



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 AM UTC

PDB ID : 1K8A / pdb_00001k8a
Title : Co-crystal structure of Carbomycin A bound to the 50S ribosomal subunit of *Haloarcula marismortui*
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.
Deposited on : 2001-10-23
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

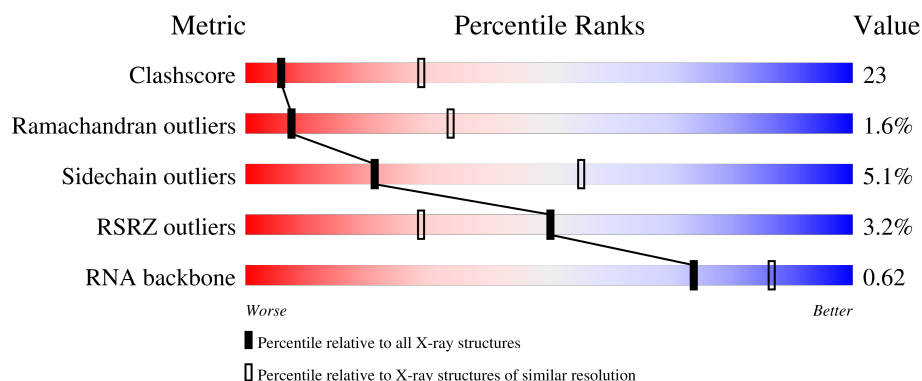
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

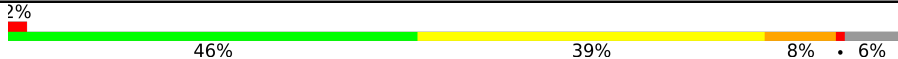
The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	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
33	NA	B	8383	-	-	-	X
34	CL	A	8523	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98560 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	? 3377779

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

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

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 5 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	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 18 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

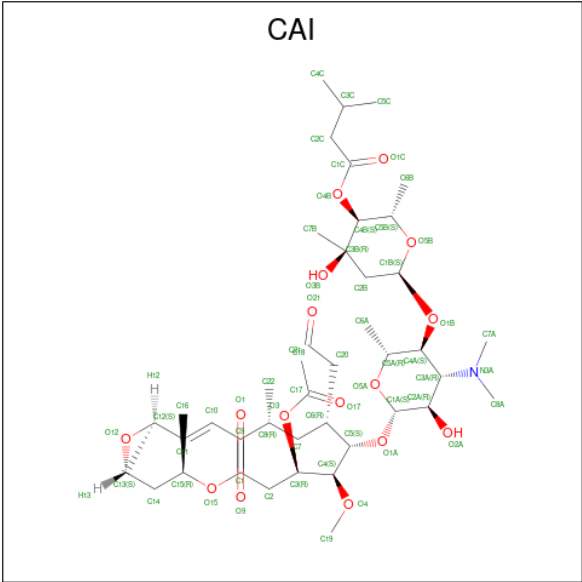
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is CARBOMYCIN A (CCD ID: CAI) (formula: C₄₂H₆₇NO₁₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			59	42	1	16		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	111	Total	Mg	0	0
			111	111		
32	B	1	Total	Mg	0	0
			1	1		
32	C	2	Total	Mg	0	0
			2	2		
32	D	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	69	Total Na 69 69	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	2	Total Na 2 2	0	0
33	R	1	Total Na 1 1	0	0
33	S	1	Total Na 1 1	0	0
33	T	1	Total Na 1 1	0	0
33	U	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	10	Total Cl 10 10	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	Z	1	Total 1	Cl 1	0	0
34	4	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5858	Total 5858	O 5858	0	0
37	B	141	Total 141	O 141	0	0
37	C	138	Total 138	O 138	0	0
37	D	154	Total 154	O 154	0	0
37	E	177	Total 177	O 177	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	49	Total 49	O 49	0	0
37	G	44	Total 44	O 44	0	0
37	H	26	Total 26	O 26	0	0
37	I	21	Total 21	O 21	0	0
37	J	79	Total 79	O 79	0	0
37	K	53	Total 53	O 53	0	0
37	L	59	Total 59	O 59	0	0
37	M	87	Total 87	O 87	0	0
37	N	130	Total 130	O 130	0	0
37	O	69	Total 69	O 69	0	0
37	P	44	Total 44	O 44	0	0
37	Q	68	Total 68	O 68	0	0
37	R	51	Total 51	O 51	0	0
37	S	81	Total 81	O 81	0	0
37	T	37	Total 37	O 37	0	0
37	U	37	Total 37	O 37	0	0
37	V	28	Total 28	O 28	0	0
37	W	14	Total 14	O 14	0	0
37	X	69	Total 69	O 69	0	0
37	Y	28	Total 28	O 28	0	0
37	Z	100	Total 100	O 100	0	0

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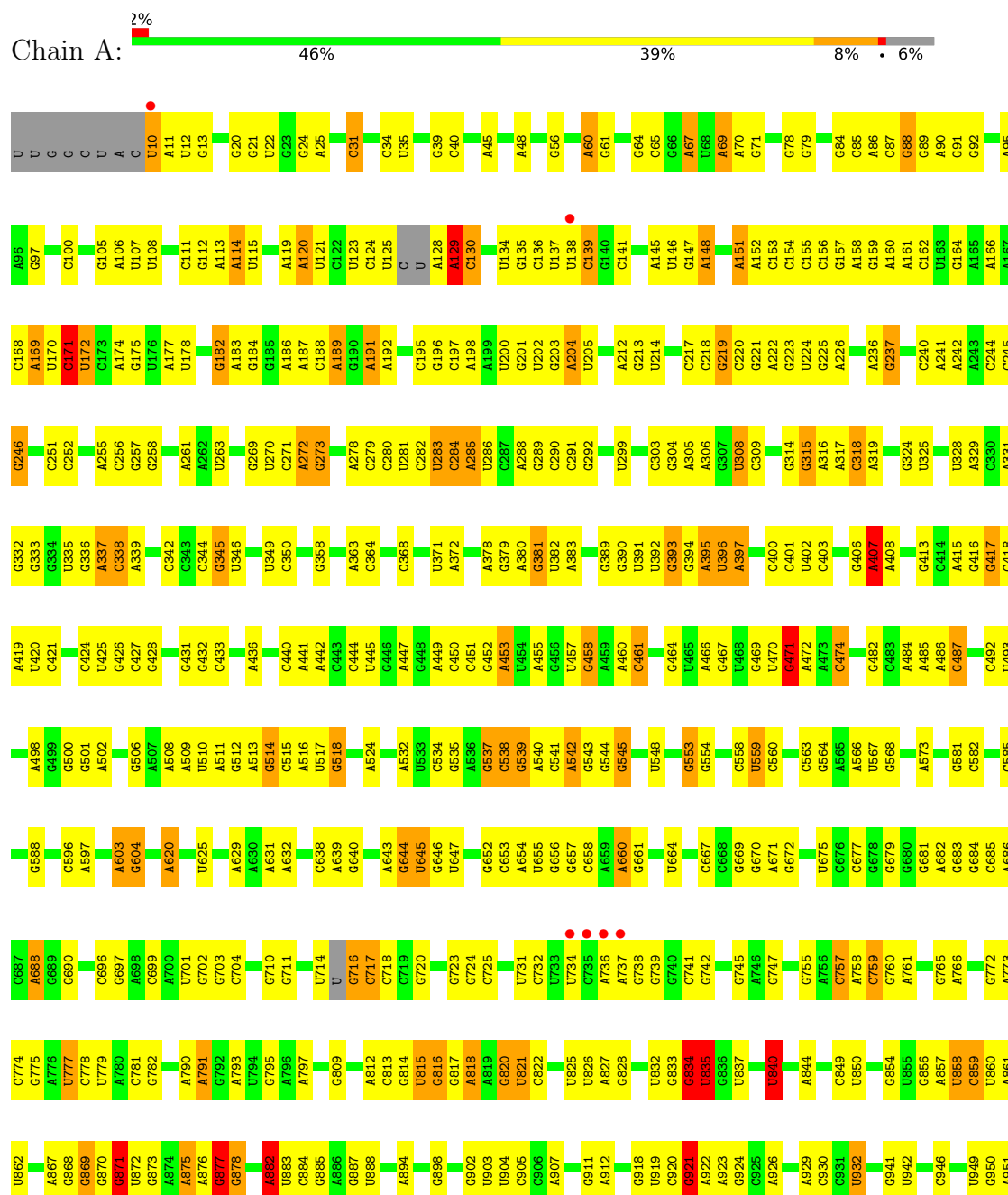
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	41	Total 41	O 41	0	0
37	2	58	Total 58	O 58	0	0
37	3	41	Total 41	O 41	0	0
37	4	68	Total 68	O 68	0	0

