49	0.43
27:Z:153:GLN:O	27:Z:156:GLY:N	2.39	0.43
31:4:69:TYR:HB3	31:4:78:HIS:CE1	2.54	0.43
1:A:407:A:H2'	1:A:408:A:C8	2.54	0.43
1:A:506:G:H22	1:A:509:A:H5"	1.83	0.43
1:A:558:C:C2'	1:A:559:U:C5'	2.95	0.43
1:A:625:U:O2'	1:A:627:G:N7	2.37	0.43
1:A:1156:C:H3'	1:A:1156:C:C6	2.52	0.43
1:A:1318:A:H2'	1:A:1319:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1393:A:OP1	39:A:5109:HOH:O	2.21	0.43
1:A:1450:C:C4'	1:A:1451:C:OP2	2.61	0.43
1:A:1742:A:C6	1:A:1743:G:C6	3.07	0.43
1:A:1835:U:C2	1:A:1839:A:N7	2.87	0.43
1:A:1878:G:O2'	1:A:1879:U:P	2.77	0.43
1:A:1881:A:C2	1:A:1882:C:C4	3.06	0.43
1:A:1969:A:O5'	1:A:1969:A:H8	2.00	0.43
1:A:2392:C:H4'	39:R:2875:HOH:O	2.18	0.43
1:A:2412:G:N2	1:A:2415:A:OP2	2.48	0.43
1:A:2712:G:H5'	39:A:4699:HOH:O	2.19	0.43
1:A:2848:G:O4'	1:A:2906:A:C2	2.71	0.43
2:B:3004:G:O2'	16:O:44:ARG:NH2	2.51	0.43
4:C:43:VAL:HG21	4:C:59:GLU:HG3	2.00	0.43
4:C:191:GLY:HA2	4:C:194:MET:CE	2.48	0.43
4:C:211:LYS:NZ	39:C:8574:HOH:O	2.51	0.43
7:F:15:GLU:HA	7:F:16:PRO:HD3	1.88	0.43
7:F:21:VAL:CG1	7:F:131:THR:O	2.66	0.43
7:F:45:THR:HG22	7:F:75:LEU:HD11	2.01	0.43
11:J:158:ASN:ND2	39:J:8385:HOH:O	2.51	0.43
13:L:87:ARG:NH1	39:L:4066:HOH:O	2.50	0.43
14:M:104:ASP:HB2	39:M:8455:HOH:O	2.17	0.43
17:P:44:ASN:HB2	35:P:8508:CL:CL	2.56	0.43
21:T:23:LYS:HG2	21:T:67:ARG:HA	2.00	0.43
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.45	0.43
25:X:32:CYS:N	39:X:5420:HOH:O	2.51	0.43
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.52	0.43
31:4:65:THR:HB	31:4:83:TRP:H	1.84	0.43
1:A:183:A:C6	1:A:184:G:C6	3.07	0.43
1:A:951:A:C2'	1:A:952:G:H5'	2.48	0.43
1:A:1055:G:OP2	11:J:94:ARG:NH1	2.51	0.43
1:A:1322:G:H2'	1:A:1323:G:O4'	2.18	0.43
1:A:1726:G:N2	1:A:2050:G:C4	2.87	0.43
1:A:1778:A:C2'	1:A:1779:A:H5'	2.45	0.43
1:A:2587:U:O5'	1:A:2587:U:H6	2.02	0.43
1:A:2635:A:C5	1:A:2636:C:C5	3.07	0.43
1:A:2894:C:O2'	1:A:2895:C:H5'	2.18	0.43
4:C:123:GLY:HA2	4:C:159:VAL:O	2.19	0.43
4:C:223:ARG:CG	39:C:8604:HOH:O	2.57	0.43
5:D:27:ASN:HD22	5:D:27:ASN:H	1.66	0.43
5:D:105:PHE:CD1	5:D:115:VAL:CG1	3.02	0.43
5:D:320:GLN:HG3	5:D:321:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:83:ALA:O	6:E:84:VAL:C	2.57	0.43
7:F:173:GLU:O	7:F:174:VAL:C	2.57	0.43
10:I:12:ILE:HG22	10:I:12:ILE:O	2.18	0.43
11:J:136:VAL:HA	39:J:8342:HOH:O	2.19	0.43
16:O:141:ARG:NH1	16:O:146:HIS:CD2	2.87	0.43
20:S:99:ALA:O	20:S:104:PHE:HD1	2.02	0.43
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.49	0.43
28:1:42:CYS:SG	28:1:43:GLY:N	2.92	0.43
1:A:74:A:C2	1:A:104:G:C2	3.06	0.43
1:A:365:G:C5	1:A:366:U:C5	3.07	0.43
1:A:573:A:O2'	1:A:574:C:H5'	2.19	0.43
1:A:1228:C:C4	1:A:1229:C:C4	3.06	0.43
1:A:1322:G:C4	1:A:1323:G:C8	3.07	0.43
1:A:1381:A:H4'	1:A:1382:G:O5'	2.18	0.43
1:A:1477:C:H4'	1:A:1868:G:H5"	2.01	0.43
1:A:1758:U:H2'	1:A:1759:A:O4'	2.19	0.43
1:A:2245:C:O5'	1:A:2245:C:H6	2.02	0.43
1:A:2316:G:H5'	39:A:5562:HOH:O	2.19	0.43
1:A:2318:C:H3'	1:A:2318:C:C6	2.53	0.43
1:A:2403:C:H3'	39:A:4689:HOH:O	2.18	0.43
2:B:3011:A:C8	16:O:8:VAL:CG2	3.02	0.43
2:B:3063:C:O2'	2:B:3064:C:H5'	2.19	0.43
4:C:232:ARG:O	4:C:233:THR:CG2	2.67	0.43
7:F:94:ALA:O	7:F:95:THR:O	2.36	0.43
15:N:28:MET:O	15:N:32:ARG:HG3	2.19	0.43
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.18	0.43
16:O:67:ALA:HA	16:O:71:TRP:HB3	2.01	0.43
17:P:18:ALA:HB2	39:P:3062:HOH:O	2.19	0.43
19:R:61:GLY:HA3	19:R:73:VAL:CG1	2.48	0.43
20:S:92:LEU:CD2	20:S:145:LEU:HD21	2.43	0.43
22:U:52:ARG:O	22:U:53:GLY:O	2.36	0.43
1:A:13:G:H2'	1:A:14:C:H6	1.84	0.43
1:A:335:U:H4'	22:U:92:ASP:OD2	2.19	0.43
1:A:796:A:C2	1:A:797:A:C4	3.07	0.43
1:A:862:U:OP1	39:A:8933:HOH:O	2.21	0.43
1:A:1134:G:H5'	11:J:151:MET:HE3	2.01	0.43
1:A:1189:A:O2'	1:A:1209:C:O4'	2.27	0.43
1:A:1205:U:C2'	1:A:1206:U:C5'	2.97	0.43
1:A:1259:A:N6	39:A:3045:HOH:O	2.52	0.43
1:A:1500:U:C2	1:A:1502:A:OP2	2.72	0.43
1:A:1718:G:OP1	18:Q:20:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:A:H2'	1:A:1799:G:O5'	2.19	0.43
1:A:1838:U:H4'	39:A:8668:HOH:O	2.19	0.43
1:A:1902:G:O2'	1:A:1903:U:H5'	2.19	0.43
1:A:2011:A:C6	1:A:2013:G:O6	2.72	0.43
1:A:2033:G:N2	1:A:2037:C:O2	2.47	0.43
1:A:2081:A:H2'	1:A:2082:G:O4'	2.19	0.43
1:A:2568:A:C2'	1:A:2569:A:H5'	2.49	0.43
1:A:2635:A:O2'	1:A:2636:C:H5'	2.19	0.43
1:A:2685:C:H2'	1:A:2686:C:C6	2.53	0.43
1:A:2831:C:O2'	39:A:6212:HOH:O	2.21	0.43
39:A:9260:HOH:O	20:S:117:HIS:HB3	2.19	0.43
2:B:3036:C:H2'	2:B:3037:C:H5'	2.00	0.43
4:C:95:PRO:HA	4:C:153:ARG:HA	2.00	0.43
5:D:301:VAL:CG1	5:D:302:PRO:HD2	2.49	0.43
6:E:94:THR:HB	39:E:8359:HOH:O	2.19	0.43
6:E:124:VAL:HA	6:E:230:GLY:O	2.18	0.43
8:G:166:VAL:C	8:G:167:TYR:CD1	2.93	0.43
11:J:166:ASN:N	11:J:166:ASN:ND2	2.67	0.43
13:L:106:GLY:HA3	39:L:5264:HOH:O	2.19	0.43
20:S:111:ILE:HG12	20:S:145:LEU:HD11	2.01	0.43
22:U:50:VAL:O	22:U:56:ALA:HA	2.19	0.43
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.19	0.43
27:Z:184:GLU:OE2	27:Z:204:ARG:HD2	2.19	0.43
1:A:24:G:N2	1:A:518:G:H1'	2.34	0.42
1:A:133:U:H5'	1:A:1465:A:OP1	2.19	0.42
1:A:621:C:H5'	27:Z:132:ASP:OD2	2.19	0.42
1:A:685:C:O2	1:A:748:C:H4'	2.18	0.42
1:A:746:A:H4'	1:A:747:G:H5'	2.01	0.42
1:A:1168:C:H5'	39:A:6872:HOH:O	2.19	0.42
1:A:1188:A:P	39:A:6358:HOH:O	2.76	0.42
1:A:1294:A:O3'	14:M:16:GLY:HA2	2.18	0.42
1:A:1369:A:N1	1:A:2054:A:H5"	2.34	0.42
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.40	0.42
1:A:1969:A:OP2	39:A:3242:HOH:O	2.21	0.42
1:A:2034:U:H2'	1:A:2035:C:H6	1.84	0.42
1:A:2554:U:C6	1:A:2577:A:N6	2.87	0.42
1:A:2708:G:N2	13:L:1:MET:O	2.51	0.42
1:A:2768:A:H3'	1:A:2768:A:N3	2.34	0.42
1:A:2778:A:H1'	8:G:153:ARG:NH1	2.34	0.42
2:B:3004:G:OP1	2:B:3059:C:O2'	2.37	0.42
4:C:51:ARG:NH1	4:C:120:ARG:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:133:ASN:HD22	7:F:134:LEU:N	2.17	0.42
11:J:47:GLU:HA	11:J:146:TRP:CH2	2.54	0.42
12:K:40:ASN:OD1	12:K:106:GLY:HA2	2.19	0.42
13:L:32:ILE:HD11	13:L:56:SER:HB3	2.00	0.42
15:N:48:ARG:NH2	39:N:8560:HOH:O	2.52	0.42
17:P:47:ARG:CD	17:P:115:ARG:O	2.67	0.42
18:Q:59:ARG:HG2	18:Q:59:ARG:NH1	2.34	0.42
23:V:6:CYS:O	23:V:8:TYR:N	2.52	0.42
25:X:21:LEU:HD21	25:X:48:VAL:HG11	2.00	0.42
27:Z:151:SER:HB3	27:Z:154:ARG:CB	2.45	0.42
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.49	0.42
31:4:7:PHE:HE2	31:4:22:VAL:HG21	1.84	0.42
1:A:27:U:H2'	1:A:28:G:O4'	2.19	0.42
1:A:284:C:N4	39:A:6654:HOH:O	2.52	0.42
1:A:558:C:H2'	1:A:559:U:H5'	2.01	0.42
1:A:756:A:H2'	1:A:757:C:C6	2.53	0.42
1:A:766:A:HO2'	1:A:767:A:H8	1.65	0.42
1:A:1097:A:H5"	25:X:125:HIS:NE2	2.34	0.42
1:A:1773:G:C8	28:1:16:PRO:HA	2.53	0.42
1:A:2414:A:H2'	1:A:2415:A:C8	2.54	0.42
1:A:2536:C:OP1	39:A:9616:HOH:O	2.21	0.42
1:A:2584:G:H4'	39:A:6583:HOH:O	2.18	0.42
5:D:56:ASP:HB3	5:D:322:ARG:HH21	1.84	0.42
7:F:95:THR:CG2	7:F:174:VAL:HG22	2.49	0.42
8:G:9:GLU:HG3	8:G:10:ASP:N	2.34	0.42
14:M:124:ASP:OD1	14:M:149:ARG:NH2	2.52	0.42
20:S:126:LYS:O	20:S:127:PRO:C	2.55	0.42
21:T:22:ASN:ND2	21:T:68:LEU:HB2	2.34	0.42
22:U:39:ASN:HD22	22:U:39:ASN:C	2.23	0.42
26:Y:31:ILE:O	26:Y:31:ILE:HG22	2.19	0.42
27:Z:216:ARG:CD	39:Z:8571:HOH:O	2.58	0.42
1:A:236:A:H4'	1:A:237:G:OP1	2.19	0.42
1:A:401:C:O2'	15:N:92:THR:HB	2.18	0.42
1:A:475:G:C5'	6:E:73:LEU:HD23	2.49	0.42
1:A:710:G:OP1	39:A:6107:HOH:O	2.21	0.42
1:A:821:U:H2'	1:A:822:C:C6	2.54	0.42
1:A:850:U:C5	1:A:851:C:C5	3.07	0.42
1:A:1447:U:C5	1:A:1504:A:H2	2.37	0.42
1:A:1613:C:O2	39:A:5451:HOH:O	2.20	0.42
1:A:1723:G:H2'	39:A:9130:HOH:O	2.20	0.42
1:A:1861:C:OP1	4:C:224:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2363:G:O2'	19:R:11:ARG:HG3	2.19	0.42
1:A:2543:G:O2'	1:A:2544:G:H5'	2.19	0.42
3:5:75:C:H2'	3:5:76:DA:H1'	2.01	0.42
4:C:223:ARG:NH2	39:C:8574:HOH:O	2.52	0.42
6:E:233:THR:HG21	6:E:235:PHE:CE1	2.54	0.42
6:E:246:ARG:HH11	6:E:246:ARG:CB	2.26	0.42
9:H:78:GLU:HG3	39:H:5966:HOH:O	2.19	0.42
9:H:98:VAL:O	39:H:3461:HOH:O	2.22	0.42
12:K:52:GLN:CG	12:K:53:ILE:N	2.75	0.42
15:N:91:ILE:HG23	39:N:8641:HOH:O	2.19	0.42
16:O:66:LEU:HD12	16:O:66:LEU:HA	1.86	0.42
16:O:165:ALA:HA	39:O:8517:HOH:O	2.20	0.42
20:S:82:GLU:HG3	20:S:83:LYS:N	2.33	0.42
20:S:149:GLU:HA	20:S:150:PRO:HD3	1.89	0.42
23:V:9:CYS:CA	23:V:52:THR:HG23	2.46	0.42
1:A:48:A:C2'	39:A:3838:HOH:O	2.66	0.42
1:A:830:G:H2'	1:A:831:U:O4'	2.19	0.42
1:A:1184:C:N1	39:A:5710:HOH:O	2.47	0.42
1:A:1447:U:H3'	1:A:1506:U:O2	2.20	0.42
1:A:1476:A:O2'	1:A:1868:G:H5'	2.19	0.42
1:A:1672:G:H4'	39:A:9377:HOH:O	2.19	0.42
1:A:1833:U:C2	1:A:1834:C:C5	3.07	0.42
39:A:5675:HOH:O	5:D:2:GLN:NE2	2.51	0.42
4:C:48:ASP:HA	4:C:49:PRO:HD3	1.73	0.42
5:D:313:PRO:O	5:D:314:ALA:C	2.57	0.42
7:F:95:THR:C	7:F:97:GLN:N	2.68	0.42
8:G:34:TRP:HA	39:G:4572:HOH:O	2.19	0.42
9:H:47:LEU:HB2	9:H:108:LEU:HD11	2.02	0.42
11:J:31:PHE:HE2	11:J:87:LYS:O	2.02	0.42
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.54	0.42
11:J:56:ILE:HG21	11:J:61:LEU:HD11	2.01	0.42
11:J:57:ARG:O	11:J:61:LEU:CD2	2.64	0.42
12:K:39:VAL:HG13	12:K:106:GLY:O	2.18	0.42
12:K:131:THR:O	12:K:134:GLU:HB2	2.18	0.42
15:N:87:MET:HG2	31:4:46:ILE:CG2	2.36	0.42
16:O:184:ILE:HG22	16:O:185:GLU:HG3	2.00	0.42
20:S:68:HIS:HA	20:S:76:ASP:O	2.19	0.42
21:T:13:LYS:NZ	39:T:8319:HOH:O	2.40	0.42
25:X:48:VAL:CG1	25:X:48:VAL:O	2.66	0.42
27:Z:106:THR:HG23	27:Z:107:PRO:HD2	2.01	0.42
29:2:26:SER:HB3	29:2:35:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:G:C6	1:A:119:A:N7	2.88	0.42
1:A:164:G:O3'	14:M:30:ARG:HB2	2.19	0.42
1:A:275:G:C2	1:A:376:C:N3	2.88	0.42
1:A:537:G:C6	1:A:2060:A:C2	3.07	0.42
1:A:676:C:OP1	6:E:38:ALA:HA	2.20	0.42
1:A:876:A:N3	1:A:876:A:H2'	2.34	0.42
1:A:906:C:C2	1:A:1300:G:N2	2.88	0.42
1:A:912:A:C4	1:A:1294:A:C2	3.07	0.42
1:A:1006:A:H5"	39:A:3021:HOH:O	2.20	0.42
1:A:1044:C:C5'	39:A:8543:HOH:O	2.68	0.42
1:A:1205:U:C2'	1:A:1206:U:H5"	2.49	0.42
1:A:1270:U:H2'	1:A:1271:A:C8	2.55	0.42
1:A:1382:G:C6	1:A:1401:G:C2	3.08	0.42
1:A:1741:U:H5'	1:A:1742:A:OP1	2.19	0.42
1:A:1745:G:N2	1:A:2033:G:OP2	2.45	0.42
1:A:1972:U:H2'	1:A:1973:A:C5'	2.50	0.42
1:A:2107:U:OP2	39:A:3733:HOH:O	2.21	0.42
1:A:2327:A:H2'	1:A:2328:U:C6	2.54	0.42
1:A:2364:A:P	19:R:11:ARG:NH1	2.92	0.42
1:A:2749:U:H3'	1:A:2750:G:H5"	2.01	0.42
39:A:5226:HOH:O	27:Z:144:ARG:NH1	2.49	0.42
2:B:3010:C:P	39:B:8521:HOH:O	2.76	0.42
5:D:154:VAL:HG12	5:D:156:LYS:HG2	2.00	0.42
5:D:254:GLN:CB	39:D:8537:HOH:O	2.67	0.42
6:E:166:ILE:HD13	6:E:207:LEU:HD13	2.01	0.42
8:G:8:PRO:O	8:G:11:VAL:N	2.48	0.42
8:G:93:MET:HE1	8:G:165:GLY:N	2.35	0.42
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.50	0.42
16:O:47:LEU:HD23	16:O:47:LEU:HA	1.78	0.42
17:P:32:ARG:O	17:P:35:LYS:HB2	2.18	0.42
20:S:18:LEU:HB2	20:S:143:VAL:HG13	2.02	0.42
21:T:23:LYS:HE2	39:T:8333:HOH:O	2.20	0.42
30:3:7:THR:HG23	30:3:49:GLU:OE1	2.19	0.42
30:3:48:ASP:O	30:3:49:GLU:HB2	2.19	0.42
1:A:138:U:H5"	1:A:139:C:OP2	2.20	0.42
1:A:795:G:H1'	1:A:817:G:N2	2.34	0.42
1:A:921:G:H4'	1:A:924:G:C6	2.53	0.42
1:A:1592:G:H2'	1:A:1593:C:C6	2.55	0.42
1:A:1741:U:O2'	1:A:2723:G:H4'	2.20	0.42
1:A:1752:G:H1'	1:A:1754:A:N6	2.35	0.42
1:A:2712:G:H1'	39:A:5320:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2765:C:H2'	1:A:2766:A:C8	2.54	0.42
39:A:4048:HOH:O	15:N:86:MET:CE	2.60	0.42
4:C:83:GLY:O	4:C:94:LEU:HB3	2.19	0.42
15:N:69:LYS:HG3	15:N:127:LYS:HG3	2.01	0.42
16:O:48:VAL:HG13	16:O:55:ASP:HB3	1.96	0.42
16:O:50:LEU:HD12	16:O:50:LEU:HA	1.81	0.42
17:P:44:ASN:HA	17:P:65:LEU:O	2.20	0.42
26:Y:47:ALA:HB1	26:Y:82:GLU:HA	2.02	0.42
1:A:282:C:C2'	1:A:283:U:H5'	2.48	0.42
1:A:622:G:OP2	27:Z:148:GLY:HA3	2.20	0.42
1:A:917:U:O5'	1:A:917:U:H6	2.02	0.42
1:A:1157:C:C6	1:A:1157:C:C3'	3.02	0.42
1:A:1453:G:N2	1:A:1675:C:C2	2.88	0.42
1:A:1573:A:H2'	1:A:1574:C:O4'	2.18	0.42
1:A:1603:A:H5'	1:A:1605:G:C4'	2.49	0.42
1:A:1635:U:P	39:A:5642:HOH:O	2.77	0.42
1:A:1697:G:O2'	1:A:1698:U:H5'	2.20	0.42