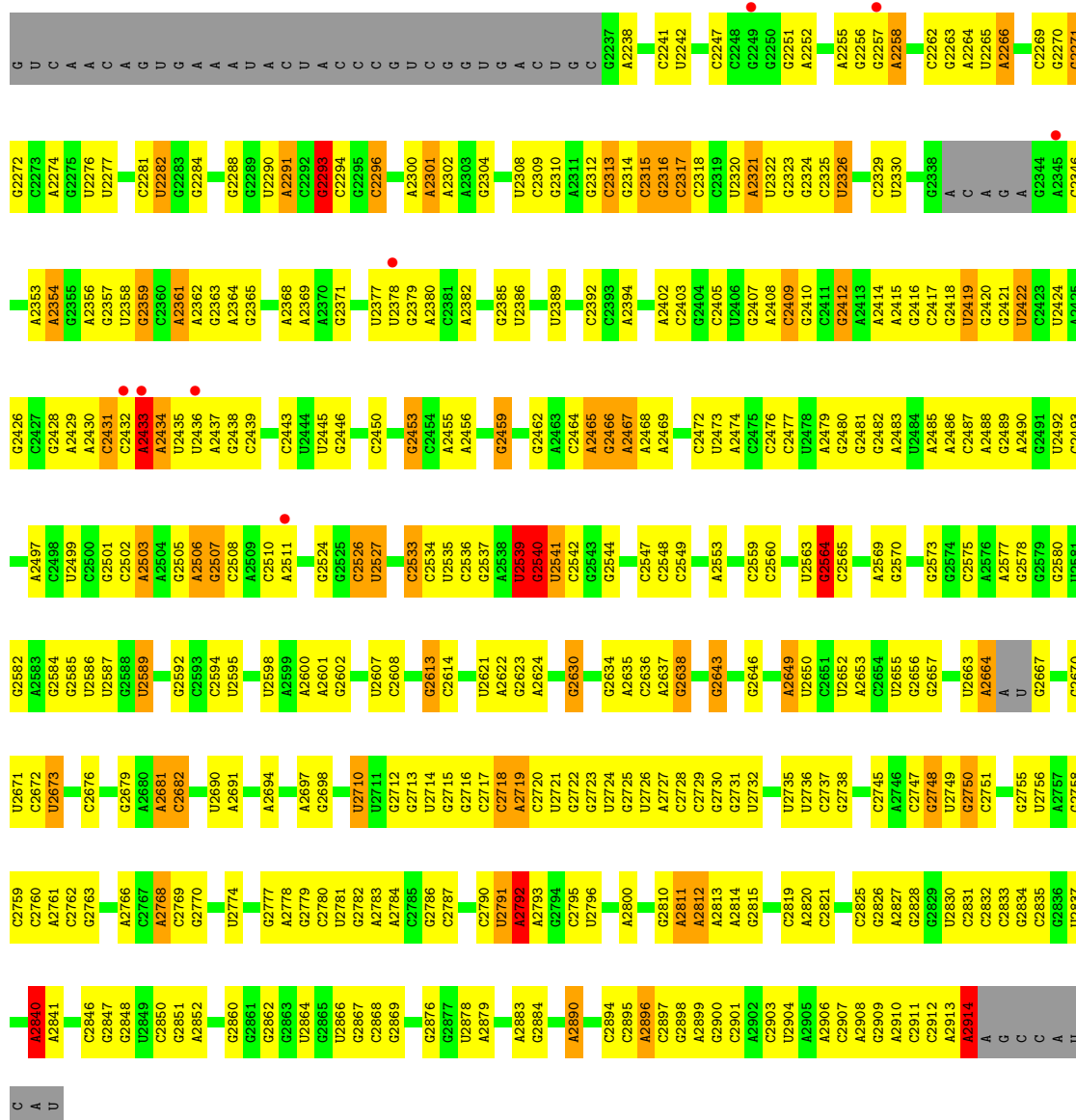
3 Residue-property plots

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

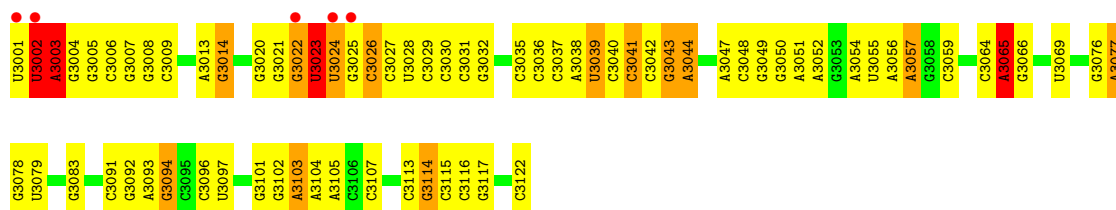
• Molecule 1: 23S rRNA





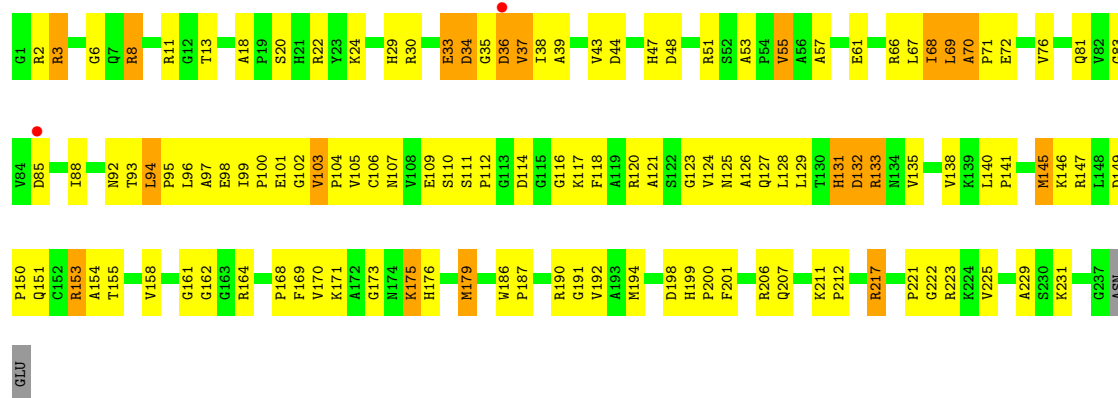


• Molecule 2: 5S rRNA



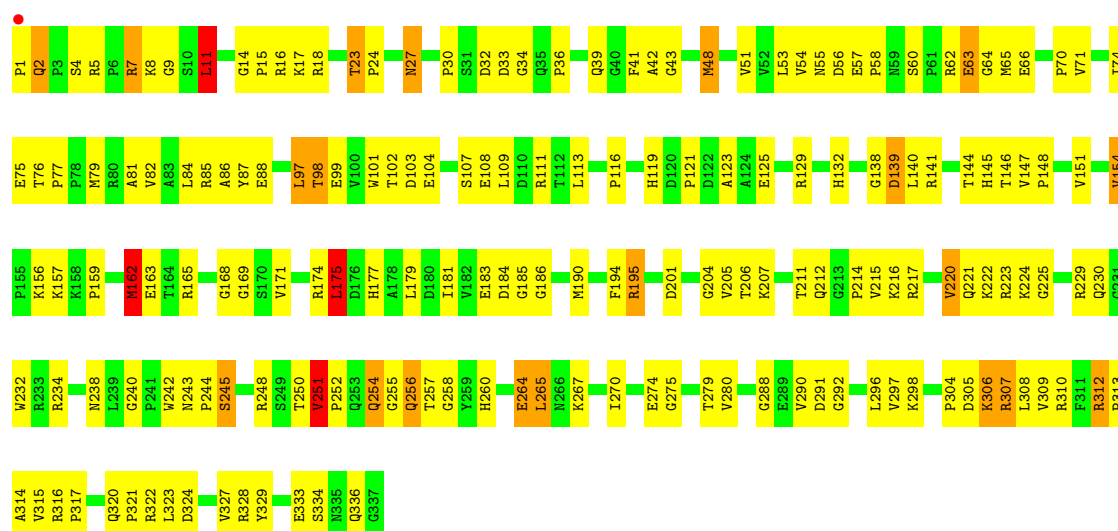
• Molecule 3: RIBOSOMAL PROTEIN L2





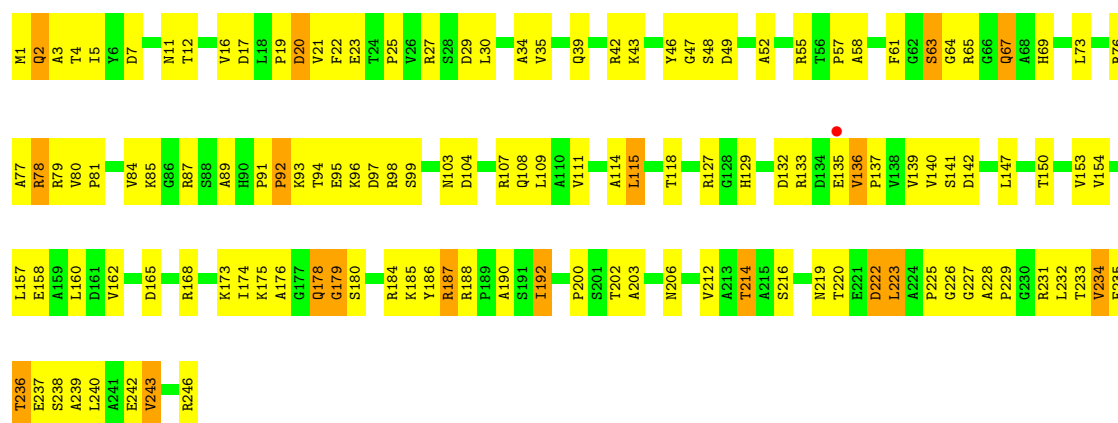
• Molecule 4: RIBOSOMAL PROTEIN L3

Chain D: 47% 46% 6%

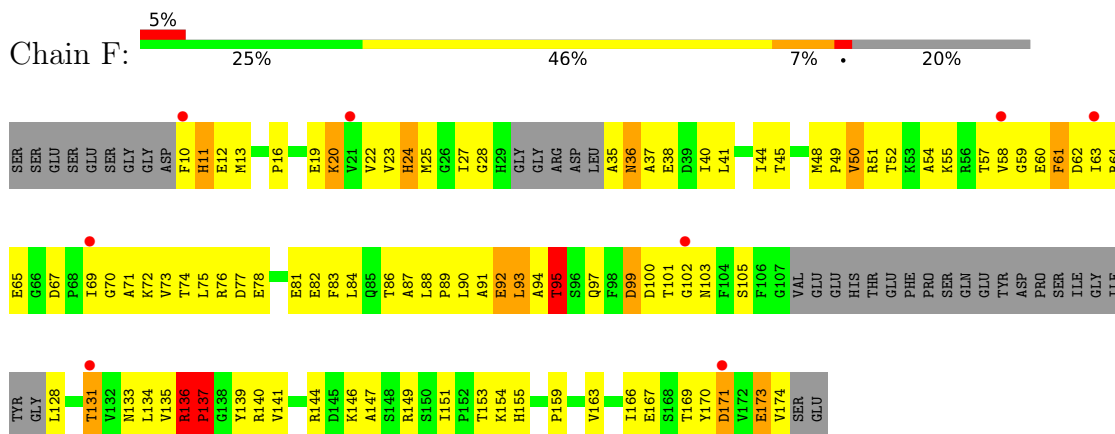


• Molecule 5: RIBOSOMAL PROTEIN L4

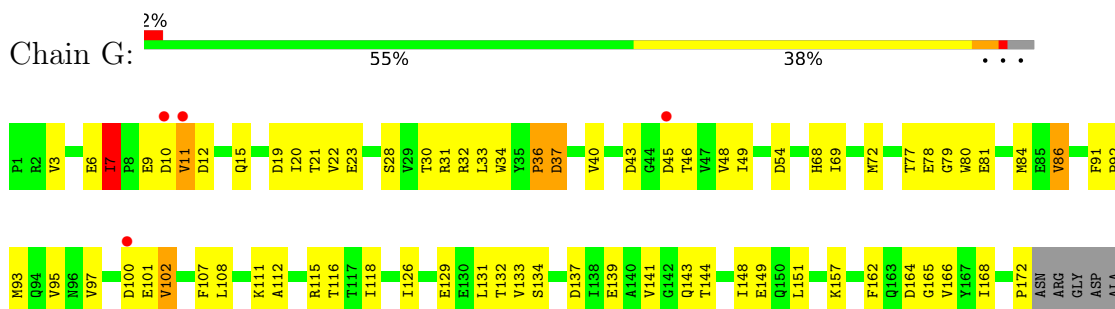
Chain E: 47% 46% 7%



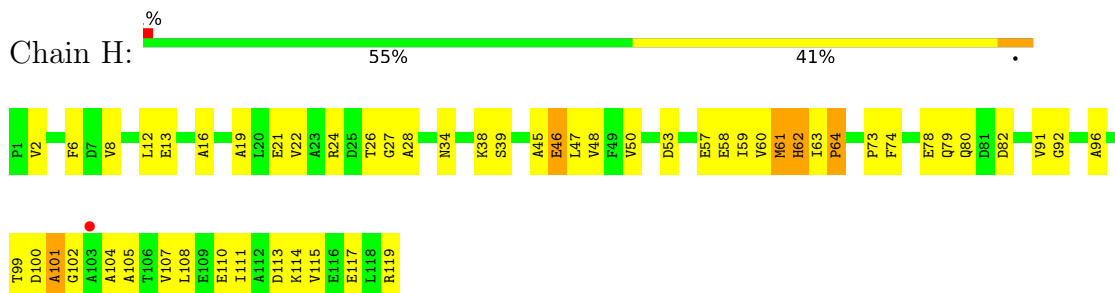
• Molecule 6: RIBOSOMAL PROTEIN L5



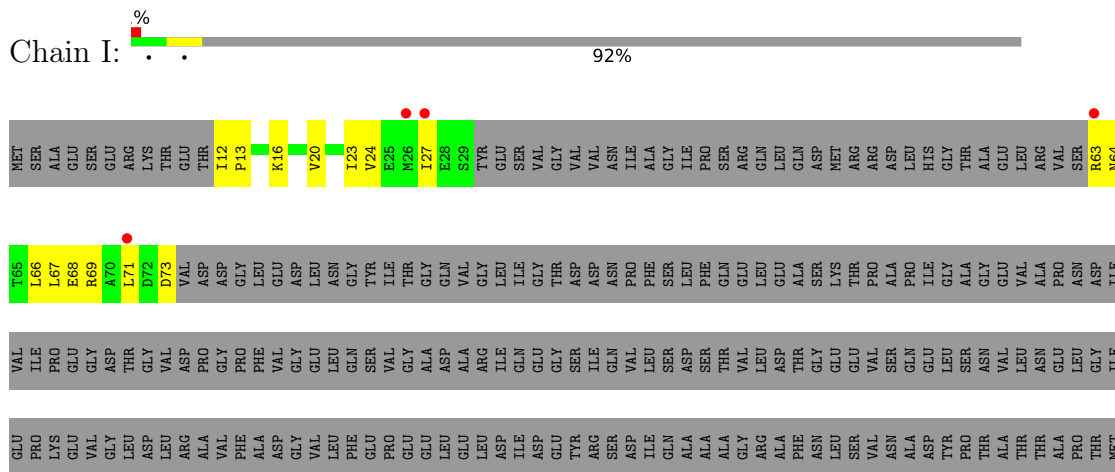
- Molecule 7: RIBOSOMAL PROTEIN L6

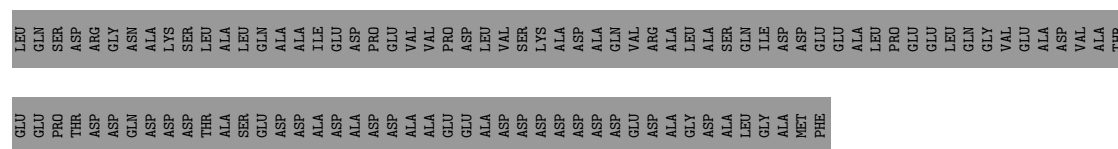


- Molecule 8: RIBOSOMAL PROTEIN L7AE

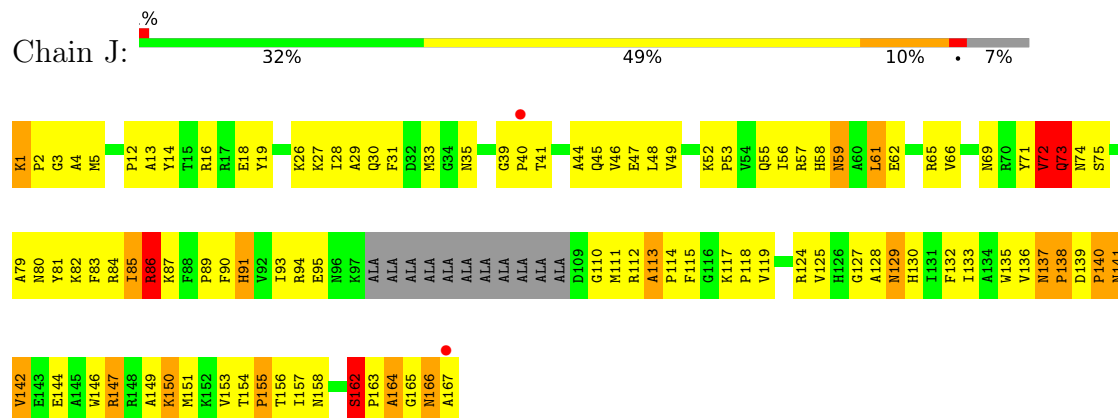


- Molecule 9: RIBOSOMAL PROTEIN L10

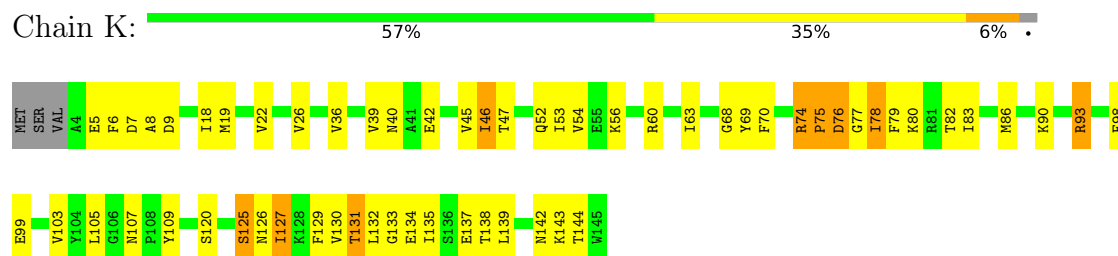




• Molecule 10: RIBOSOMAL PROTEIN L10E



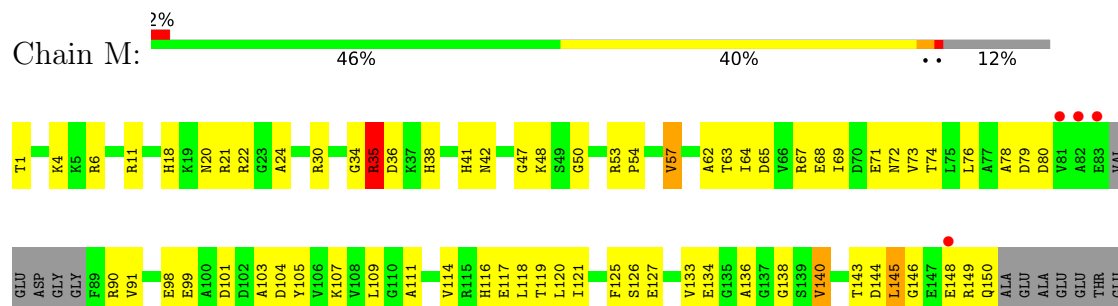
• Molecule 11: RIBOSOMAL PROTEIN L13



• Molecule 12: RIBOSOMAL PROTEIN L14

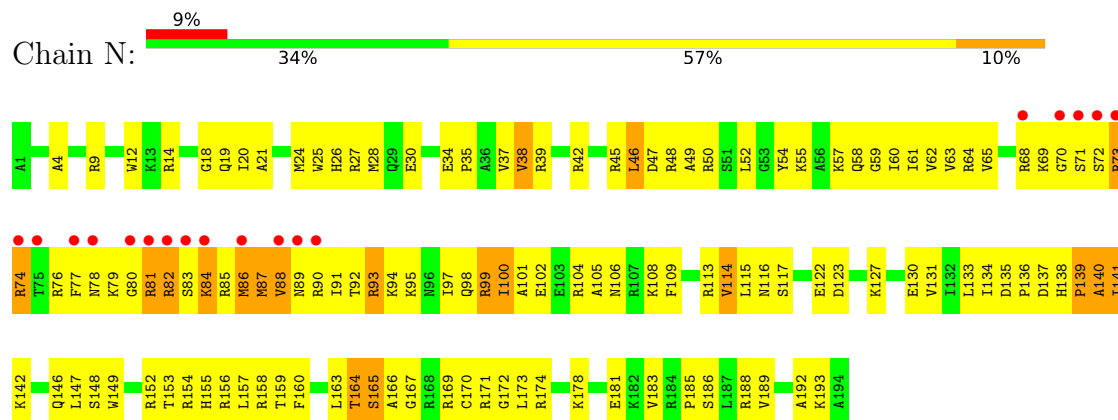


• Molecule 13: RIBOSOMAL PROTEIN L15

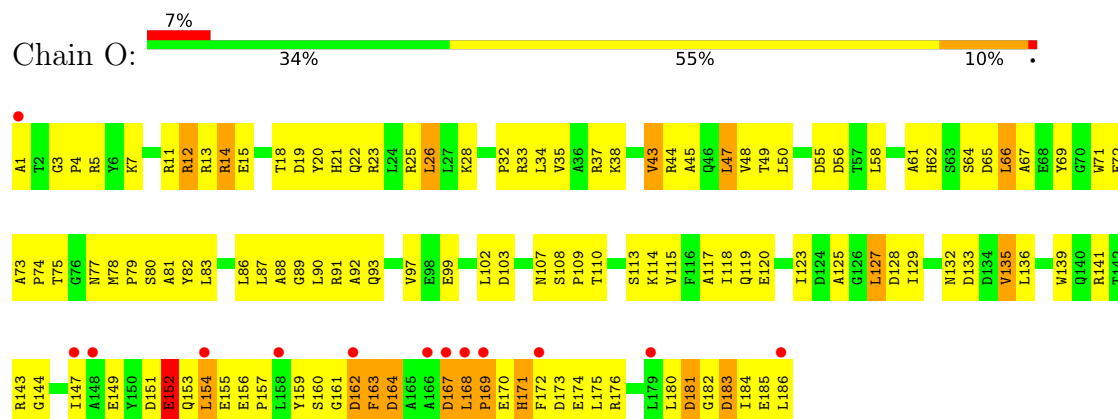


ASP
ALA
ASP
ALA
ASP
GLU
GLU

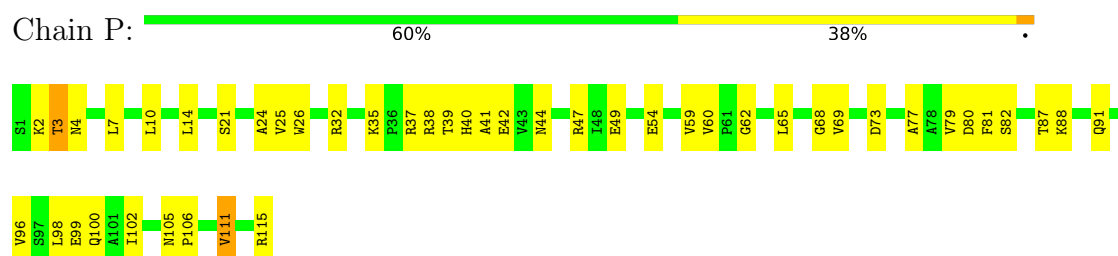
• Molecule 14: RIBOSOMAL PROTEIN L15E



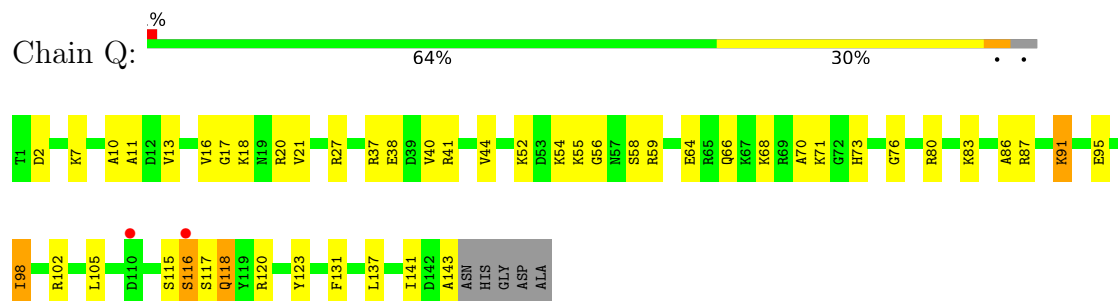
• Molecule 15: RIBOSOMAL PROTEIN L18



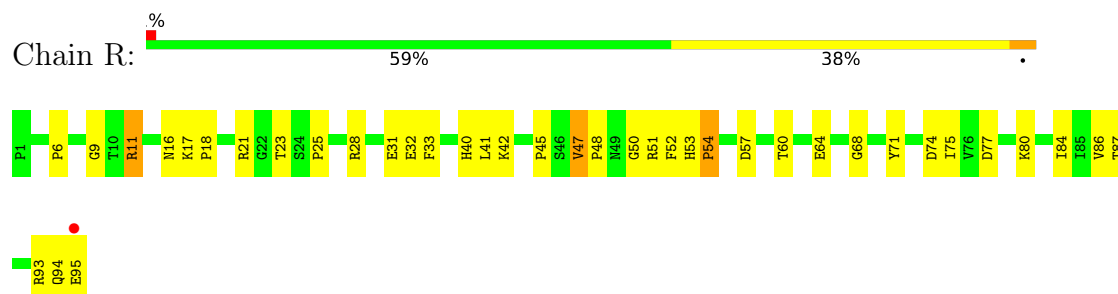
• Molecule 16: RIBOSOMAL PROTEIN L18E



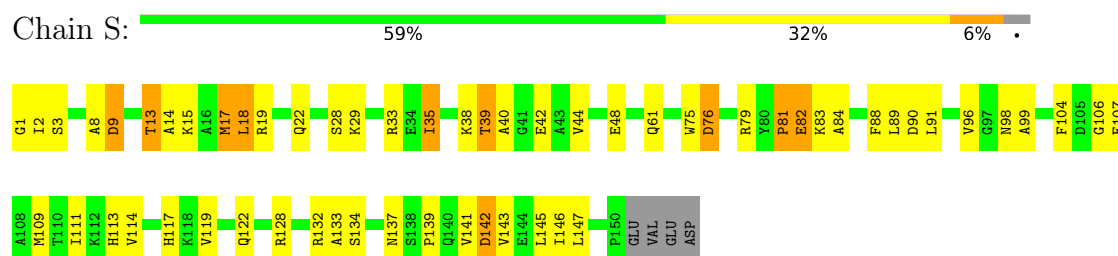
• Molecule 17: RIBOSOMAL PROTEIN L19E



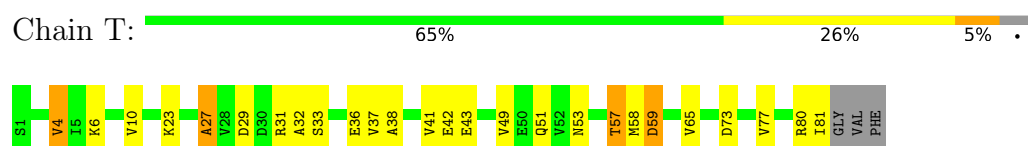
- Molecule 18: RIBOSOMAL PROTEIN L21E



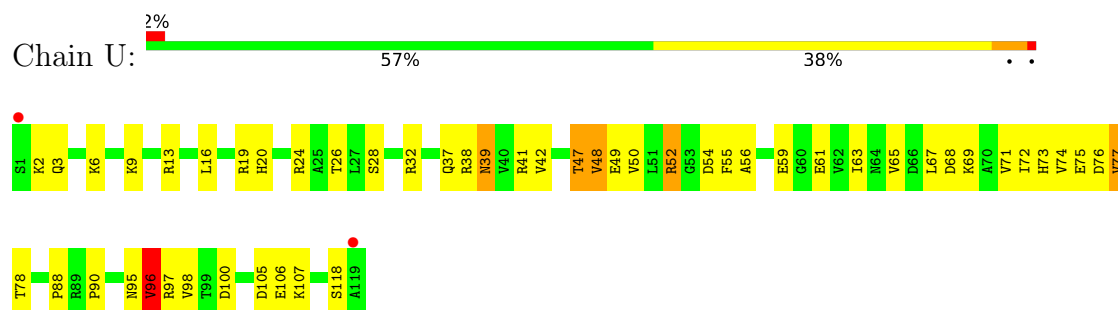
- Molecule 19: RIBOSOMAL PROTEIN L22



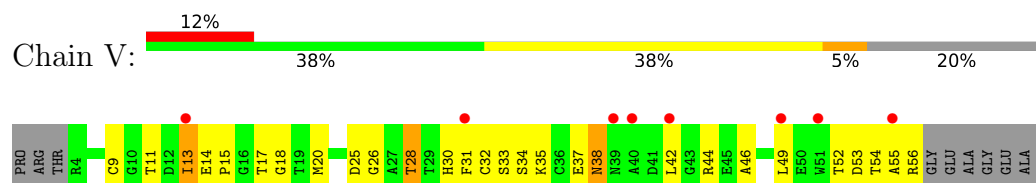
- Molecule 20: RIBOSOMAL PROTEIN L23



- Molecule 21: RIBOSOMAL PROTEIN L24

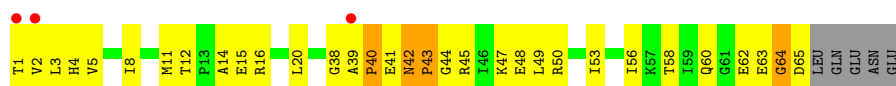


- Molecule 22: RIBOSOMAL PROTEIN L24E



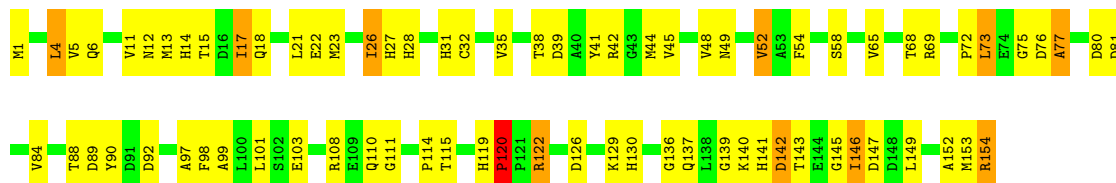
- Molecule 23: RIBOSOMAL PROTEIN L29





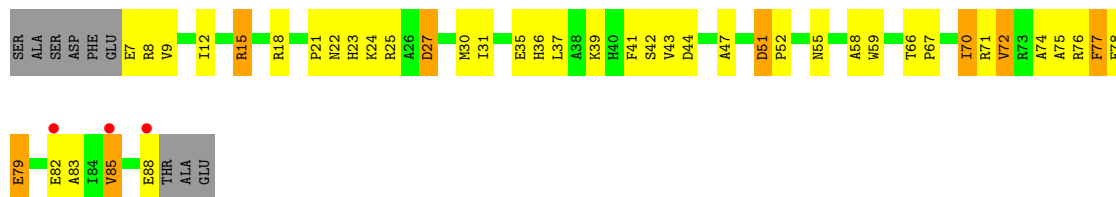
● Molecule 24: RIBOSOMAL PROTEIN L30

Chain X: 51% 42% 6%



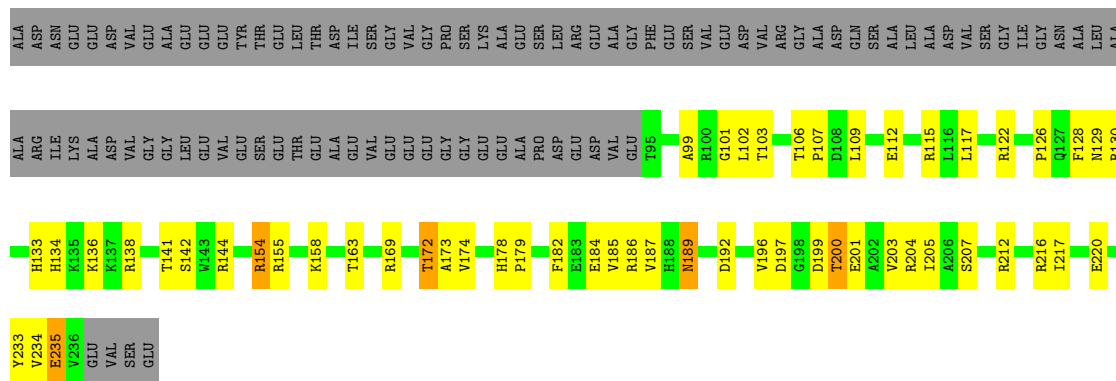
● Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y: 3% 43% 38% 9% 10%



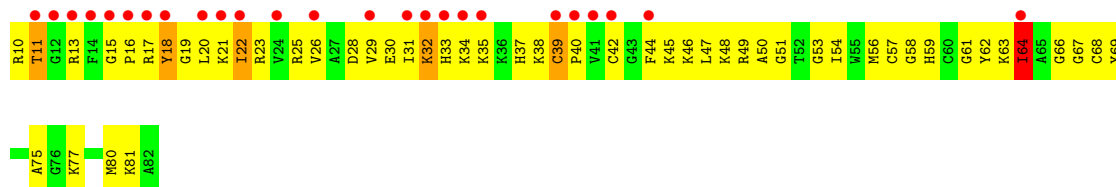
● Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z: 36% 21% 41%



● Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1: 34% 27% 64% 7%



● Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2:  59% 38% .



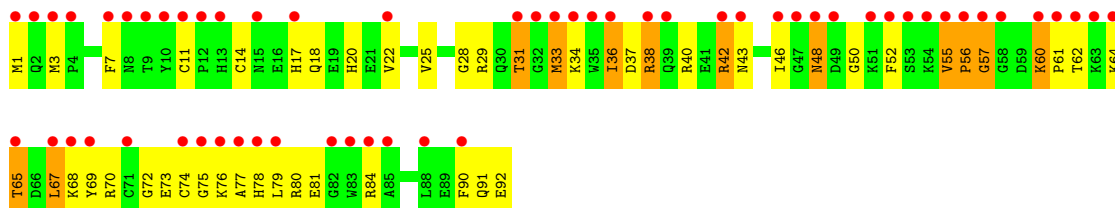
• Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 3:  54% 40% . .



• Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4:  63% 45% 42% 13%



4 Data and refinement statistics

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)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.00) 93.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.265 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	98560	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	5/66076 (0.0%)	0.78	70/103052 (0.1%)
2	B	0.56	0/2905	0.85	9/4528 (0.2%)
3	C	0.65	1/1787 (0.1%)	1.18	12/2409 (0.5%)
4	D	0.66	1/2689 (0.0%)	1.15	19/3652 (0.5%)
5	E	0.70	0/1883	1.15	15/2551 (0.6%)
6	F	0.51	0/1111	1.00	5/1498 (0.3%)
7	G	0.63	0/1382	0.99	7/1880 (0.4%)
8	H	0.56	0/896	0.98	2/1219 (0.2%)
9	I	0.54	0/241	0.81	0/324
10	J	0.68	0/1246	1.36	18/1686 (1.1%)
11	K	0.68	0/1135	1.03	3/1530 (0.2%)
12	L	0.64	0/1003	1.14	10/1351 (0.7%)
13	M	0.59	0/1126	1.11	5/1504 (0.3%)
14	N	0.87	1/1633 (0.1%)	1.27	13/2180 (0.6%)
15	O	0.58	0/1473	1.19	15/1999 (0.8%)
16	P	0.68	0/873	1.07	4/1181 (0.3%)
17	Q	0.61	0/1143	1.00	3/1521 (0.2%)