1:A:1766:U:O4'	1:A:1779:A:N6	2.53	0.42
1:A:1768:C:C2'	1:A:1769:C:H5'	2.49	0.42
1:A:1816:C:H2'	1:A:1817:U:O4'	2.19	0.42
1:A:2008:U:OP2	39:A:3578:HOH:O	2.21	0.42
1:A:2032:U:O2'	1:A:2033:G:H5"	2.20	0.42
2:B:3078:G:N2	2:B:3103:A:OP2	2.42	0.42
4:C:123:GLY:HA3	4:C:162:GLY:HA2	2.01	0.42
5:D:5:ARG:HD2	5:D:8:LYS:NZ	2.35	0.42
5:D:51:VAL:HG13	5:D:53:LEU:HD13	2.02	0.42
5:D:75:GLU:CD	5:D:290:VAL:HG22	2.39	0.42
5:D:137:LEU:HD11	5:D:140:LEU:HD21	2.01	0.42
6:E:236:THR:HG22	6:E:239:ALA:CB	2.49	0.42
15:N:122:GLU:OE2	15:N:127:LYS:HE2	2.20	0.42
16:O:108:SER:HA	16:O:109:PRO:HD3	1.75	0.42
16:O:110:THR:HB	16:O:113:SER:OG	2.19	0.42
17:P:18:ALA:HB2	17:P:26:TRP:HB2	2.01	0.42
24:W:12:THR:O	24:W:13:PRO:C	2.58	0.42
1:A:64:G:H2'	1:A:65:C:C6	2.55	0.42
1:A:81:G:OP1	22:U:43:ASN:HA	2.20	0.42
1:A:539:G:H2'	1:A:540:A:C8	2.55	0.42
1:A:883:U:H6	39:A:9290:HOH:O	2.02	0.42
1:A:1156:C:C6	1:A:1156:C:C3'	3.02	0.42
1:A:1175:G:H1'	1:A:1193:A:H2'	2.02	0.42
1:A:1183:C:N4	1:A:1184:C:H41	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:U:O2'	1:A:1206:U:H5"	2.20	0.42
1:A:1947:G:H2'	1:A:1948:G:C8	2.54	0.42
1:A:2106:C:H1'	1:A:2484:U:O2	2.19	0.42
1:A:2515:C:H2'	1:A:2516:G:O4'	2.20	0.42
1:A:2546:U:H5	5:D:2:GLN:HE22	1.68	0.42
1:A:2729:C:O2'	1:A:2730:G:C5'	2.67	0.42
39:A:6463:HOH:O	19:R:9:GLY:HA2	2.18	0.42
2:B:3023:U:H6	2:B:3023:U:C5'	2.29	0.42
5:D:280:VAL:CG1	5:D:334:SER:HA	2.50	0.42
5:D:305:ASP:O	5:D:306:LYS:HB2	2.19	0.42
6:E:1:MET:CG	6:E:2:GLN:H	2.27	0.42
6:E:94:THR:HG22	6:E:95:GLU:N	2.35	0.42
6:E:142:ASP:OD1	6:E:236:THR:HG23	2.20	0.42
9:H:49:PHE:HE1	9:H:98:VAL:CG2	2.32	0.42
9:H:63:ILE:HB	9:H:64:PRO:CD	2.44	0.42
13:L:21:ALA:O	13:L:96:VAL:HG22	2.20	0.42
14:M:66:VAL:HG23	14:M:67:ARG:N	2.35	0.42
16:O:110:THR:HA	16:O:111:PRO:HD3	1.81	0.42
19:R:50:GLY:CA	19:R:87:THR:HG23	2.50	0.42
21:T:11:THR:H	21:T:14:ALA:HB3	1.84	0.42
27:Z:189:ASN:HB2	39:Z:8525:HOH:O	2.20	0.42
1:A:1098:A:OP1	25:X:128:VAL:HG22	2.20	0.42
1:A:1130:U:H5'	39:A:7133:HOH:O	2.20	0.42
1:A:1133:A:H2'	1:A:1134:G:O4'	2.20	0.42
1:A:1367:A:C2'	1:A:1368:U:H5'	2.49	0.42
1:A:1383:U:OP1	39:A:5948:HOH:O	2.21	0.42
1:A:1461:U:H2'	1:A:1462:C:C6	2.55	0.42
1:A:1593:C:H5'	18:Q:116:SER:O	2.20	0.42
1:A:1647:G:H2'	1:A:1648:G:O4'	2.20	0.42
1:A:2316:G:C5'	39:A:5562:HOH:O	2.67	0.42
1:A:2398:A:H2'	1:A:2399:G:H5'	2.00	0.42
1:A:2563:U:H2'	1:A:2565:C:O5'	2.20	0.42
5:D:212:GLN:HB2	5:D:257:THR:CG2	2.45	0.42
7:F:42:GLY:HA2	39:F:5828:HOH:O	2.20	0.42
9:H:78:GLU:HB2	39:H:2750:HOH:O	2.19	0.42
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.35	0.42
12:K:37:ALA:HA	12:K:102:ARG:O	2.19	0.42
14:M:105:TYR:CG	39:M:8442:HOH:O	2.71	0.42
16:O:119:GLN:O	16:O:123:ILE:HG13	2.20	0.42
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.68	0.42
18:Q:103:THR:O	18:Q:106:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:1:THR:CG2	24:W:2:VAL:H	2.14	0.42
25:X:47:LYS:NZ	39:X:3920:HOH:O	2.27	0.42
26:Y:20:GLU:CD	26:Y:21:PRO:HD2	2.40	0.42
27:Z:203:VAL:HG12	27:Z:228:VAL:HG22	2.02	0.42
27:Z:213:LYS:HE3	27:Z:213:LYS:HB2	1.87	0.42
28:1:59:HIS:CE1	39:1:4742:HOH:O	2.72	0.42
29:2:21:ARG:NH2	29:2:43:ALA:O	2.53	0.42
30:3:6:ALA:O	30:3:9:LYS:HB2	2.20	0.42
31:4:88:LEU:HD12	31:4:88:LEU:HA	1.70	0.42
1:A:183:A:H5'	15:N:157:LEU:HD12	2.02	0.42
1:A:483:C:C4	1:A:484:A:C6	3.08	0.42
1:A:508:A:H2'	1:A:509:A:H5"	2.01	0.42
1:A:642:G:OP2	39:A:8945:HOH:O	2.21	0.42
1:A:820:G:H5'	1:A:821:U:C5'	2.50	0.42
1:A:1052:G:C5	1:A:1063:G:C6	3.08	0.42
1:A:1523:G:C6	1:A:1524:U:O4	2.72	0.42
1:A:1736:A:C2	1:A:2044:G:C2	3.08	0.42
1:A:1878:G:C4'	39:A:5591:HOH:O	2.67	0.42
1:A:2029:C:H2'	1:A:2030:A:O4'	2.20	0.42
1:A:2507:G:H2'	1:A:2510:C:H42	1.85	0.42
1:A:2834:G:C5	1:A:2847:G:N2	2.87	0.42
4:C:48:ASP:OD2	4:C:51:ARG:HG3	2.20	0.42
5:D:144:THR:CG2	5:D:145:HIS:N	2.83	0.42
7:F:55:LYS:O	39:F:4069:HOH:O	2.22	0.42
11:J:39:GLY:O	11:J:41:THR:N	2.53	0.42
13:L:34:VAL:O	13:L:35:HIS:C	2.58	0.42
25:X:3:ALA:O	25:X:54:PHE:HA	2.19	0.42
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.78	0.42
31:4:3:MET:HG3	31:4:4:PRO:HD2	2.02	0.42
1:A:128:A:H3'	1:A:128:A:C8	2.55	0.41
1:A:226:A:H1'	1:A:393:G:C5	2.55	0.41
1:A:668:C:C2	1:A:679:G:N2	2.88	0.41
1:A:911:G:H8	1:A:911:G:O5'	2.02	0.41
1:A:1246:A:H8	1:A:1246:A:H5'	1.85	0.41
1:A:1743:G:H1'	39:A:4368:HOH:O	2.19	0.41
1:A:2694:A:H5"	8:G:90:HIS:CE1	2.55	0.41
1:A:2716:G:OP1	5:D:262:ARG:NH2	2.53	0.41
1:A:2816:A:H5"	1:A:2817:G:H5'	2.02	0.41
39:A:8898:HOH:O	28:1:34:LYS:HD3	2.20	0.41
14:M:12:THR:HG21	14:M:16:GLY:O	2.19	0.41
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.68	0.41
22:U:26:THR:HA	22:U:39:ASN:HB3	2.01	0.41
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.68	0.41
1:A:553:G:C1'	1:A:1325:G:H5'	2.50	0.41
1:A:785:U:H4'	1:A:1485:A:N1	2.35	0.41
1:A:1289:C:C6	39:A:5873:HOH:O	2.57	0.41
1:A:1490:G:H1'	1:A:1658:A:N1	2.35	0.41
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.52	0.41
1:A:1771:U:H4'	28:1:20:LEU:HD21	2.01	0.41
1:A:2478:U:H2'	1:A:2479:A:C8	2.55	0.41
1:A:2869:G:H2'	1:A:2870:C:C6	2.54	0.41
1:A:2912:C:H3'	39:A:5835:HOH:O	2.19	0.41
39:A:9662:HOH:O	15:N:87:MET:HE3	2.20	0.41
2:B:3011:A:C2	2:B:3069:U:O4'	2.73	0.41
8:G:43:ASP:O	8:G:45:ASP:N	2.53	0.41
8:G:162:PHE:CD1	8:G:162:PHE:N	2.88	0.41
11:J:26:LYS:HG3	11:J:58:HIS:HB2	2.02	0.41
14:M:97:VAL:HG21	14:M:106:VAL:CG1	2.49	0.41
26:Y:30:MET:CE	26:Y:55:ASN:OD1	2.68	0.41
1:A:431:G:O2'	1:A:432:G:H5'	2.20	0.41
1:A:588:G:O6	25:X:154:ARG:NH1	2.53	0.41
1:A:634:G:O3'	1:A:1359:U:H4'	2.19	0.41
1:A:718:C:C2'	1:A:719:C:H5'	2.49	0.41
1:A:1578:C:O2	1:A:1619:G:C2	2.73	0.41
1:A:2096:A:H3'	1:A:2096:A:N3	2.35	0.41
1:A:2279:G:N3	39:A:9328:HOH:O	2.37	0.41
1:A:2314:G:HO2'	1:A:2361:A:C1'	2.33	0.41
1:A:2837:U:O4	39:A:4552:HOH:O	2.21	0.41
5:D:147:VAL:O	5:D:150:ALA:HB3	2.20	0.41
6:E:146:ASP:O	6:E:147:LEU:C	2.57	0.41
8:G:84:MET:HE3	8:G:148:ILE:HG21	2.01	0.41
8:G:114:ARG:HB3	8:G:151:LEU:HD11	2.02	0.41
8:G:145:ALA:HB1	8:G:168:ILE:HD11	2.01	0.41
9:H:99:THR:O	9:H:99:THR:CG2	2.67	0.41
11:J:47:GLU:HG2	11:J:133:ILE:CD1	2.48	0.41
15:N:185:PRO:HG2	15:N:189:VAL:HG11	2.01	0.41
16:O:74:PRO:HG2	16:O:159:TYR:OH	2.21	0.41
29:2:31:LYS:O	29:2:32:LYS:C	2.59	0.41
1:A:96:A:H2	24:W:6:GLN:OE1	2.02	0.41
1:A:188:C:H5"	15:N:163:LEU:HD21	2.02	0.41
1:A:218:C:OP2	1:A:220:C:N4	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:C:O2	1:A:240:C:H2'	2.20	0.41
1:A:644:G:C2	1:A:762:C:H1'	2.55	0.41
1:A:1080:C:H3'	1:A:1080:C:C6	2.56	0.41
1:A:1119:G:H8	12:K:52:GLN:HE22	1.68	0.41
1:A:1456:C:H2'	1:A:1457:U:C1'	2.50	0.41
1:A:1501:A:C6	1:A:1502:A:C6	3.08	0.41
1:A:1751:G:OP1	39:A:9296:HOH:O	2.22	0.41
1:A:1804:A:O2'	1:A:1805:G:H5'	2.19	0.41
1:A:2113:G:C6	1:A:2114:C:C4	3.08	0.41
1:A:2318:C:H6	1:A:2318:C:O5'	2.03	0.41
1:A:2478:U:O2'	1:A:2479:A:H5'	2.20	0.41
1:A:2531:U:C5	1:A:2532:A:C6	3.09	0.41
1:A:2900:G:C2'	1:A:2901:C:H5'	2.51	0.41
2:B:3057:A:H8	7:F:141:VAL:HG21	1.84	0.41
4:C:30:ARG:HE	4:C:30:ARG:HB3	1.67	0.41
4:C:220:PRO:HD2	4:C:223:ARG:HD3	2.00	0.41
6:E:236:THR:C	39:E:8456:HOH:O	2.59	0.41
9:H:30:LYS:HB2	9:H:97:ALA:HB3	2.02	0.41
9:H:58:GLU:CD	15:N:27:ARG:HH22	2.21	0.41
10:I:65:THR:O	10:I:69:ARG:HB2	2.20	0.41
12:K:56:LYS:O	12:K:60:ARG:HG3	2.21	0.41
12:K:131:THR:HG23	12:K:133:GLY:H	1.85	0.41
14:M:1:THR:HB	14:M:6:ARG:NH1	2.36	0.41
14:M:89:PHE:N	14:M:89:PHE:CD1	2.87	0.41
15:N:40:ILE:HA	39:N:8537:HOH:O	2.19	0.41
15:N:85:ARG:C	15:N:87:MET:HG3	2.41	0.41
20:S:106:GLY:HA2	20:S:109:MET:HE2	2.02	0.41
22:U:16:LEU:HD23	22:U:16:LEU:HA	1.88	0.41
22:U:107:LYS:NZ	39:U:4056:HOH:O	2.43	0.41
26:Y:77:PHE:CD1	26:Y:78:GLU:HB2	2.55	0.41
30:3:16:ASN:C	30:3:18:ASN:N	2.74	0.41
31:4:31:THR:HB	31:4:33:MET:HE2	2.03	0.41
1:A:417:G:O2'	1:A:2443:C:C2	2.69	0.41
1:A:763:C:H2'	1:A:764:C:H6	1.85	0.41
1:A:1074:G:H4'	1:A:1260:G:C6	2.56	0.41
1:A:1138:G:C4	1:A:1226:G:N2	2.88	0.41
1:A:1218:U:H2'	1:A:1219:U:C6	2.55	0.41
1:A:1246:A:C5	1:A:1248:A:C5	3.09	0.41
1:A:1653:A:OP1	4:C:52:SER:OG	2.27	0.41
1:A:1820:G:O6	1:A:2030:A:C2	2.73	0.41
1:A:2318:C:C6	1:A:2318:C:C3'	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:A:N7	1:A:2416:G:H1'	2.35	0.41
1:A:2664:A:H8	1:A:2664:A:OP1	2.03	0.41
1:A:2698:G:H2'	1:A:2699:A:C8	2.56	0.41
2:B:3084:G:O2'	2:B:3085:A:H5'	2.21	0.41
9:H:26:THR:HB	9:H:102:GLY:C	2.41	0.41
9:H:78:GLU:CB	39:H:2750:HOH:O	2.68	0.41
11:J:33:MET:SD	11:J:65:ARG:HD2	2.60	0.41
15:N:131:VAL:O	15:N:133:LEU:HD12	2.19	0.41
20:S:72:VAL:HG11	20:S:75:TRP:HB3	2.03	0.41
24:W:29:ASN:O	24:W:33:VAL:HG23	2.21	0.41
26:Y:25:ARG:O	26:Y:26:ALA:C	2.59	0.41
29:2:21:ARG:NH1	29:2:37:CYS:O	2.54	0.41
1:A:178:U:H4'	39:A:9011:HOH:O	2.21	0.41
1:A:658:C:O2'	1:A:662:U:OP1	2.34	0.41
1:A:661:G:C4	1:A:686:A:C2	3.09	0.41
1:A:849:C:O2'	1:A:850:U:H5'	2.21	0.41
1:A:1119:G:H8	12:K:52:GLN:NE2	2.17	0.41
1:A:1277:C:N4	1:A:1278:A:N6	2.67	0.41
1:A:1938:G:H2'	1:A:1939:U:O4'	2.20	0.41
1:A:2289:G:C6	1:A:2290:U:C4	3.09	0.41
1:A:2553:A:N3	1:A:2553:A:H2'	2.35	0.41
1:A:2657:G:N2	1:A:2658:G:H1'	2.35	0.41
1:A:2752:C:C2	1:A:2753:G:C8	3.08	0.41
1:A:2846:C:H4'	5:D:156:LYS:HB3	2.01	0.41
39:A:6463:HOH:O	19:R:10:THR:N	2.53	0.41
2:B:3011:A:N7	16:O:8:VAL:HG23	2.35	0.41
5:D:41:PHE:HA	5:D:79:MET:HE2	2.02	0.41
5:D:202:VAL:HA	5:D:310:ARG:O	2.21	0.41
5:D:226:LYS:O	5:D:230:GLN:HG2	2.20	0.41
6:E:191:SER:OG	6:E:192:ILE:N	2.52	0.41
7:F:44:ILE:HG12	7:F:83:PHE:CE1	2.56	0.41
8:G:35:TYR:N	39:G:4572:HOH:O	2.47	0.41
11:J:113:ALA:N	11:J:114:PRO:CD	2.83	0.41
14:M:18:HIS:CD2	14:M:18:HIS:O	2.74	0.41
15:N:108:LYS:HA	15:N:108:LYS:HD3	1.84	0.41
25:X:118:LEU:HD11	25:X:150:LEU:HD23	2.02	0.41
25:X:122:ARG:CG	25:X:152:ALA:O	2.69	0.41
1:A:336:G:H4'	1:A:337:A:OP2	2.21	0.41
1:A:382:U:O2'	1:A:430:A:H1'	2.21	0.41
1:A:654:A:OP2	17:P:38:ARG:HD3	2.20	0.41
1:A:906:C:C2	1:A:907:A:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1688:G:H2'	1:A:1689:A:OP1	2.21	0.41
1:A:1789:G:H2'	1:A:1790:C:O5'	2.20	0.41
1:A:1892:C:N4	1:A:1893:C:N4	2.68	0.41
1:A:2247:C:C5'	39:A:6807:HOH:O	2.68	0.41
1:A:2404:G:OP1	19:R:68:GLY:HA3	2.21	0.41
1:A:2608:C:H3'	39:A:7268:HOH:O	2.20	0.41
1:A:2614:C:C2'	1:A:2615:U:H5'	2.50	0.41
1:A:2765:C:H2'	1:A:2766:A:H8	1.86	0.41
1:A:2834:G:C5	1:A:2847:G:C2	3.09	0.41
2:B:3039:U:H3	2:B:3042:C:H5"	1.86	0.41
4:C:72:GLU:HG3	28:1:66:GLY:HA2	2.02	0.41
5:D:115:VAL:HA	5:D:116:PRO:HD3	1.93	0.41
6:E:33:LYS:HE2	39:E:8365:HOH:O	2.20	0.41
6:E:162:VAL:CG1	6:E:162:VAL:O	2.69	0.41
7:F:174:VAL:CG1	39:F:6555:HOH:O	2.66	0.41
8:G:20:ILE:HD12	8:G:33:LEU:HD12	2.02	0.41
11:J:167:ALA:HA	39:J:8372:HOH:O	2.21	0.41
12:K:4:ALA:O	12:K:5:GLU:O	2.38	0.41
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.51	0.41
15:N:32:ARG:NH2	39:N:8595:HOH:O	2.54	0.41
16:O:5:ARG:HG3	19:R:18:PRO:CB	2.51	0.41
16:O:154:LEU:HG	16:O:155:GLU:H	1.86	0.41
17:P:18:ALA:CB	39:P:3062:HOH:O	2.69	0.41
19:R:33:PHE:HB2	19:R:71:TYR:CE2	2.55	0.41
20:S:25:PHE:O	20:S:29:LYS:HG3	2.20	0.41
20:S:91:LEU:O	20:S:94:ASN:HB3	2.19	0.41
21:T:57:THR:C	21:T:59:ASP:N	2.72	0.41
25:X:65:VAL:CA	25:X:68:THR:HG22	2.51	0.41
1:A:69:A:H5'	1:A:69:A:H8	1.86	0.41
1:A:390:G:C4	1:A:391:U:C6	3.09	0.41
1:A:440:C:C4	1:A:441:A:C6	3.09	0.41
1:A:556:C:H2'	1:A:557:C:C6	2.56	0.41
1:A:1292:G:HO2'	1:A:1293:U:H6	1.66	0.41
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.20	0.41
1:A:1884:G:O6	4:C:190:ARG:CD	2.69	0.41
1:A:1968:A:O2'	1:A:1969:A:H5'	2.21	0.41
1:A:2097:G:C4	1:A:2612:A:C2	3.09	0.41
1:A:2271:G:N3	1:A:2271:G:H2'	2.36	0.41
4:C:165:THR:HG22	39:C:8617:HOH:O	2.21	0.41
5:D:86:ALA:HB2	5:D:128:ILE:HD13	2.02	0.41
6:E:177:GLY:CA	39:E:8314:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:59:GLY:C	7:F:61:PHE:N	2.74	0.41
7:F:81:GLU:C	7:F:83:PHE:N	2.74	0.41
11:J:57:ARG:HG3	11:J:57:ARG:NH1	2.35	0.41
11:J:150:LYS:CG	39:J:8382:HOH:O	2.67	0.41