18	R	0.65	0/748	1.18	6/1005 (0.6%)
19	S	0.76	1/1172 (0.1%)	1.15	10/1578 (0.6%)
20	T	0.55	0/648	1.01	5/875 (0.6%)
21	U	0.57	0/957	1.11	6/1289 (0.5%)
22	V	1.00	1/417 (0.2%)	1.17	2/562 (0.4%)
23	W	0.57	0/502	1.04	3/675 (0.4%)
24	X	0.76	0/1218	1.09	7/1655 (0.4%)
25	Y	0.68	0/664	1.07	4/895 (0.4%)
26	Z	0.69	0/1146	1.07	2/1536 (0.1%)
27	1	1.10	2/575 (0.3%)	1.25	7/763 (0.9%)
28	2	0.70	0/437	1.12	2/578 (0.3%)
29	3	0.53	0/398	0.83	0/527
30	4	1.32	5/771 (0.6%)	1.13	6/1024 (0.6%)
All	All	0.59	17/98255 (0.0%)	0.89	270/147027 (0.2%)

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	165
2	B	0	3
All	All	1	168

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	145	MET	SD-CE	7.54	1.98	1.79
1	A	2539	U	C5'-C4'	7.30	1.62	1.51
30	4	1	MET	SD-CE	7.01	1.97	1.79
1	A	2540	G	O5'-C5'	6.89	1.52	1.42
30	4	33	MET	SD-CE	6.64	1.96	1.79
1	A	2105	C	C3'-O3'	6.30	1.51	1.42
14	N	86	MET	SD-CE	6.20	1.95	1.79
30	4	36	ILE	CA-CB	5.95	1.63	1.54
22	V	13	ILE	CA-CB	5.94	1.61	1.54
1	A	2486	A	O3'-P	5.89	1.70	1.61
27	1	22	ILE	CA-CB	5.77	1.60	1.54
1	A	2106	C	C3'-O3'	-5.29	1.34	1.42
30	4	31	THR	CA-CB	5.26	1.62	1.53
19	S	17	MET	SD-CE	-5.18	1.66	1.79
27	1	56	MET	SD-CE	5.08	1.92	1.79
30	4	48	ASN	CA-C	5.05	1.59	1.52
4	D	162	MET	SD-CE	-5.01	1.67	1.79