15:N:147:LEU:O	15:N:150:ILE:HG22	2.21	0.41
16:O:37:ARG:CZ	39:O:8533:HOH:O	2.69	0.41
16:O:165:ALA:O	39:O:8517:HOH:O	2.22	0.41
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.56	0.41
25:X:38:THR:HG22	25:X:39:ASP:N	2.34	0.41
1:A:13:G:H2'	1:A:14:C:C6	2.56	0.41
1:A:178:U:H2'	1:A:179:C:H6	1.86	0.41
1:A:275:G:C2	1:A:376:C:C2	3.09	0.41
1:A:308:U:C5'	22:U:97:ARG:NH2	2.83	0.41
1:A:326:G:C6	1:A:327:A:C5	3.09	0.41
1:A:429:A:C6	1:A:430:A:C6	3.09	0.41
1:A:500:G:H4'	20:S:17:MET:O	2.21	0.41
1:A:563:C:H2'	1:A:564:G:H5'	2.03	0.41
1:A:567:U:H5"	39:X:5817:HOH:O	2.20	0.41
1:A:589:U:H2'	1:A:590:A:H8	1.85	0.41
1:A:613:C:C5'	39:A:3428:HOH:O	2.68	0.41
1:A:918:G:C2	1:A:926:A:C2	3.08	0.41
1:A:935:G:O2'	1:A:936:C:H5'	2.21	0.41
1:A:956:G:H5'	2:B:3081:C:H4'	2.03	0.41
1:A:1014:A:H5"	2:B:3101:G:O2'	2.20	0.41
1:A:1072:G:OP2	27:Z:154:ARG:NH2	2.52	0.41
1:A:1123:A:N1	1:A:1238:C:H5'	2.35	0.41
1:A:1523:G:C4	1:A:1524:U:C5	3.09	0.41
1:A:1687:C:O2	29:2:9:GLY:HA2	2.21	0.41
1:A:1761:U:H4'	18:Q:82:GLY:O	2.20	0.41
1:A:1842:A:C4	1:A:1979:G:C6	3.09	0.41
1:A:1847:A:OP1	4:C:175:LYS:HG3	2.20	0.41
1:A:2580:G:C6	1:A:2581:U:N3	2.89	0.41
39:A:4882:HOH:O	4:C:164:ARG:CZ	2.69	0.41
4:C:51:ARG:O	4:C:52:SER:HB2	2.20	0.41
5:D:62:ARG:CA	5:D:65:MET:CE	2.84	0.41
5:D:217:ARG:NE	5:D:257:THR:HG22	2.35	0.41
6:E:1:MET:CG	6:E:2:GLN:N	2.84	0.41
6:E:118:THR:HG22	6:E:137:PRO:HB3	2.03	0.41
7:F:52:THR:N	7:F:70:GLY:O	2.54	0.41
7:F:55:LYS:N	39:F:4069:HOH:O	2.54	0.41
8:G:31:ARG:NH1	39:G:5919:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:166:VAL:C	39:G:3134:HOH:O	2.59	0.41
11:J:54:VAL:HG21	11:J:155:PRO:HD3	2.01	0.41
11:J:75:SER:HB3	11:J:79:ALA:CB	2.49	0.41
11:J:151:MET:HA	11:J:151:MET:HE3	2.03	0.41
11:J:162:SER:HA	39:J:8341:HOH:O	2.21	0.41
12:K:73:LYS:O	12:K:136:SER:HB3	2.21	0.41
13:L:99:ASP:OD1	13:L:99:ASP:C	2.59	0.41
15:N:65:VAL:O	15:N:128:TRP:HA	2.20	0.41
15:N:178:LYS:HD2	39:N:8619:HOH:O	2.21	0.41
20:S:126:LYS:HG3	20:S:127:PRO:O	2.21	0.41
22:U:38:ARG:NH1	22:U:38:ARG:HG3	2.36	0.41
30:3:16:ASN:C	30:3:18:ASN:H	2.24	0.41
31:4:84:ARG:CD	39:4:8550:HOH:O	2.69	0.41
1:A:21:G:C2	1:A:523:C:C2	3.08	0.41
1:A:344:C:H2'	1:A:345:G:O4'	2.21	0.41
1:A:451:C:N4	1:A:452:G:C6	2.89	0.41
1:A:590:A:H2'	1:A:591:A:H5'	2.02	0.41
1:A:814:G:H2'	1:A:815:U:O4'	2.21	0.41
1:A:929:A:H8	1:A:929:A:O5'	2.04	0.41
1:A:1185:U:C4'	39:A:6930:HOH:O	2.69	0.41
1:A:1538:C:H2'	1:A:1539:U:O4'	2.21	0.41
1:A:1540:G:N2	1:A:1646:G:H1'	2.36	0.41
1:A:1584:C:C2	1:A:1612:A:C2	3.09	0.41
1:A:1707:G:N2	1:A:1709:G:H3'	2.36	0.41
1:A:2244:A:H3'	1:A:2245:C:C6	2.55	0.41
1:A:2413:A:H62	16:O:109:PRO:CG	2.34	0.41
1:A:2634:G:H2'	1:A:2635:A:H8	1.86	0.41
1:A:2681:A:H4'	1:A:2682:C:H5'	2.03	0.41
2:B:3051:A:H5'	16:O:160:SER:HB3	2.03	0.41
5:D:176:ASP:O	5:D:177:HIS:C	2.59	0.41
11:J:94:ARG:NH2	39:J:8331:HOH:O	2.54	0.41
13:L:16:SER:O	13:L:31:VAL:HG23	2.21	0.41
15:N:154:ARG:CD	39:N:8639:HOH:O	2.64	0.41
20:S:44:VAL:HG13	20:S:89:LEU:HD22	2.02	0.41
24:W:12:THR:H	24:W:15:GLU:HB2	1.86	0.41
25:X:122:ARG:HG3	25:X:152:ALA:O	2.21	0.41
27:Z:106:THR:HG22	27:Z:107:PRO:O	2.21	0.41
29:2:15:THR:OG1	29:2:16:HIS:N	2.54	0.41
31:4:9:THR:O	31:4:17:HIS:HA	2.21	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.40
1:A:547:A:H3'	39:A:4421:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:A:H2'	1:A:757:C:H6	1.86	0.40
1:A:1038:G:C2'	1:A:1039:G:H5'	2.51	0.40
1:A:1174:A:C5'	1:A:1176:C:OP2	2.68	0.40
1:A:1201:C:C6	39:A:5699:HOH:O	2.71	0.40
1:A:1299:G:N2	39:A:4159:HOH:O	2.53	0.40
1:A:1299:G:N7	14:M:6:ARG:NH1	2.69	0.40
1:A:1682:A:C5'	39:A:8958:HOH:O	2.65	0.40
1:A:1815:A:H3'	1:A:1816:C:C6	2.56	0.40
1:A:2039:A:OP2	39:A:5554:HOH:O	2.22	0.40
1:A:2354:A:O5'	1:A:2354:A:H2'	2.20	0.40
1:A:2368:A:H8	39:O:8531:HOH:O	2.02	0.40
1:A:2682:C:C2	1:A:2713:G:N2	2.89	0.40
1:A:2750:G:O2'	1:A:2751:C:H5'	2.21	0.40
4:C:211:LYS:NZ	39:C:8620:HOH:O	2.43	0.40
5:D:224:LYS:O	5:D:225:GLY:C	2.60	0.40
8:G:5:LEU:HD21	8:G:66:GLN:HG3	2.02	0.40
9:H:17:LEU:O	9:H:21:GLU:HG3	2.20	0.40
9:H:79:GLN:HB2	9:H:82:ASP:OD2	2.21	0.40
11:J:156:THR:HG22	11:J:157:ILE:N	2.36	0.40
13:L:19:THR:HG22	13:L:20:CYS:N	2.36	0.40
13:L:19:THR:HB	13:L:94:ALA:HB2	2.03	0.40
14:M:7:GLN:CD	39:M:8464:HOH:O	2.60	0.40
15:N:52:LEU:HD13	15:N:116:ASN:HB3	2.04	0.40
17:P:17:ALA:CB	17:P:102:ILE:HG23	2.51	0.40
18:Q:18:LYS:O	18:Q:21:VAL:HG22	2.21	0.40
20:S:89:LEU:HD23	20:S:89:LEU:HA	1.67	0.40
20:S:96:VAL:O	20:S:96:VAL:HG12	2.20	0.40
25:X:66:LEU:HA	25:X:66:LEU:HD23	1.74	0.40
30:3:9:LYS:HE2	30:3:9:LYS:HB3	1.91	0.40
1:A:88:G:H5'	1:A:88:G:C8	2.46	0.40
1:A:661:G:C5	1:A:662:U:C4	3.10	0.40
1:A:823:U:O4	1:A:824:G:C6	2.75	0.40
1:A:1162:G:N1	1:A:1163:G:C5	2.89	0.40
1:A:1181:A:C8	1:A:1182:C:C5	3.10	0.40
1:A:1327:G:C6	1:A:1331:A:C6	3.09	0.40
1:A:1810:C:C2	1:A:1811:A:C8	3.10	0.40
1:A:1873:G:H3'	39:C:8584:HOH:O	2.21	0.40
1:A:2029:C:C2'	1:A:2030:A:H5'	2.51	0.40
1:A:2379:G:C5	1:A:2381:C:N4	2.90	0.40
1:A:2385:G:H2'	1:A:2386:U:H6	1.84	0.40
1:A:2715:G:OP1	5:D:16:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2838:A:H2'	1:A:2839:C:O4'	2.21	0.40
39:A:3016:HOH:O	18:Q:91:LYS:HD2	2.20	0.40
5:D:92:TYR:CD1	5:D:92:TYR:N	2.89	0.40
5:D:98:THR:O	5:D:99:GLU:HG3	2.21	0.40
6:E:162:VAL:CG1	6:E:192:ILE:CD1	2.99	0.40
7:F:65:GLU:CG	39:F:6752:HOH:O	2.65	0.40
8:G:84:MET:HA	8:G:167:TYR:O	2.21	0.40
8:G:93:MET:HE1	8:G:107:PHE:HE1	1.86	0.40
9:H:12:LEU:HD23	9:H:12:LEU:O	2.20	0.40
14:M:142:LEU:HA	14:M:142:LEU:HD12	1.86	0.40
22:U:47:THR:HB	22:U:100:ASP:HB3	2.02	0.40
22:U:48:VAL:HG21	22:U:96:VAL:CG1	2.51	0.40
22:U:48:VAL:HG11	22:U:96:VAL:CG1	2.52	0.40
25:X:72:PRO:HA	25:X:112:LEU:HD23	2.04	0.40
27:Z:136:LYS:HB3	27:Z:139:VAL:HG23	2.02	0.40
1:A:21:G:H5"	20:S:2:ILE:HA	1.96	0.40
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.40
1:A:168:C:C2'	1:A:169:A:H5'	2.51	0.40
1:A:477:A:N6	1:A:478:C:N4	2.69	0.40
1:A:532:A:C6	1:A:2661:U:C4'	3.04	0.40
1:A:563:C:C2'	1:A:564:G:H5'	2.51	0.40
1:A:566:A:H2'	1:A:567:U:O4'	2.21	0.40
1:A:784:A:C4	1:A:863:G:N2	2.89	0.40
1:A:1000:C:P	39:A:4195:HOH:O	2.77	0.40
1:A:1200:A:C1'	39:A:6805:HOH:O	2.68	0.40
1:A:1241:G:O2'	12:K:85:GLY:HA3	2.21	0.40
1:A:1370:G:C1'	39:A:9638:HOH:O	2.69	0.40
1:A:1427:A:C2	39:A:4280:HOH:O	2.71	0.40
1:A:1942:A:H2'	1:A:1943:C:H6	1.86	0.40
1:A:2003:U:O5'	1:A:2003:U:H6	2.03	0.40
1:A:2295:G:C4	1:A:2314:G:N2	2.89	0.40
1:A:2597:U:OP2	39:A:3318:HOH:O	2.21	0.40
1:A:2629:C:C4	1:A:2630:G:N7	2.89	0.40
1:A:2715:G:H4'	5:D:13:PHE:CZ	2.56	0.40
1:A:2724:U:O4	1:A:2725:G:N1	2.55	0.40
1:A:2838:A:H1'	1:A:2844:C:O2	2.22	0.40
1:A:2898:G:O2'	1:A:2899:A:H5'	2.21	0.40
2:B:3050:G:C6	2:B:3051:A:C6	3.09	0.40
2:B:3079:U:O2	2:B:3079:U:H2'	2.22	0.40
4:C:42:VAL:HG21	4:C:74:VAL:CG1	2.52	0.40
5:D:248:ARG:O	5:D:251:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:81:GLU:O	7:F:85:GLN:HG3	2.22	0.40
8:G:6:GLU:HG2	8:G:46:THR:HG22	2.04	0.40
8:G:137:ASP:O	8:G:141:VAL:HG23	2.21	0.40
13:L:35:HIS:HB2	39:L:5729:HOH:O	2.19	0.40
16:O:29:SER:HA	39:O:8553:HOH:O	2.20	0.40
22:U:27:LEU:HG	22:U:39:ASN:HA	2.04	0.40
22:U:49:GLU:OE2	22:U:51:LEU:HD21	2.22	0.40
25:X:26:ILE:HG22	39:X:5420:HOH:O	2.20	0.40
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.85	0.40
1:A:230:C:H2'	1:A:231:G:H8	1.85	0.40
1:A:247:A:C5	1:A:262:A:C6	3.09	0.40
1:A:292:G:H8	1:A:292:G:O5'	2.05	0.40
1:A:652:G:O6	39:A:9209:HOH:O	2.21	0.40
1:A:784:A:C2	1:A:863:G:N3	2.89	0.40
1:A:812:A:H2'	1:A:813:C:O4'	2.21	0.40
1:A:936:C:O2'	1:A:937:C:H5'	2.21	0.40
1:A:1058:A:H2'	1:A:1060:C:C5'	2.51	0.40
1:A:1452:G:H2'	1:A:1453:G:O4'	2.21	0.40
1:A:1838:U:H3'	39:A:4996:HOH:O	2.21	0.40
1:A:2670:G:O2'	1:A:2671:U:H5'	2.22	0.40
1:A:2721:U:H4'	13:L:87:ARG:HG3	2.04	0.40
1:A:2755:G:H1'	39:A:4158:HOH:O	2.22	0.40
39:A:5640:HOH:O	5:D:216:LYS:HD2	2.21	0.40
39:A:8919:HOH:O	15:N:52:LEU:HD23	2.21	0.40
4:C:74:VAL:H	28:1:65:ALA:HB3	1.86	0.40
7:F:38:GLU:HB3	7:F:49:PRO:HG2	2.03	0.40
10:I:19:GLU:OE1	10:I:19:GLU:HA	2.22	0.40
11:J:47:GLU:CG	11:J:133:ILE:CD1	2.99	0.40
15:N:134:ILE:HG23	15:N:141:ILE:HD13	2.04	0.40
15:N:158:ARG:NH2	39:N:8630:HOH:O	2.29	0.40
16:O:47:LEU:HD12	16:O:92:ALA:HB1	2.03	0.40
17:P:50:ARG:HD2	17:P:51:TYR:CZ	2.55	0.40
17:P:102:ILE:HD13	17:P:102:ILE:HG21	1.87	0.40
22:U:38:ARG:HG3	22:U:38:ARG:HH11	1.86	0.40
22:U:48:VAL:HG13	22:U:49:GLU:N	2.37	0.40
25:X:26:ILE:CG2	39:X:5420:HOH:O	2.68	0.40
26:Y:12:ILE:HG23	26:Y:12:ILE:HD12	1.75	0.40
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.61	0.40
1:A:219:G:O5'	1:A:220:C:H5"	2.21	0.40
1:A:236:A:H2'	1:A:236:A:O5'	2.21	0.40
1:A:288:A:H2'	1:A:289:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:G:C5	1:A:324:G:C2	3.10	0.40
1:A:657:G:C2'	39:A:8532:HOH:O	2.69	0.40
1:A:810:G:H2'	1:A:811:C:C6	2.56	0.40
1:A:1067:A:O2'	25:X:12:ASN:HA	2.21	0.40
1:A:1183:C:N4	1:A:1184:C:N4	2.70	0.40
1:A:1197:G:C6	1:A:1198:U:C4	3.10	0.40
1:A:1707:G:H2'	1:A:1709:G:OP2	2.22	0.40
1:A:1886:A:N3	39:A:4299:HOH:O	2.37	0.40
1:A:2005:G:C6	1:A:2008:U:C4	3.09	0.40
1:A:2044:G:C6	1:A:2045:G:C5	3.10	0.40
1:A:2054:A:H2	20:S:128:ARG:HH22	1.62	0.40
1:A:2297:U:P	39:A:6939:HOH:O	2.79	0.40
4:C:36:ASP:OD2	4:C:85:ASP:HB2	2.22	0.40
6:E:25:PRO:HA	39:E:8361:HOH:O	2.21	0.40
11:J:46:VAL:CG1	11:J:160:ASP:O	2.69	0.40
11:J:133:ILE:HD12	11:J:133:ILE:HG23	1.80	0.40
13:L:84:ASP:O	23:V:16:GLY:HA2	2.22	0.40
16:O:23:ARG:O	16:O:27:LEU:HG	2.22	0.40
16:O:115:VAL:HG23	16:O:116:PHE:N	2.37	0.40
18:Q:7:LYS:HD3	18:Q:21:VAL:CG2	2.51	0.40
18:Q:71:LYS:O	18:Q:71:LYS:HG3	2.21	0.40
19:R:7:LEU:N	19:R:7:LEU:HD23	2.35	0.40
19:R:16:ASN:HD22	19:R:16:ASN:HA	1.71	0.40
19:R:50:GLY:HA3	19:R:87:THR:OG1	2.22	0.40
20:S:123:GLN:NE2	39:S:8537:HOH:O	2.53	0.40
23:V:36:CYS:O	23:V:39:ASN:N	2.53	0.40
24:W:4:HIS:HB2	24:W:7:GLU:HG3	2.03	0.40
25:X:35:VAL:HG23	25:X:41:TYR:CG	2.57	0.40
25:X:92:ASP:O	25:X:93:ILE:C	2.58	0.40
28:1:81:LYS:O	28:1:82:ALA:O	2.40	0.40
31:4:70:ARG:HG2	31:4:70:ARG:HH11	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:5574:HOH:O	39:W:2786:HOH:O[4_565]	2.14	0.06
39:A:3438:HOH:O	39:A:9956:HOH:O[5_445]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	C	235/239 (98%)	204 (87%)	23 (10%)	8 (3%)	3 24
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	4 28
6	E	244/246 (99%)	206 (84%)	34 (14%)	4 (2%)	9 43
7	F	134/176 (76%)	95 (71%)	26 (19%)	13 (10%)	0 3
8	G	170/177 (96%)	160 (94%)	9 (5%)	1 (1%)	25 64
9	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9 42
10	I	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
11	J	152/167 (91%)	130 (86%)	13 (9%)	9 (6%)	1 12
12	K	140/145 (97%)	125 (89%)	11 (8%)	4 (3%)	4 28
13	L	130/132 (98%)	110 (85%)	15 (12%)	5 (4%)	3 22
14	M	141/164 (86%)	114 (81%)	25 (18%)	2 (1%)	11 46
15	N	192/194 (99%)	167 (87%)	22 (12%)	3 (2%)	9 43
16	O	184/186 (99%)	153 (83%)	23 (12%)	8 (4%)	2 20
17	P	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	8 41
18	Q	141/148 (95%)	129 (92%)	12 (8%)	0	100 100
19	R	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	14 51
20	S	148/154 (96%)	132 (89%)	15 (10%)	1 (1%)	22 61
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12 47
22	U	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	5 31
23	V	51/66 (77%)	45 (88%)	5 (10%)	1 (2%)	7 38
24	W	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	4 26
25	X	152/154 (99%)	141 (93%)	8 (5%)	3 (2%)	7 38
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	3 22
27	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100 100
28	1	71/73 (97%)	58 (82%)	11 (16%)	2 (3%)	5 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	2	54/56 (96%)	47 (87%)	7 (13%)	0	100 100
30	3	42/48 (88%)	42 (100%)	0	0	100 100
31	4	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	6 35
All	All	3633/4235 (86%)	3196 (88%)	347 (10%)	90 (2%)	5 32