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.64	64.07	108.00
1	A	1164	U	OP2-P-O3'	-14.30	65.11	108.00
1	A	1563	G	C2'-C3'-O3'	13.46	129.69	109.50
10	J	141	ASN	N-CA-C	-12.89	97.65	113.50
15	O	135	VAL	N-CA-C	-12.34	101.00	113.47
10	J	74	ASN	N-CA-C	-11.81	95.23	113.89
14	N	141	ILE	N-CA-C	-11.09	102.27	111.81
1	A	1979	G	C2'-C3'-O3'	10.76	125.64	109.50
10	J	1	LYS	CA-C-N	9.50	129.45	119.85
10	J	1	LYS	C-N-CA	9.50	129.45	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1942	A	C5'-C4'-C3'	9.37	130.06	116.00
18	R	17	LYS	N-CA-C	-9.27	98.43	109.93
6	F	136	ARG	CA-C-N	9.04	131.14	119.84
6	F	136	ARG	C-N-CA	9.04	131.14	119.84
1	A	1563	G	C4'-C3'-O3'	8.84	122.65	109.40
3	C	222	GLY	N-CA-C	-8.59	104.39	113.58
7	G	11	VAL	N-CA-C	8.48	122.35	109.20
2	B	3025	G	O3'-P-O5'	8.32	116.49	104.00
18	R	47	VAL	CA-C-N	8.31	127.89	119.24
18	R	47	VAL	C-N-CA	8.31	127.89	119.24
4	D	157	LYS	N-CA-C	-8.21	103.86	114.04
28	2	21	ARG	N-CA-C	8.12	121.31	111.40
14	N	139	PRO	N-CA-C	-8.06	99.81	111.33
4	D	151	VAL	CA-C-N	8.03	127.60	119.24
4	D	151	VAL	C-N-CA	8.03	127.60	119.24
14	N	42	ARG	CA-C-N	8.03	128.33	119.90
14	N	42	ARG	C-N-CA	8.03	128.33	119.90
4	D	154	VAL	CA-C-N	7.74	127.29	119.24
4	D	154	VAL	C-N-CA	7.74	127.29	119.24
10	J	156	THR	N-CA-C	-7.71	99.07	110.48
21	U	52	ARG	N-CA-C	7.68	123.38	114.62
14	N	74	ARG	N-CA-C	7.63	120.95	108.52
21	U	3	GLN	CA-C-N	7.58	127.12	119.24
21	U	3	GLN	C-N-CA	7.58	127.12	119.24
5	E	175	LYS	N-CA-C	7.52	120.02	110.24
18	R	51	ARG	N-CA-C	7.43	120.59	110.55
30	4	55	VAL	CA-C-N	7.41	129.10	119.84
30	4	55	VAL	C-N-CA	7.41	129.10	119.84
10	J	155	PRO	N-CA-C	7.32	121.47	111.22
5	E	89	ALA	N-CA-C	7.29	119.86	111.11
6	F	100	ASP	N-CA-C	-7.22	104.47	113.28
15	O	169	PRO	N-CA-C	-7.20	104.55	114.27
10	J	147	ARG	N-CA-C	-7.18	103.49	111.82
15	O	13	ARG	N-CA-C	-7.18	105.05	113.88
14	N	70	GLY	N-CA-C	7.16	124.15	112.84
14	N	73	ARG	N-CA-C	-7.15	93.69	107.57
3	C	48	ASP	CA-C-N	7.14	126.84	119.56
3	C	48	ASP	C-N-CA	7.14	126.84	119.56
25	Y	22	ASN	N-CA-C	7.12	119.94	111.33
1	A	2102	G	C5'-C4'-C3'	7.05	125.77	115.20
15	O	153	GLN	N-CA-C	-6.98	103.70	113.20
2	B	3023	U	C2'-C3'-O3'	-6.97	103.25	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	198	ASP	N-CA-C	6.97	121.87	113.23
10	J	137	ASN	N-CA-C	-6.95	101.05	110.36
10	J	113	ALA	CA-C-N	6.94	128.15	120.45
10	J	113	ALA	C-N-CA	6.94	128.15	120.45
4	D	251	VAL	CA-C-N	6.79	128.33	119.84
4	D	251	VAL	C-N-CA	6.79	128.33	119.84
5	E	80	VAL	CA-C-N	6.72	126.23	119.24
5	E	80	VAL	C-N-CA	6.72	126.23	119.24
19	S	3	SER	N-CA-C	-6.72	99.09	109.24
23	W	42	ASN	CA-C-N	6.71	128.23	119.84
23	W	42	ASN	C-N-CA	6.71	128.23	119.84
15	O	117	ALA	N-CA-C	-6.70	104.06	111.36
3	C	70	ALA	N-CA-C	6.70	119.33	109.42
24	X	126	ASP	N-CA-C	6.70	121.16	113.19
16	P	82	SER	N-CA-C	-6.65	101.75	110.33
14	N	100	ILE	N-CA-C	-6.63	104.05	110.42
18	R	86	VAL	N-CA-C	6.60	117.07	108.35
4	D	242	TRP	N-CA-C	-6.60	103.70	111.03
5	E	179	GLY	N-CA-C	-6.58	104.51	113.27
5	E	78	ARG	N-CA-C	6.57	118.85	108.79
1	A	840	U	N1-C1'-C2'	6.53	121.79	112.00
12	L	55	VAL	N-CA-C	6.51	118.10	108.65
5	E	64	GLY	N-CA-C	6.48	120.51	113.58
28	2	11	LYS	N-CA-C	6.41	119.70	108.56
2	B	3026	C	O3'-P-O5'	6.38	113.57	104.00
13	M	57	VAL	N-CA-C	-6.38	106.11	112.17
10	J	91	HIS	N-CA-C	6.36	118.31	109.15
15	O	102	LEU	N-CA-C	6.36	118.53	108.67
4	D	230	GLN	N-CA-C	6.36	120.29	112.54
14	N	90	ARG	N-CA-C	6.33	121.00	113.28
1	A	2096	A	C4'-C3'-O3'	-6.33	103.51	113.00
17	Q	56	GLY	N-CA-C	-6.33	101.22	110.90
4	D	265	LEU	N-CA-C	6.32	119.83	110.48
2	B	3039	U	N1-C1'-C2'	6.30	121.45	112.00
16	P	2	LYS	N-CA-C	-6.29	102.06	110.55
4	D	23	THR	CA-C-N	6.27	126.24	119.78
4	D	23	THR	C-N-CA	6.27	126.24	119.78
15	O	20	TYR	N-CA-C	6.27	120.19	112.54
24	X	115	THR	N-CA-C	6.25	119.09	108.90
1	A	129	A	C2'-C3'-O3'	6.24	123.06	113.70
13	M	47	GLY	N-CA-C	6.23	118.46	111.85
2	B	3039	U	C4'-C3'-O3'	-6.21	103.69	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	78	THR	N-CA-C	6.17	118.79	109.41
2	B	3023	U	O3'-P-O5'	-6.16	94.75	104.00
19	S	9	ASP	CA-C-N	6.15	126.04	119.28
19	S	9	ASP	C-N-CA	6.15	126.04	119.28
1	A	2106	C	C4'-C3'-O3'	-6.11	103.84	113.00
1	A	834	G	C2'-C3'-O3'	-6.10	104.55	113.70
19	S	18	LEU	N-CA-C	-6.08	100.28	109.95
7	G	7	ILE	CA-C-N	6.07	126.01	119.76
7	G	7	ILE	C-N-CA	6.07	126.01	119.76
4	D	11	LEU	N-CA-C	-6.06	105.46	112.92
3	C	103	VAL	N-CA-C	6.06	115.20	108.05
11	K	68	GLY	N-CA-C	6.05	120.28	112.18
7	G	48	VAL	N-CA-C	6.03	116.62	108.17
19	S	142	ASP	N-CA-C	-6.03	100.32	109.85
6	F	151	ILE	CA-C-N	6.02	125.97	119.76
6	F	151	ILE	C-N-CA	6.02	125.97	119.76
1	A	1651	C	N1-C1'-C2'	6.01	121.02	112.00
7	G	112	ALA	CA-C-N	6.01	125.77	119.76
7	G	112	ALA	C-N-CA	6.01	125.77	119.76
19	S	76	ASP	N-CA-C	6.00	120.40	112.72
20	T	57	THR	N-CA-C	6.00	119.36	110.48
1	A	2539	U	P-O3'-C3'	6.00	129.20	120.20
16	P	79	VAL	N-CA-C	-6.00	104.66	110.72
14	N	114	VAL	N-CA-C	5.99	116.79	109.30
1	A	2486	A	C3'-C2'-O2'	5.99	119.68	110.70
12	L	38	SER	N-CA-C	-5.97	99.27	109.24
30	4	60	LYS	N-CA-C	-5.96	102.56	110.07
25	Y	79	GLU	N-CA-C	5.92	120.35	113.18
2	B	3002	U	C4'-C3'-O3'	5.92	118.28	109.40
1	A	2122	C	C3'-C2'-O2'	5.91	119.57	110.70
24	X	75	GLY	N-CA-C	5.91	120.45	112.17
19	S	90	ASP	N-CA-C	-5.89	104.77	111.14
19	S	137	ASN	N-CA-C	5.89	119.55	110.42
1	A	2106	C	N1-C1'-C2'	-5.89	103.17	112.00
3	C	118	PHE	N-CA-C	5.88	119.67	110.32
12	L	71	ALA	N-CA-C	5.83	116.25	108.38
1	A	2539	U	C3'-C2'-O2'	5.83	119.44	110.70
15	O	14	ARG	N-CA-C	-5.82	104.84	111.07
12	L	8	VAL	N-CA-C	5.82	116.86	108.48
13	M	145	LEU	N-CA-C	-5.79	105.11	111.82
10	J	162	SER	CA-C-N	-5.78	112.61	119.84
10	J	162	SER	C-N-CA	-5.78	112.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	122	GLN	N-CA-C	-5.74	99.77	108.67
1	A	1942	A	C5'-C4'-O4'	5.74	118.41	109.80
4	D	48	MET	N-CA-C	5.72	118.54	109.50
27	1	64	ILE	N-CA-C	5.72	118.06	109.20
7	G	37	ASP	N-CA-C	5.71	119.55	112.24
3	C	231	LYS	N-CA-C	-5.70	106.28	113.18
1	A	389	G	C5'-C4'-C3'	-5.70	107.45	116.00
14	N	88	VAL	CB-CA-C	-5.69	101.96	111.29
1	A	2293	G	C3'-C2'-O2'	5.68	119.23	110.70
2	B	3003	A	C5'-C4'-C3'	5.68	123.72	115.20
15	O	3	GLY	CA-C-N	5.67	125.52	119.28
15	O	3	GLY	C-N-CA	5.67	125.52	119.28
1	A	2419	U	N1-C1'-C2'	5.67	120.50	112.00
1	A	1911	C	C3'-C2'-O2'	5.66	119.19	110.70
10	J	110	GLY	N-CA-C	-5.62	99.85	113.18
1	A	2296	C	C3'-C2'-O2'	5.61	119.11	110.70
30	4	72	GLY	N-CA-C	5.61	120.84	114.67
1	A	1592	G	N9-C1'-C2'	5.59	120.39	112.00
1	A	1205	U	C3'-C2'-O2'	5.58	119.07	110.70
4	D	147	VAL	CA-C-N	5.56	125.92	119.47
4	D	147	VAL	C-N-CA	5.56	125.92	119.47
5	E	178	GLN	N-CA-C	5.55	119.67	113.01
1	A	2431	C	C1'-C2'-O2'	5.55	116.72	108.40
14	N	82	ARG	N-CA-C	-5.55	102.27	110.48
12	L	78	LYS	CA-C-N	5.54	125.84	119.92
12	L	78	LYS	C-N-CA	5.54	125.84	119.92
18	R	68	GLY	N-CA-C	-5.53	100.08	113.18
1	A	2433	A	C1'-C2'-O2'	5.53	116.69	108.40
16	P	69	VAL	N-CA-C	5.51	116.42	108.48
1	A	2465	A	N9-C1'-C2'	-5.50	105.75	114.00
1	A	755	G	O4'-C4'-C3'	-5.50	98.50	104.00
1	A	1165	G	N9-C1'-C2'	5.49	120.24	112.00
12	L	46	LYS	N-CA-C	5.49	118.68	109.95
2	B	3003	A	C4'-C3'-C2'	-5.48	97.12	102.60
1	A	2301	A	N9-C1'-C2'	5.47	120.20	112.00
19	S	35	ILE	N-CA-C	5.46	119.08	112.80
4	D	220	VAL	N-CA-C	-5.45	104.11	110.05
24	X	120	PRO	N-CA-C	-5.45	105.24	110.47
1	A	2622	A	C3'-C2'-O2'	5.44	118.86	110.70
8	H	62	HIS	N-CA-C	5.43	118.12	111.82
20	T	59	ASP	N-CA-C	-5.43	106.82	113.50
4	D	222	LYS	N-CA-C	-5.43	102.42	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	129	ASN	CA-C-N	-5.42	115.25	122.72
10	J	129	ASN	C-N-CA	-5.42	115.25	122.72
11	K	75	PRO	N-CA-C	-5.39	106.83	113.84
22	V	18	GLY	N-CA-C	5.37	120.76	112.81
3	C	8	ARG	N-CA-C	-5.37	105.43	111.28
1	A	2540	G	C1'-O4'-C4'	-5.37	104.53	109.90
10	J	86	ARG	N-CA-C	5.37	119.67	113.18
20	T	4	VAL	CB-CA-C	-5.37	104.99	112.02
27	1	32	LYS	N-CA-C	-5.36	105.35	111.14
3	C	133	ARG	N-CA-C	-5.35	106.59	113.23
1	A	882	A	C3'-C2'-O2'	-5.34	106.58	114.60
1	A	1979	G	C3'-C2'-O2'	5.33	122.60	114.60
1	A	2105	C	O3'-P-O5'	5.33	112.00	104.00
3	C	33	GLU	N-CA-C	-5.33	104.72	111.11
1	A	2664	A	N9-C1'-C2'	5.33	119.99	112.00
1	A	393	G	N9-C1'-C2'	5.31	119.96	112.00
1	A	2835	C	C4'-C3'-O3'	-5.31	105.04	113.00
1	A	2792	A	C3'-C2'-O2'	5.30	118.65	110.70
5	E	176	ALA	N-CA-C	-5.30	101.06	109.76
30	4	42	ARG	N-CA-C	5.30	116.74	111.07
27	1	32	LYS	CA-C-N	5.29	127.63	120.38
27	1	32	LYS	C-N-CA	5.29	127.63	120.38
1	A	189	A	N9-C1'-C2'	5.29	119.93	112.00
1	A	2136	G	C2'-C3'-O3'	5.29	121.63	113.70
23	W	64	GLY	N-CA-C	-5.29	107.74	115.72
12	L	111	GLY	CA-C-N	5.28	125.28	120.21
12	L	111	GLY	C-N-CA	5.28	125.28	120.21
15	O	168	LEU	N-CA-C	5.28	120.15	108.64
25	Y	51	ASP	CA-C-N	5.28	126.44	119.84
25	Y	51	ASP	C-N-CA	5.28	126.44	119.84
1	A	2540	G	O5'-C5'-C4'	-5.27	103.59	111.50
27	1	22	ILE	N-CA-C	5.27	115.72	110.23
10	J	73	GLN	N-CA-C	-5.27	104.01	110.65
5	E	192	ILE	N-CA-C	5.27	116.38	109.21
1	A	407	A	O4'-C4'-C3'	-5.26	98.74	104.00
1	A	1723	G	C4'-C3'-O3'	-5.25	105.12	113.00
1	A	820	G	N9-C1'-C2'	5.25	119.87	112.00
1	A	1681	G	C2'-C3'-O3'	-5.25	105.83	113.70
12	L	14	LYS	N-CA-C	-5.25	102.28	110.10
24	X	17	ILE	N-CA-C	-5.24	106.02	111.58
1	A	2102	G	O3'-P-O5'	5.24	111.86	104.00
27	1	18	TYR	N-CA-C	5.23	121.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1450	C	C2'-C3'-O3'	-5.23	105.86	113.70
20	T	27	ALA	N-CA-C	-5.22	100.21	108.73
1	A	2103	A	C5'-C4'-O4'	-5.22	101.27	109.10
1	A	2914	A	C2'-C3'-O3'	5.22	121.53	113.70
1	A	2536	C	N1-C1'-C2'	5.22	119.82	112.00
13	M	42	ASN	N-CA-C	5.21	118.91	112.24
26	Z	196	VAL	N-CA-C	5.20	116.19	108.23
1	A	1419	U	N1-C1'-C2'	5.20	119.80	112.00
1	A	1058	A	N9-C1'-C2'	5.20	119.80	112.00
4	D	175	LEU	N-CA-C	-5.20	105.51	111.07
20	T	4	VAL	N-CA-C	5.19	115.41	110.53
1	A	854	G	C4'-C3'-O3'	-5.18	105.23	113.00
1	A	2103	A	C4'-C3'-O3'	5.18	117.17	109.40
5	E	93	LYS	N-CA-C	5.18	117.51	108.76
15	O	171	HIS	N-CA-C	-5.18	105.75	111.71
1	A	148	A	C3'-C2'-O2'	5.17	118.46	110.70
1	A	2539	U	C1'-C2'-O2'	-5.17	100.65	108.40
1	A	1359	U	N1-C1'-C2'	5.16	119.75	112.00
24	X	143	THR	N-CA-C	-5.15	105.78	111.71
26	Z	101	GLY	N-CA-C	5.14	123.25	112.45
1	A	1504	A	C4'-C3'-O3'	-5.14	105.30	113.00
17	Q	70	ALA	N-CA-C	-5.13	105.77	112.23
1	A	471	G	N9-C1'-C2'	5.12	119.67	112.00
21	U	77	VAL	CB-CA-C	-5.12	107.49	113.22
1	A	171	C	C3'-C2'-O2'	5.12	118.37	110.70
30	4	67	LEU	N-CA-C	5.11	117.93	109.85
13	M	20	ASN	N-CA-C	5.11	118.96	111.04
14	N	92	THR	N-CA-C	-5.11	101.43	109.50
1	A	2315	C	C5'-C4'-C3'	-5.11	108.34	116.00
22	V	38	ASN	N-CA-C	5.09	117.73	111.82
1	A	2466	G	N9-C1'-C2'	5.09	119.63	112.00
24	X	49	ASN	N-CA-C	5.08	121.62	110.80
11	K	9	ASP	N-CA-C	-5.08	106.35	112.54
15	O	66	LEU	N-CA-C	-5.08	105.39	112.45
1	A	335	U	C4'-C3'-O3'	-5.07	105.39	113.00
27	1	39	CYS	N-CA-C	5.05	116.06	109.64
21	U	96	VAL	N-CA-C	5.05	116.87	108.99
1	A	171	C	C4'-C3'-O3'	-5.04	105.44	113.00
5	E	92	PRO	N-CA-C	-5.04	103.36	111.38
3	C	146	LYS	N-CA-C	5.04	116.94	108.73
5	E	63	SER	CA-C-N	-5.03	117.96	123.30
5	E	63	SER	C-N-CA	-5.03	117.96	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	133	ASP	N-CA-C	5.03	121.52	110.80
15	O	152	GLU	N-CA-C	-5.03	105.99	111.82
1	A	921	G	N9-C1'-C2'	5.02	119.53	112.00
1	A	2479	A	C3'-C2'-O2'	5.02	118.23	110.70
5	E	20	ASP	N-CA-C	5.02	117.40	111.33
1	A	871	G	O4'-C1'-C2'	-5.02	102.58	107.60
8	H	8	VAL	N-CA-C	5.01	112.51	107.55
17	Q	118	GLN	N-CA-C	-5.01	105.73	111.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	A	Sidechain
1	A	1023	C	Sidechain
1	A	1027	G	Sidechain
1	A	1042	U	Sidechain
1	A	1127	C	Sidechain
1	A	1136	U	Sidechain
1	A	1191	A	Sidechain
1	A	1206	U	Sidechain
1	A	1237	U	Sidechain
1	A	1261	A	Sidechain
1	A	1264	U	Sidechain
1	A	1269	G	Sidechain
1	A	1288	U	Sidechain
1	A	1309	U	Sidechain
1	A	1336	U	Sidechain
1	A	1347	U	Sidechain
1	A	1376	G	Sidechain
1	A	1387	G	Sidechain
1	A	1408	U	Sidechain
1	A	1430	G	Sidechain
1	A	1432	U	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	146	U	Sidechain
1	A	1487	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1614	G	Sidechain
1	A	162	C	Sidechain
1	A	1635	U	Sidechain
1	A	1643	C	Sidechain
1	A	1655	G	Sidechain
1	A	1671	U	Sidechain
1	A	1681	G	Sidechain
1	A	1685	A	Sidechain
1	A	1688	G	Sidechain
1	A	170	U	Sidechain
1	A	171	C	Sidechain
1	A	172	U	Sidechain
1	A	1720	C	Sidechain
1	A	1728	G	Sidechain
1	A	1736	A	Sidechain
1	A	174	A	Sidechain
1	A	1777	G	Sidechain
1	A	1819	G	Sidechain
1	A	182	G	Sidechain
1	A	1823	G	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1851	G	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1879	U	Sidechain
1	A	191	A	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	1993	C	Sidechain
1	A	2001	G	Sidechain
1	A	2035	C	Sidechain
1	A	204	A	Sidechain
1	A	2053	G	Sidechain
1	A	2063	U	Sidechain
1	A	2068	G	Sidechain
1	A	2101	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2106	C	Sidechain
1	A	2120	U	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	22	U	Sidechain
1	A	2266	A	Sidechain
1	A	2282	U	Sidechain
1	A	2288	G	Sidechain
1	A	2293	G	Sidechain
1	A	2304	G	Sidechain
1	A	2308	U	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2316	G	Sidechain
1	A	2326	U	Sidechain
1	A	2358	U	Sidechain
1	A	2359	G	Sidechain
1	A	2364	A	Sidechain
1	A	2378	U	Sidechain
1	A	2394	A	Sidechain
1	A	2409	C	Sidechain
1	A	2412	G	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2436	U	Sidechain
1	A	2439	C	Sidechain
1	A	2453	G	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2535	U	Sidechain
1	A	2539	U	Sidechain
1	A	2544	G	Sidechain
1	A	2564	G	Sidechain
1	A	2573	G	Sidechain
1	A	2575	C	Sidechain
1	A	261	A	Sidechain
1	A	2630	G	Sidechain
1	A	2643	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2655	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2710	U	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2810	G	Sidechain
1	A	2811	A	Sidechain
1	A	2840	A	Sidechain
1	A	2864	U	Sidechain
1	A	315	G	Sidechain
1	A	333	G	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	453	A	Sidechain
1	A	458	G	Sidechain
1	A	460	A	Sidechain
1	A	471	G	Sidechain
1	A	474	C	Sidechain
1	A	48	A	Sidechain
1	A	502	A	Sidechain
1	A	517	U	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	554	G	Sidechain
1	A	720	G	Sidechain
1	A	723	G	Sidechain
1	A	742	G	Sidechain
1	A	757	C	Sidechain
1	A	759	C	Sidechain
1	A	761	A	Sidechain
1	A	781	C	Sidechain
1	A	782	G	Sidechain
1	A	791	A	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	818	A	Sidechain
1	A	827	A	Sidechain
1	A	835	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	859	C	Sidechain
1	A	860	U	Sidechain
1	A	867	A	Sidechain
1	A	871	G	Sidechain
1	A	877	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	888	U	Sidechain
1	A	904	U	Sidechain
1	A	919	U	Sidechain
1	A	932	U	Sidechain
1	A	946	C	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain
2	B	3005	G	Sidechain
2	B	3065	A	Sidechain
2	B	3094	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29799	1357	0
2	B	2600	0	1326	83	0
3	C	1754	0	1763	132	0
4	D	2624	0	2533	200	0