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	11	HIS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU
9	H	101	ALA
11	J	162	SER
13	L	119	GLN
14	M	80	ASP
16	O	154	LEU
16	O	164	ASP
16	O	183	ASP
19	R	23	THR
25	X	14	HIS
4	C	10	GLY
4	C	34	ASP
4	C	37	VAL
5	D	34	GLY
5	D	169	GLY
7	F	16	PRO
7	F	171	ASP
11	J	164	ALA
12	K	5	GLU
12	K	89	HIS
12	K	143	LYS
16	O	9	PRO
16	O	162	ASP
22	U	53	GLY
23	V	7	ASP
24	W	43	PRO
25	X	77	ALA
25	X	133	LYS
26	Y	87	ALA

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Mol	Chain	Res	Type
31	4	57	GLY
4	C	20	SER
4	C	87	GLU
4	C	132	ASP
4	C	229	ALA
5	D	83	ALA
5	D	107	SER
5	D	184	ASP
5	D	291	ASP
6	E	201	SER
7	F	20	LYS
7	F	82	GLU
7	F	85	GLN
7	F	137	PRO
7	F	170	TYR
8	G	44	GLY
9	H	71	GLY
11	J	40	PRO
11	J	72	VAL
13	L	126	SER
22	U	93	THR
22	U	114	SER
28	1	74	VAL
28	1	81	LYS
5	D	185	GLY
7	F	60	GLU
11	J	91	HIS
11	J	138	PRO
11	J	155	PRO
14	M	100	ALA
15	N	140	ALA
16	O	12	ARG
16	O	138	ASP
16	O	181	ASP
21	T	58	MET
24	W	40	PRO
26	Y	77	PHE
31	4	56	PRO
6	E	244	ALA
7	F	61	PHE
11	J	154	THR
12	K	50	GLU

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Mol	Chain	Res	Type
15	N	165	SER
5	D	2	GLN
6	E	175	LYS
17	P	20	SER
26	Y	42	SER
4	C	170	VAL
6	E	225	PRO
11	J	54	VAL
15	N	88	VAL
13	L	62	PRO
13	L	122	GLY
5	D	225	GLY
13	L	36	GLY
20	S	106	GLY
17	P	46	GLY

5.3.2 Protein sidechains (i)

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
4	C	179/181 (99%)	167 (93%)	12 (7%)	16 50
5	D	282/282 (100%)	264 (94%)	18 (6%)	17 52
6	E	193/193 (100%)	173 (90%)	20 (10%)	7 28
7	F	117/147 (80%)	107 (92%)	10 (8%)	10 38
8	G	152/155 (98%)	145 (95%)	7 (5%)	27 63
9	H	92/92 (100%)	89 (97%)	3 (3%)	38 71
10	I	27/283 (10%)	26 (96%)	1 (4%)	34 68
11	J	122/122 (100%)	112 (92%)	10 (8%)	11 41
12	K	118/121 (98%)	107 (91%)	11 (9%)	9 33
13	L	106/106 (100%)	102 (96%)	4 (4%)	33 67
14	M	112/126 (89%)	108 (96%)	4 (4%)	35 69
15	N	166/166 (100%)	156 (94%)	10 (6%)	19 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	O	149/149 (100%)	142 (95%)	7 (5%)	26 62
17	P	93/93 (100%)	88 (95%)	5 (5%)	22 58
18	Q	113/116 (97%)	108 (96%)	5 (4%)	28 64
19	R	79/79 (100%)	75 (95%)	4 (5%)	24 60
20	S	117/121 (97%)	112 (96%)	5 (4%)	29 64
21	T	71/73 (97%)	70 (99%)	1 (1%)	67 86
22	U	105/105 (100%)	100 (95%)	5 (5%)	25 61
23	V	44/52 (85%)	44 (100%)	0	100 100
24	W	51/56 (91%)	51 (100%)	0	100 100
25	X	130/130 (100%)	122 (94%)	8 (6%)	18 53
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13 45
27	Z	120/195 (62%)	109 (91%)	11 (9%)	9 33
28	1	56/56 (100%)	50 (89%)	6 (11%)	6 27
29	2	46/46 (100%)	44 (96%)	2 (4%)	29 64
30	3	42/44 (96%)	41 (98%)	1 (2%)	49 77
31	4	79/79 (100%)	76 (96%)	3 (4%)	33 67
All	All	3027/3441 (88%)	2849 (94%)	178 (6%)	19 54

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	8	ARG
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	94	LEU
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
4	C	220	PRO
5	D	7	ARG
5	D	11	LEU
5	D	16	ARG

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Mol	Chain	Res	Type
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	190	MET
5	D	245	SER
5	D	249	SER
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	42	ARG
6	E	67	GLN
6	E	76	ARG
6	E	78	ARG
6	E	91	PRO
6	E	94	THR
6	E	95	GLU
6	E	115	LEU
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	237	GLU
6	E	240	LEU
6	E	243	VAL
7	F	24	HIS
7	F	50	VAL
7	F	61	PHE
7	F	99	ASP
7	F	100	ASP
7	F	131	THR
7	F	133	ASN

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Mol	Chain	Res	Type
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	1	PRO
8	G	7	ILE
8	G	12	ASP
8	G	16	ASP
8	G	36	PRO
8	G	102	VAL
8	G	164	ASP
9	H	1	PRO
9	H	64	PRO
9	H	100	ASP
10	I	64	ASN
11	J	1	LYS
11	J	30	GLN
11	J	59	ASN
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	86	ARG
11	J	129	ASN
11	J	142	VAL
11	J	150	LYS
12	K	46	ILE
12	K	47	THR
12	K	52	GLN
12	K	74	ARG
12	K	76	ASP
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	127	ILE
12	K	131	THR
13	L	7	ASP
13	L	10	GLN
13	L	49	LEU
13	L	98	VAL
14	M	30	ARG
14	M	35	ARG
14	M	80	ASP

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Mol	Chain	Res	Type
14	M	117	GLU
15	N	38	VAL
15	N	46	LEU
15	N	48	ARG
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	115	LEU
15	N	159	THR
15	N	164	THR
16	O	26	LEU
16	O	43	VAL
16	O	47	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	38	ARG
17	P	98	LEU
17	P	109	SER
17	P	115	ARG
18	Q	52	LYS
18	Q	81	LYS
18	Q	91	LYS
18	Q	98	ILE
18	Q	136	ASP
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	56	PRO
20	S	82	GLU
20	S	132	ARG
21	T	10	VAL
22	U	26	THR
22	U	39	ASN
22	U	48	VAL
22	U	73	HIS

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Mol	Chain	Res	Type
22	U	96	VAL
25	X	4	LEU
25	X	26	ILE
25	X	35	VAL
25	X	73	LEU
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	49	ARG
26	Y	72	VAL
26	Y	76	ARG
27	Z	103	THR
27	Z	154	ARG
27	Z	163	THR
27	Z	172	THR
27	Z	186	ARG
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
27	Z	204	ARG
27	Z	231	PRO
27	Z	235	GLU
28	1	11	THR
28	1	32	LYS
28	1	44	PHE
28	1	49	ARG
28	1	60	CYS
28	1	64	ILE
29	2	21	ARG
29	2	26	SER
30	3	18	ASN
31	4	42	ARG
31	4	56	PRO
31	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	47	HIS

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Mol	Chain	Res	Type
4	C	92	ASN
4	C	125	ASN
4	C	127	GLN
4	C	188	ASN
4	C	199	HIS
5	D	27	ASN
5	D	55	ASN
5	D	145	HIS
5	D	221	GLN
5	D	238	ASN
5	D	260	HIS
5	D	318	ASN
5	D	332	ASN
6	E	39	GLN
6	E	44	GLN
6	E	129	HIS
7	F	47	GLN
7	F	103	ASN
7	F	133	ASN
8	G	90	HIS
8	G	106	ASN
8	G	143	GLN
9	H	80	GLN
10	I	64	ASN
11	J	8	ASN
11	J	35	ASN
11	J	36	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	158	ASN
11	J	166	ASN
12	K	25	GLN
12	K	52	GLN
12	K	107	ASN
13	L	10	GLN
14	M	18	HIS

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Mol	Chain	Res	Type
14	M	41	HIS
14	M	58	GLN
14	M	116	HIS
15	N	58	GLN
15	N	176	GLN
16	O	107	ASN
16	O	119	GLN
16	O	140	GLN
17	P	53	GLN
17	P	100	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	122	GLN
20	S	123	GLN
21	T	53	ASN
21	T	55	GLN
22	U	39	ASN
22	U	95	ASN
23	V	39	ASN
24	W	60	GLN
25	X	2	HIS
25	X	14	HIS
25	X	87	HIS
25	X	110	GLN
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
26	Y	40	HIS
27	Z	121	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN

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Mol	Chain	Res	Type
28	1	33	HIS
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	18	ASN
30	3	41	HIS
30	3	45	ASN
31	4	15	ASN
31	4	30	GLN
31	4	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	259 (9%)	44 (1%)
2	B	121/122 (99%)	19 (15%)	5 (4%)
3	5	1/3 (33%)	0	0
All	All	2869/3047 (94%)	278 (9%)	49 (1%)

All (278) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A

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Mol	Chain	Res	Type
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	317	A
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	457	U
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A

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Mol	Chain	Res	Type
1	A	688	A
1	A	701	U
1	A	705	C
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	1006	A
1	A	1008	C
1	A	1015	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1083	C
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G

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Mol	Chain	Res	Type
1	A	1120	U
1	A	1129	C
1	A	1130	U
1	A	1138	G
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1242	A
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1457	U
1	A	1460	G
1	A	1474	C
1	A	1488	U
1	A	1504	A
1	A	1505	U
1	A	1506	U
1	A	1507	C
1	A	1524	U
1	A	1525	G
1	A	1526	A

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Mol	Chain	Res	Type
1	A	1528	A
1	A	1562	C
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1732	A
1	A	1737	A
1	A	1741	U
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1819	G
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1996	U
1	A	2004	U
1	A	2008	U

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Mol	Chain	Res	Type
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
1	A	2110	G
1	A	2238	A
1	A	2243	C
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2316	G
1	A	2317	C
1	A	2320	U
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2379	G
1	A	2422	U
1	A	2462	G
1	A	2465	A
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2509	A
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A

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Mol	Chain	Res	Type
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2637	A
1	A	2648	U
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2718	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2914	A
2	B	3002	U
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3040	C
2	B	3041	C
2	B	3043	G

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Mol	Chain	Res	Type
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3094	G
2	B	3114	G
2	B	3122	C

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C
1	A	338	C
1	A	542	A
1	A	603	A
1	A	644	G
1	A	681	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	869	G
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1137	G
1	A	1164	U
1	A	1165	G
1	A	1232	A
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1438	G
1	A	1446	U
1	A	1450	C
1	A	1504	A
1	A	1563	G

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Mol	Chain	Res	Type
1	A	1667	A
1	A	1692	C
1	A	1738	C
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2005	G
1	A	2011	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2649	A
1	A	2718	C
1	A	2791	U
2	B	3023	U
2	B	3024	U
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 234 ligands modelled in this entry, 232 are monoatomic - leaving 2 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	$\#\|Z\|>2$
37	PUY	5	78	36	32,37,37	3.07	12 (37%)	33,53,53	2.02	9 (27%)
36	PO4	5	77	3,37	0,2,4	-	-	0,1,6	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PUY	5	78	36	-	4/20/40/40	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	78	PUY	CE2-CZ	7.77	1.54	1.38
37	5	78	PUY	CD1-CG	6.66	1.53	1.38
37	5	78	PUY	CD2-CG	6.07	1.51	1.38
37	5	78	PUY	C-N3'	6.02	1.47	1.34
37	5	78	PUY	OM-CMZ	-4.70	1.28	1.42
37	5	78	PUY	CE1-CZ	4.59	1.47	1.38
37	5	78	PUY	C9-N6	-4.13	1.36	1.45
37	5	78	PUY	C10-N6	-3.65	1.37	1.45
37	5	78	PUY	CE1-CD1	2.54	1.43	1.38
37	5	78	PUY	CB-CG	2.54	1.57	1.51
37	5	78	PUY	C8-N7	-2.21	1.30	1.34
37	5	78	PUY	OM-CZ	2.02	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	5	78	PUY	CG-CB-CA	-5.27	103.18	114.13
37	5	78	PUY	CMZ-OM-CZ	5.08	128.54	117.51
37	5	78	PUY	O-C-N3'	-4.19	115.18	122.93
37	5	78	PUY	CB-CA-C	-3.14	101.63	108.97
37	5	78	PUY	C3'-N3'-C	-2.90	118.83	123.21
37	5	78	PUY	CE1-CD1-CG	-2.73	117.27	121.03
37	5	78	PUY	CD2-CG-CD1	2.47	122.05	118.17
37	5	78	PUY	C-CA-N	-2.47	99.86	109.40
37	5	78	PUY	CB-CG-CD1	-2.33	116.27	120.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	5	78	PUY	N3'-C-CA-CB
37	5	78	PUY	C3'-C4'-C5'-O5'
37	5	78	PUY	O-C-N3'-C3'
37	5	78	PUY	O4'-C4'-C5'-O5'

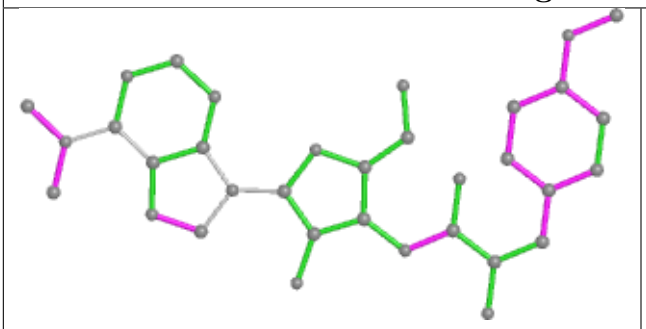
There are no ring outliers.

1 monomer is involved in 1 short contact:

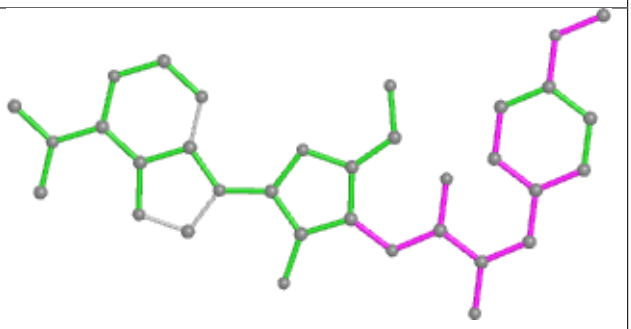
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PO4	1	0

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 then 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.

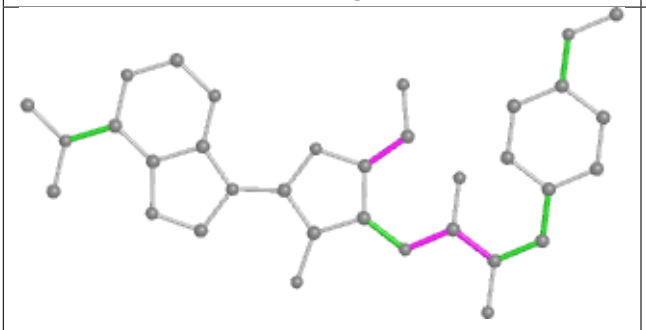
Ligand PUY 5 78



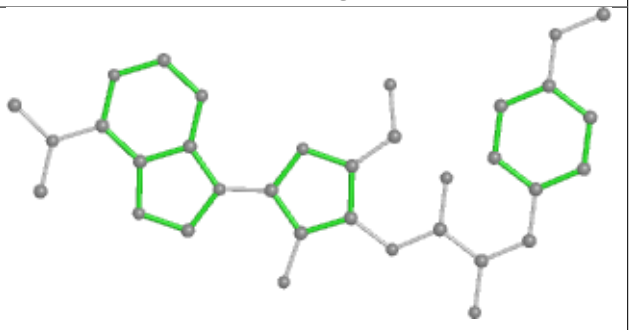
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	A	2754/2922 (94%)	-0.20	32 (1%) 79 67	24, 50, 96, 142	0
2	B	122/122 (100%)	0.04	4 (3%) 46 30	36, 65, 94, 147	0
3	5	3/3 (100%)	-0.00	0 100 100	53, 53, 56, 62	0
4	C	237/239 (99%)	0.11	10 (4%) 36 23	29, 59, 91, 111	0
5	D	337/337 (100%)	-0.20	1 (0%) 94 92	23, 55, 83, 90	0
6	E	246/246 (100%)	-0.21	0 100 100	29, 54, 76, 85	0
7	F	140/176 (79%)	1.04	26 (18%) 1 1	62, 101, 118, 131	0
8	G	172/177 (97%)	0.31	4 (2%) 60 47	40, 69, 91, 96	0
9	H	119/119 (100%)	0.55	10 (8%) 11 6	58, 81, 101, 106	0
10	I	29/348 (8%)	1.63	11 (37%) 0 0	82, 96, 102, 103	0
11	J	156/167 (93%)	-0.08	1 (0%) 89 83	33, 54, 85, 93	0
12	K	142/145 (97%)	-0.26	0 100 100	32, 48, 71, 87	0
13	L	132/132 (100%)	-0.28	0 100 100	28, 51, 73, 82	0
14	M	145/164 (88%)	0.66	28 (19%) 1 1	24, 76, 110, 119	0
15	N	194/194 (100%)	-0.23	0 100 100	37, 52, 69, 78	0
16	O	186/186 (100%)	0.37	13 (6%) 16 9	43, 70, 109, 120	0
17	P	115/115 (100%)	-0.11	0 100 100	48, 61, 81, 85	0
18	Q	143/148 (96%)	0.03	1 (0%) 87 81	40, 62, 75, 80	0
19	R	95/95 (100%)	-0.15	0 100 100	29, 49, 59, 74	0
20	S	150/154 (97%)	-0.30	0 100 100	31, 47, 66, 72	0
21	T	81/84 (96%)	0.10	3 (3%) 41 26	53, 70, 85, 90	0
22	U	119/119 (100%)	0.46	4 (3%) 45 29	48, 63, 85, 94	0
23	V	53/66 (80%)	-0.13	0 100 100	43, 57, 74, 81	0
24	W	65/70 (92%)	0.72	5 (7%) 13 7	61, 81, 110, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	154/154 (100%)	-0.40	0 100 100	37, 49, 67, 76	0
26	Y	82/91 (90%)	0.11	3 (3%) 41 26	38, 62, 81, 97	0
27	Z	142/240 (59%)	-0.12	1 (0%) 87 81	30, 51, 74, 89	0
28	1	73/73 (100%)	-0.04	2 (2%) 54 39	52, 66, 80, 84	0
29	2	56/56 (100%)	-0.31	0 100 100	25, 40, 46, 48	0
30	3	46/48 (95%)	0.09	0 100 100	43, 65, 86, 95	0
31	4	92/92 (100%)	0.30	5 (5%) 25 14	36, 62, 72, 78	0
All	All	6580/7282 (90%)	-0.05	164 (2%) 57 43	23, 56, 97, 147	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	M	104	ASP	6.4
16	O	186	LEU	5.4
10	I	27	ILE	5.3
14	M	105	TYR	5.0
10	I	23	ILE	4.5
2	B	3001	U	4.5
22	U	119	ALA	4.4
24	W	1	THR	4.3
1	A	1172	G	4.2
1	A	735	C	4.2
7	F	57	THR	4.2
1	A	1177	A	4.1
24	W	43	PRO	4.1
14	M	59	GLU	4.0
7	F	18	ILE	3.9
14	M	97	VAL	3.8
7	F	26	GLY	3.8
9	H	102	GLY	3.8
1	A	1173	A	3.7
2	B	3122	C	3.7
9	H	101	ALA	3.7
10	I	24	VAL	3.7
7	F	69	ILE	3.6
10	I	20	VAL	3.6
14	M	106	VAL	3.6
14	M	60	GLU	3.5
14	M	91	VAL	3.5
9	H	19	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1525	G	3.5
14	M	61	ALA	3.5
2	B	3023	U	3.4
4	C	32	VAL	3.4
2	B	3025	G	3.4
1	A	282	C	3.3
4	C	37	VAL	3.3
1	A	1175	G	3.3
28	1	59	HIS	3.2
7	F	134	LEU	3.2
24	W	39	ALA	3.2
9	H	106	THR	3.2
1	A	1171	A	3.1
1	A	1951	G	3.1
16	O	147	ILE	3.1
24	W	38	GLY	3.1
14	M	93	VAL	3.1
14	M	73	VAL	3.0
7	F	24	HIS	3.0
7	F	44	ILE	3.0
1	A	2238	A	3.0
1	A	1198	U	3.0
14	M	96	VAL	3.0
7	F	25	MET	2.9
14	M	58	GLN	2.9
16	O	159	TYR	2.9
14	M	79	ASP	2.9
7	F	88	LEU	2.9
5	D	1	PRO	2.9
31	4	72	GLY	2.8
14	M	140	VAL	2.8
7	F	62	ASP	2.8
7	F	49	PRO	2.8
16	O	162	ASP	2.8
14	M	89	PHE	2.8
1	A	2237	G	2.8
16	O	146	HIS	2.7
1	A	285	A	2.7
9	H	16	ALA	2.7
10	I	64	ASN	2.6
10	I	28	GLU	2.6
7	F	41	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1526	A	2.6
14	M	142	LEU	2.6
27	Z	108	ASP	2.6
1	A	970	U	2.6
16	O	157	PRO	2.6
7	F	56	ARG	2.6
1	A	1162	G	2.6
14	M	62	ALA	2.6
10	I	12	ILE	2.6
10	I	65	THR	2.5
14	M	100	ALA	2.5
14	M	57	VAL	2.5
7	F	84	LEU	2.5
22	U	99	THR	2.5
4	C	31	LYS	2.5
16	O	160	SER	2.5
1	A	1205	U	2.5
1	A	1279	U	2.5
7	F	73	VAL	2.5
16	O	140	GLN	2.5
31	4	92	GLU	2.5
7	F	58	VAL	2.5
16	O	67	ALA	2.5
7	F	40	ILE	2.5
7	F	68	PRO	2.5
7	F	17	ARG	2.5
31	4	62	THR	2.5
1	A	960	G	2.5
14	M	76	LEU	2.4
9	H	99	THR	2.4
14	M	80	ASP	2.4
1	A	130	C	2.4
1	A	1188	A	2.4
16	O	183	ASP	2.4
4	C	97	ALA	2.4
9	H	103	ALA	2.4
1	A	2004	U	2.4
31	4	22	VAL	2.4
1	A	1527	A	2.4
9	H	22	VAL	2.4
1	A	2249	G	2.4
8	G	154	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
11	J	72	VAL	2.4
1	A	713	U	2.3
21	T	67	ARG	2.3
16	O	143	ARG	2.3
9	H	100	ASP	2.3
7	F	87	ALA	2.3
14	M	144	ASP	2.3
4	C	98	GLU	2.3
28	1	44	PHE	2.3
8	G	100	ASP	2.3
9	H	26	THR	2.2
24	W	41	GLU	2.2
14	M	123	ASP	2.2
14	M	120	LEU	2.2
22	U	35	TYR	2.2
7	F	106	PHE	2.2
18	Q	57	ASN	2.2
4	C	65	ARG	2.2
7	F	63	ILE	2.2
21	T	81	ILE	2.2
7	F	85	GLN	2.1
4	C	38	ILE	2.1
4	C	35	GLY	2.1
14	M	94	ARG	2.1
7	F	92	GLU	2.1
8	G	122	THR	2.1
26	Y	9	VAL	2.1
4	C	36	ASP	2.1
16	O	137	ALA	2.1
1	A	2239	C	2.1
22	U	42	VAL	2.1
10	I	17	GLN	2.1
31	4	65	THR	2.1
14	M	127	GLU	2.1
8	G	124	VAL	2.1
16	O	138	ASP	2.1
4	C	237	GLY	2.1
26	Y	10	VAL	2.1
1	A	1161	A	2.1
7	F	10	PHE	2.0
1	A	284	C	2.0
10	I	26	MET	2.0

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Mol	Chain	Res	Type	RSRZ
21	T	50	GLU	2.0
1	A	1199	A	2.0
14	M	125	PHE	2.0
26	Y	41	PHE	2.0
14	M	92	ASP	2.0
7	F	27	ILE	2.0
10	I	69	ARG	2.0
1	A	1190	G	2.0
1	A	1665	G	2.0
1	A	1204	C	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
34	NA	A	8384	1/1	0.23	0.79	103,103,103,103	0
34	NA	A	8370	1/1	0.47	0.40	93,93,93,93	0
34	NA	S	8386	1/1	0.51	0.47	48,48,48,48	0
34	NA	B	8351	1/1	0.54	0.26	67,67,67,67	0
34	NA	B	8383	1/1	0.60	0.26	63,63,63,63	0
35	CL	A	8505	1/1	0.67	0.30	65,65,65,65	0
34	NA	T	8312	1/1	0.71	0.57	122,122,122,122	0
34	NA	A	8323	1/1	0.71	0.49	62,62,62,62	0
35	CL	O	8507	1/1	0.71	0.51	102,102,102,102	0
35	CL	4	8504	1/1	0.71	0.35	69,69,69,69	0
35	CL	P	8508	1/1	0.72	0.62	113,113,113,113	0
32	MG	A	8103	1/1	0.75	0.39	57,57,57,57	0
32	MG	A	8066	1/1	0.75	0.27	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8303	1/1	0.76	0.41	42,42,42,42	0
35	CL	A	8511	1/1	0.77	0.42	92,92,92,92	0
34	NA	A	8371	1/1	0.78	0.23	32,32,32,32	0
32	MG	A	8089	1/1	0.79	0.25	104,104,104,104	0
34	NA	A	8382	1/1	0.81	0.46	52,52,52,52	0
35	CL	A	8510	1/1	0.81	0.71	101,101,101,101	0
34	NA	A	8366	1/1	0.82	0.19	58,58,58,58	0
32	MG	A	8070	1/1	0.82	0.79	101,101,101,101	0
32	MG	Z	8109	1/1	0.82	0.12	32,32,32,32	0
34	NA	A	8357	1/1	0.84	0.07	43,43,43,43	0
32	MG	A	8052	1/1	0.84	0.14	24,24,24,24	0
32	MG	A	8100	1/1	0.84	0.13	51,51,51,51	0
34	NA	A	8341	1/1	0.84	0.14	40,40,40,40	0
32	MG	A	8046	1/1	0.85	0.13	62,62,62,62	0
32	MG	1	8105	1/1	0.85	0.33	32,32,32,32	0
35	CL	A	8515	1/1	0.85	0.46	131,131,131,131	0
34	NA	J	8322	1/1	0.86	0.17	26,26,26,26	0
35	CL	A	8513	1/1	0.86	0.35	81,81,81,81	0
34	NA	A	8333	1/1	0.86	0.10	14,14,14,14	0
32	MG	A	8116	1/1	0.86	0.23	95,95,95,95	0
33	K	A	8201	1/1	0.86	0.22	76,76,76,76	0
35	CL	S	8506	1/1	0.86	0.29	77,77,77,77	0
34	NA	A	8375	1/1	0.86	0.56	42,42,42,42	0
34	NA	A	8360	1/1	0.87	0.44	37,37,37,37	0
34	NA	A	8307	1/1	0.87	0.17	34,34,34,34	0
34	NA	A	8359	1/1	0.87	0.46	47,47,47,47	0
32	MG	L	8069	1/1	0.88	0.13	105,105,105,105	0
32	MG	A	8115	1/1	0.88	0.17	51,51,51,51	0
32	MG	A	8102	1/1	0.88	0.19	83,83,83,83	0
34	NA	A	8363	1/1	0.88	0.39	100,100,100,100	0
37	PUY	5	78	34/34	0.88	0.37	66,69,74,75	0
34	NA	A	8326	1/1	0.89	0.17	35,35,35,35	0
35	CL	A	8503	1/1	0.89	0.24	62,62,62,62	0
34	NA	S	8337	1/1	0.89	0.28	70,70,70,70	0
34	NA	A	8365	1/1	0.89	0.20	29,29,29,29	0
32	MG	A	8018	1/1	0.90	0.13	24,24,24,24	0
34	NA	A	8368	1/1	0.90	0.08	35,35,35,35	0
32	MG	A	8108	1/1	0.90	0.10	50,50,50,50	0
32	MG	A	8064	1/1	0.90	0.17	31,31,31,31	0
32	MG	A	8085	1/1	0.90	0.12	39,39,39,39	0
34	NA	A	8328	1/1	0.90	0.26	52,52,52,52	0
34	NA	A	8329	1/1	0.90	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8332	1/1	0.90	0.26	37,37,37,37	0
32	MG	A	8042	1/1	0.91	0.09	25,25,25,25	0
34	NA	A	8355	1/1	0.91	0.23	60,60,60,60	0
32	MG	A	8033	1/1	0.91	0.10	42,42,42,42	0
35	CL	A	8517	1/1	0.91	0.24	61,61,61,61	0
35	CL	K	8502	1/1	0.91	0.27	91,91,91,91	0
32	MG	A	8092	1/1	0.91	0.20	58,58,58,58	0
34	NA	A	8330	1/1	0.91	0.14	36,36,36,36	0
34	NA	A	8362	1/1	0.91	0.27	38,38,38,38	0
34	NA	A	8316	1/1	0.91	0.23	42,42,42,42	0
32	MG	A	8075	1/1	0.91	0.07	42,42,42,42	0
32	MG	A	8044	1/1	0.92	0.23	68,68,68,68	0
35	CL	A	8522	1/1	0.92	0.44	57,57,57,57	0
35	CL	C	8509	1/1	0.92	0.20	66,66,66,66	0
34	NA	A	8385	1/1	0.92	0.25	22,22,22,22	0
34	NA	A	8369	1/1	0.92	0.30	49,49,49,49	0
32	MG	A	8034	1/1	0.92	0.04	50,50,50,50	0
34	NA	A	8356	1/1	0.92	0.60	86,86,86,86	0
32	MG	A	8030	1/1	0.92	0.13	68,68,68,68	0
34	NA	A	8339	1/1	0.92	0.08	30,30,30,30	0
32	MG	A	8104	1/1	0.93	0.11	31,31,31,31	0
34	NA	A	8377	1/1	0.93	0.36	70,70,70,70	0
35	CL	A	8512	1/1	0.93	0.13	30,30,30,30	0
32	MG	A	8024	1/1	0.93	1.03	108,108,108,108	0
33	K	A	8202	1/1	0.93	0.16	56,56,56,56	0
34	NA	A	8302	1/1	0.93	0.17	25,25,25,25	0
32	MG	A	8028	1/1	0.93	0.10	75,75,75,75	0
32	MG	A	8041	1/1	0.93	0.18	80,80,80,80	0
34	NA	A	8336	1/1	0.93	0.09	51,51,51,51	0
34	NA	A	8308	1/1	0.93	0.09	40,40,40,40	0
34	NA	A	8314	1/1	0.93	0.12	29,29,29,29	0
32	MG	A	8001	1/1	0.93	0.09	31,31,31,31	0
35	CL	Z	8520	1/1	0.93	0.21	64,64,64,64	0
32	MG	A	8087	1/1	0.93	0.19	41,41,41,41	0
34	NA	A	8372	1/1	0.93	0.18	25,25,25,25	0
38	CD	P	8405	1/1	0.93	0.33	196,196,196,196	0
32	MG	A	8099	1/1	0.94	0.14	43,43,43,43	0
34	NA	A	8313	1/1	0.94	0.14	47,47,47,47	0
32	MG	5	8114	1/1	0.94	0.20	44,44,44,44	0
34	NA	A	8343	1/1	0.94	0.07	9,9,9,9	0
34	NA	A	8354	1/1	0.94	0.17	16,16,16,16	0
34	NA	A	8315	1/1	0.94	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8076	1/1	0.94	0.43	134,134,134,134	0
32	MG	A	8053	1/1	0.94	0.12	85,85,85,85	0
32	MG	A	8060	1/1	0.94	0.23	43,43,43,43	0
34	NA	A	8327	1/1	0.94	0.19	24,24,24,24	0
35	CL	K	8521	1/1	0.94	0.18	47,47,47,47	0
32	MG	A	8071	1/1	0.94	0.07	52,52,52,52	0
34	NA	E	8304	1/1	0.94	0.09	4,4,4,4	0
32	MG	A	8107	1/1	0.94	0.03	46,46,46,46	0
32	MG	A	8050	1/1	0.94	0.11	41,41,41,41	0
32	MG	A	8113	1/1	0.94	0.10	29,29,29,29	0
34	NA	A	8367	1/1	0.94	0.10	22,22,22,22	0
32	MG	A	8097	1/1	0.94	0.52	64,64,64,64	0
34	NA	A	8353	1/1	0.95	0.07	13,13,13,13	0
34	NA	C	8345	1/1	0.95	0.17	68,68,68,68	0
32	MG	A	8055	1/1	0.95	0.12	29,29,29,29	0
32	MG	A	8094	1/1	0.95	0.09	50,50,50,50	0
34	NA	M	8380	1/1	0.95	0.35	73,73,73,73	0
32	MG	A	8056	1/1	0.95	0.20	75,75,75,75	0
32	MG	B	8095	1/1	0.95	0.17	85,85,85,85	0
32	MG	A	8072	1/1	0.95	0.26	55,55,55,55	0
34	NA	A	8317	1/1	0.95	0.06	25,25,25,25	0
34	NA	A	8319	1/1	0.95	0.11	43,43,43,43	0
32	MG	C	8065	1/1	0.95	0.09	85,85,85,85	0
32	MG	A	8059	1/1	0.95	0.13	119,119,119,119	0
32	MG	U	8073	1/1	0.95	0.14	21,21,21,21	0
32	MG	A	8027	1/1	0.95	0.06	60,60,60,60	0
32	MG	A	8045	1/1	0.95	0.14	63,63,63,63	0
32	MG	4	8078	1/1	0.95	0.07	23,23,23,23	0
32	MG	A	8035	1/1	0.95	0.07	70,70,70,70	0
32	MG	A	8106	1/1	0.95	0.12	69,69,69,69	0
35	CL	D	8519	1/1	0.95	0.33	55,55,55,55	0
35	CL	K	8501	1/1	0.95	0.12	55,55,55,55	0
34	NA	A	8301	1/1	0.95	0.14	22,22,22,22	0
34	NA	A	8373	1/1	0.95	0.07	36,36,36,36	0
34	NA	A	8374	1/1	0.95	0.29	46,46,46,46	0
32	MG	A	8068	1/1	0.95	0.09	44,44,44,44	0
34	NA	A	8340	1/1	0.95	0.23	29,29,29,29	0
32	MG	A	8090	1/1	0.95	0.22	46,46,46,46	0
32	MG	A	8111	1/1	0.95	0.26	82,82,82,82	0
34	NA	A	8344	1/1	0.95	0.06	11,11,11,11	0
34	NA	A	8350	1/1	0.95	0.22	18,18,18,18	0
32	MG	A	8039	1/1	0.96	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8088	1/1	0.96	0.10	12,12,12,12	0
32	MG	A	8051	1/1	0.96	0.10	93,93,93,93	0
34	NA	A	8364	1/1	0.96	0.18	12,12,12,12	0
32	MG	A	8021	1/1	0.96	0.10	46,46,46,46	0
32	MG	A	8032	1/1	0.96	0.07	23,23,23,23	0
32	MG	A	8112	1/1	0.96	0.18	58,58,58,58	0
32	MG	A	8043	1/1	0.96	0.07	50,50,50,50	0
34	NA	A	8334	1/1	0.96	0.06	30,30,30,30	0
34	NA	A	8305	1/1	0.96	0.08	10,10,10,10	0
32	MG	A	8096	1/1	0.96	0.16	33,33,33,33	0
32	MG	A	8006	1/1	0.96	0.05	33,33,33,33	0
34	NA	A	8311	1/1	0.96	0.19	43,43,43,43	0
34	NA	A	8342	1/1	0.96	0.18	30,30,30,30	0
32	MG	A	8117	1/1	0.96	0.08	1,1,1,1	0
32	MG	A	8098	1/1	0.96	0.24	47,47,47,47	0
34	NA	A	8381	1/1	0.96	0.11	51,51,51,51	0
32	MG	A	8057	1/1	0.96	0.11	15,15,15,15	0
32	MG	A	8014	1/1	0.96	0.10	18,18,18,18	0
32	MG	A	8101	1/1	0.96	0.13	49,49,49,49	0
32	MG	A	8081	1/1	0.96	0.15	29,29,29,29	0
34	NA	A	8320	1/1	0.96	0.09	29,29,29,29	0
32	MG	A	8005	1/1	0.96	0.10	68,68,68,68	0
36	PO4	5	77	3/5	0.96	0.12	67,67,68,68	0
34	NA	A	8358	1/1	0.96	0.49	109,109,109,109	0
34	NA	A	8325	1/1	0.96	0.13	48,48,48,48	0
32	MG	A	8015	1/1	0.97	0.07	66,66,66,66	0
34	NA	A	8321	1/1	0.97	0.22	52,52,52,52	0
34	NA	A	8378	1/1	0.97	0.21	18,18,18,18	0
34	NA	A	8379	1/1	0.97	0.14	33,33,33,33	0
34	NA	A	8361	1/1	0.97	0.22	35,35,35,35	0
32	MG	A	8067	1/1	0.97	0.12	22,22,22,22	0
34	NA	A	8324	1/1	0.97	0.10	32,32,32,32	0
34	NA	A	8310	1/1	0.97	0.15	22,22,22,22	0
32	MG	A	8083	1/1	0.97	0.04	32,32,32,32	0
32	MG	A	8049	1/1	0.97	0.30	49,49,49,49	0
32	MG	A	8017	1/1	0.97	0.04	40,40,40,40	0
34	NA	A	8352	1/1	0.97	0.15	17,17,17,17	0
34	NA	J	8309	1/1	0.97	0.15	21,21,21,21	0
32	MG	A	8011	1/1	0.97	0.05	27,27,27,27	0
34	NA	K	8346	1/1	0.97	0.14	7,7,7,7	0
32	MG	A	8110	1/1	0.97	0.17	54,54,54,54	0
34	NA	N	8347	1/1	0.97	0.10	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8331	1/1	0.97	0.19	35,35,35,35	0
32	MG	A	8004	1/1	0.97	0.05	43,43,43,43	0
34	NA	A	8318	1/1	0.97	0.15	65,65,65,65	0
32	MG	A	8031	1/1	0.97	0.05	29,29,29,29	0
32	MG	A	8093	1/1	0.98	0.10	16,16,16,16	0
32	MG	A	8061	1/1	0.98	0.05	33,33,33,33	0
32	MG	A	8062	1/1	0.98	0.07	38,38,38,38	0
32	MG	A	8063	1/1	0.98	0.12	64,64,64,64	0
34	NA	R	8348	1/1	0.98	0.07	18,18,18,18	0
32	MG	A	8016	1/1	0.98	0.08	23,23,23,23	0
34	NA	S	8338	1/1	0.98	0.21	65,65,65,65	0
32	MG	A	8029	1/1	0.98	0.12	34,34,34,34	0
32	MG	A	8010	1/1	0.98	0.09	26,26,26,26	0
32	MG	A	8003	1/1	0.98	0.13	30,30,30,30	0
32	MG	A	8048	1/1	0.98	0.09	33,33,33,33	0
32	MG	A	8019	1/1	0.98	0.07	31,31,31,31	0
34	NA	A	8335	1/1	0.98	0.23	43,43,43,43	0
34	NA	A	8306	1/1	0.98	0.39	35,35,35,35	0
32	MG	A	8013	1/1	0.98	0.15	21,21,21,21	0
35	CL	A	8514	1/1	0.98	0.15	45,45,45,45	0
32	MG	A	8022	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8023	1/1	0.98	0.07	35,35,35,35	0
32	MG	A	8079	1/1	0.98	0.08	25,25,25,25	0
34	NA	A	8376	1/1	0.98	0.12	27,27,27,27	0
32	MG	A	8036	1/1	0.98	0.06	29,29,29,29	0
32	MG	A	8082	1/1	0.98	0.07	16,16,16,16	0
34	NA	A	8349	1/1	0.98	0.21	25,25,25,25	0
32	MG	A	8054	1/1	0.98	0.10	46,46,46,46	0
35	CL	N	8518	1/1	0.98	0.15	50,50,50,50	0
32	MG	A	8037	1/1	0.98	0.09	41,41,41,41	0
32	MG	A	8086	1/1	0.98	0.11	75,75,75,75	0
32	MG	A	8002	1/1	0.98	0.06	15,15,15,15	0
32	MG	A	8040	1/1	0.98	0.07	33,33,33,33	0
32	MG	A	8058	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8025	1/1	0.98	0.05	12,12,12,12	0
32	MG	A	8091	1/1	0.98	0.05	65,65,65,65	0
32	MG	A	8008	1/1	0.98	0.12	40,40,40,40	0
38	CD	V	8401	1/1	0.98	0.11	70,70,70,70	0
32	MG	A	8080	1/1	0.99	0.07	38,38,38,38	0
32	MG	A	8020	1/1	0.99	0.07	36,36,36,36	0
32	MG	A	8047	1/1	0.99	0.09	62,62,62,62	0
32	MG	A	8009	1/1	0.99	0.05	14,14,14,14	0

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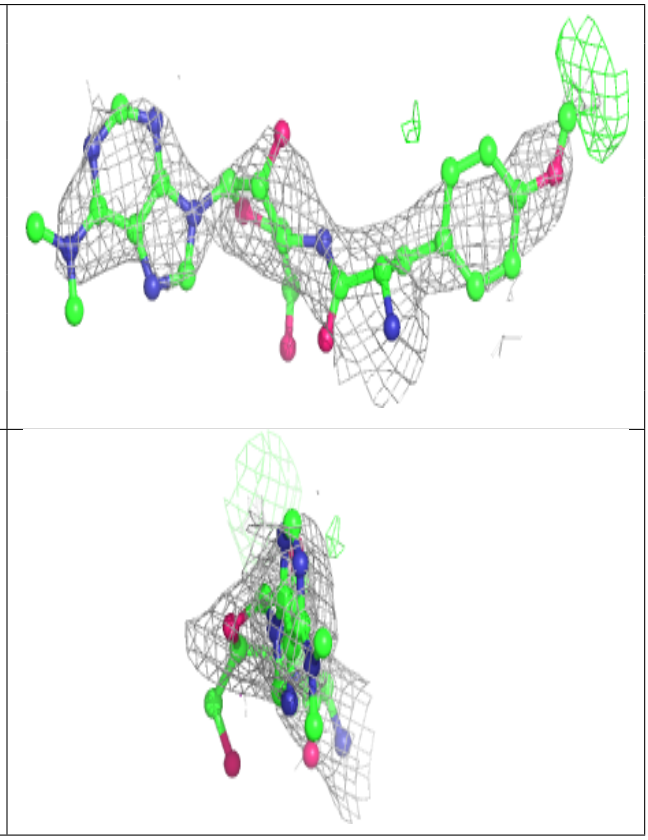
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8084	1/1	0.99	0.03	34,34,34,34	0
32	MG	A	8026	1/1	0.99	0.13	45,45,45,45	0
35	CL	A	8516	1/1	0.99	0.10	37,37,37,37	0
32	MG	A	8074	1/1	0.99	0.07	16,16,16,16	0
32	MG	A	8012	1/1	0.99	0.10	35,35,35,35	0
32	MG	A	8038	1/1	0.99	0.08	43,43,43,43	0
32	MG	A	8077	1/1	0.99	0.11	39,39,39,39	0
32	MG	A	8007	1/1	0.99	0.08	9,9,9,9	0
38	CD	1	8403	1/1	0.99	0.07	88,88,88,88	0
38	CD	2	8402	1/1	0.99	0.07	72,72,72,72	0
38	CD	4	8404	1/1	0.99	0.08	67,67,67,67	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.

Electron density around PUY 5 78:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.