5	E	1858	0	1816	155	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	90	0
8	H	885	0	854	68	0
9	I	240	0	231	21	0
10	J	1215	0	1215	170	0
11	K	1119	0	1098	76	0
12	L	993	0	1027	70	0
13	M	1114	0	1072	80	0
14	N	1605	0	1676	203	0
15	O	1444	0	1401	151	0
16	P	864	0	873	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	1133	0	1127	62	0
18	R	734	0	728	29	0
19	S	1149	0	1122	66	0
20	T	641	0	605	32	0
21	U	949	0	923	58	0
22	V	410	0	366	40	0
23	W	499	0	511	31	0
24	X	1195	0	1137	101	0
25	Y	654	0	653	49	0
26	Z	1130	0	1133	66	0
27	1	563	0	600	79	0
28	2	430	0	426	26	0
29	3	393	0	406	30	0
30	4	755	0	731	52	0
31	A	59	0	63	4	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	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	69	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	4	1	0	0	0	0
34	A	10	0	0	3	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	3	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	O	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	41	0	0	16	0
37	2	58	0	0	5	0
37	3	41	0	0	8	0
37	4	68	0	0	11	0
37	A	5858	0	0	321	0
37	B	141	0	0	15	0
37	C	138	0	0	14	0
37	D	154	0	0	33	0
37	E	177	0	0	45	0
37	F	49	0	0	22	0
37	G	44	0	0	13	0
37	H	26	0	0	12	0
37	I	21	0	0	4	0
37	J	79	0	0	23	0
37	K	53	0	0	5	0
37	L	59	0	0	12	0
37	M	87	0	0	22	0
37	N	130	0	0	29	0
37	O	69	0	0	23	0
37	P	44	0	0	11	0
37	Q	68	0	0	7	0
37	R	51	0	0	5	0
37	S	81	0	0	5	0
37	T	37	0	0	8	0
37	U	37	0	0	5	0
37	V	28	0	0	7	0
37	W	14	0	0	3	0
37	X	69	0	0	7	0
37	Y	28	0	0	10	0
37	Z	100	0	0	18	0
All	All	98560	0	59566	3455	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (3455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.61	1.15
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.46	1.15
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.24	1.14
5:E:236:THR:HG22	5:E:239:ALA:H	1.06	1.13
1:A:1160:G:H5'	1:A:1161:A:H5'	1.30	1.11
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.31	1.11
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.31	1.11
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.30	1.10
6:F:25:MET:HE2	6:F:41:LEU:HG	1.34	1.10
1:A:871:G:H5'	1:A:871:G:H8	1.03	1.10
1:A:2122:C:OP2	37:A:6114:HOH:O	1.69	1.10
1:A:2123:A:OP2	37:A:4844:HOH:O	1.72	1.08
10:J:165:GLY:HA3	37:J:8399:HOH:O	1.53	1.07
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.13	1.06
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.37	1.06
1:A:1134:G:H4'	10:J:151:MET:HE1	1.31	1.06
1:A:871:G:H5'	1:A:871:G:C8	1.90	1.05
1:A:156:C:H5''	14:N:171:ARG:HD3	1.38	1.05
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.37	1.04
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.40	1.03
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.41	1.03
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.35	1.03
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.41	1.03
14:N:164:THR:HG22	14:N:167:GLY:H	1.24	1.02
1:A:870:G:H2'	1:A:871:G:H5''	1.37	1.01
4:D:162:MET:HE1	4:D:308:LEU:HD21	1.39	1.00
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.77	1.00
17:Q:115:SER:H	17:Q:118:GLN:HE21	1.01	0.99
5:E:236:THR:HG21	37:E:8375:HOH:O	1.59	0.99
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.45	0.99
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.82	0.99
4:D:86:ALA:HA	37:D:8583:HOH:O	1.62	0.99
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.41	0.99
14:N:87:MET:CG	30:4:46:ILE:HG21	1.92	0.99
1:A:2717:C:H2'	1:A:2718:C:H5''	1.43	0.98
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.76	0.98
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.25	0.98
1:A:2121:G:H5''	37:A:3085:HOH:O	1.65	0.97
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.44	0.97
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.46	0.97
1:A:1835:U:H5	1:A:1840:A:N7	1.59	0.97
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.43	0.97
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.44	0.96
1:A:542:A:H5'	1:A:542:A:H8	1.29	0.96
24:X:88:THR:HG22	24:X:89:ASP:H	1.31	0.96
1:A:2004:U:H4'	37:A:4862:HOH:O	1.64	0.95
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.80	0.95
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.45	0.95
1:A:962:C:H1'	15:O:5:ARG:NH1	1.82	0.95
1:A:714:U:H3'	37:A:6481:HOH:O	1.66	0.95
10:J:2:PRO:HB2	37:J:8366:HOH:O	1.67	0.94
6:F:105:SER:HB2	6:F:131:THR:HG23	1.48	0.94
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.67	0.94
37:A:4420:HOH:O	14:N:14:ARG:HG2	1.66	0.94
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.67	0.93
2:B:3056:A:H2'	2:B:3057:A:H5''	1.49	0.93
1:A:871:G:H8	1:A:871:G:C5'	1.80	0.93
1:A:1242:A:H5'	11:K:82:THR:HG23	1.48	0.93
24:X:88:THR:HB	37:X:6679:HOH:O	1.69	0.93
1:A:1751:G:H2'	1:A:1752:G:H5''	1.48	0.93
14:N:35:PRO:CG	14:N:38:VAL:HG23	1.98	0.93
15:O:7:LYS:HE3	18:R:21:ARG:O	1.68	0.92
4:D:140:LEU:HA	37:D:8583:HOH:O	1.67	0.92
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.35	0.92
12:L:10:GLN:NE2	12:L:10:GLN:H	1.66	0.92
1:A:2121:G:OP2	37:A:3085:HOH:O	1.88	0.92
1:A:2533:C:H6	1:A:2533:C:H5'	1.35	0.91
2:B:3076:G:H3'	2:B:3077:A:H5''	1.52	0.91
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.35	0.91
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.53	0.91
1:A:856:G:H2'	37:A:4976:HOH:O	1.67	0.91
1:A:1205:U:H2'	1:A:1206:U:H5'	1.51	0.91
13:M:79:ASP:HB3	37:M:8564:HOH:O	1.69	0.90
1:A:960:G:H4'	37:A:6965:HOH:O	1.70	0.90
20:T:57:THR:HG22	20:T:59:ASP:H	1.37	0.90
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.00	0.90
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27:LYS:H	10:J:58:HIS:HD2	1.19	0.89
13:M:68:GLU:HA	37:M:8547:HOH:O	1.72	0.89
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.52	0.89
1:A:1919:A:H4'	37:A:4406:HOH:O	1.72	0.89
4:D:62:ARG:HA	4:D:65:MET:HE3	1.53	0.89
1:A:2526:C:O2'	1:A:2527:U:H5'	1.73	0.88
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.72	0.88
1:A:2426:G:H1'	37:A:5637:HOH:O	1.73	0.88
4:D:321:PRO:HA	37:D:8664:HOH:O	1.72	0.88
1:A:2467:A:OP1	37:A:8640:HOH:O	1.89	0.88
37:A:5838:HOH:O	6:F:99:ASP:HA	1.72	0.88
10:J:141:ASN:HA	37:J:8367:HOH:O	1.74	0.88
1:A:1701:A:H5'	37:A:5826:HOH:O	1.74	0.88
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.14	0.88
37:A:3255:HOH:O	14:N:79:LYS:HD3	1.72	0.87
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.55	0.87
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.53	0.87
13:M:133:VAL:HA	37:M:8579:HOH:O	1.73	0.87
3:C:223:ARG:HG3	37:C:8612:HOH:O	1.72	0.87
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.57	0.87
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.56	0.87
26:Z:216:ARG:HD3	37:Z:8571:HOH:O	1.74	0.87
10:J:139:ASP:HA	37:J:8371:HOH:O	1.75	0.86
5:E:140:VAL:HB	37:E:8457:HOH:O	1.74	0.86
12:L:10:GLN:H	12:L:10:GLN:HE21	1.18	0.86
14:N:24:MET:HE3	14:N:28:MET:HE3	1.55	0.86
13:M:67:ARG:O	13:M:71:GLU:HG3	1.75	0.86
24:X:149:LEU:HG	24:X:153:MET:HE2	1.56	0.86
1:A:1474:C:H6	1:A:1474:C:H5'	1.39	0.86
1:A:1667:A:H5'	1:A:1667:A:H8	1.37	0.86
1:A:2506:A:HO2'	1:A:2507:G:H8	0.87	0.86
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.38	0.86
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.73	0.86
1:A:541:C:H2'	1:A:542:A:H5''	1.55	0.86
16:P:32:ARG:O	16:P:32:ARG:HD3	1.75	0.86
19:S:9:ASP:O	19:S:13:THR:HB	1.76	0.86
29:3:41:HIS:H	29:3:45:ASN:HD22	1.23	0.86
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.90	0.85
10:J:142:VAL:HG13	37:J:8382:HOH:O	1.76	0.85
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.40	0.85
1:A:797:A:H4'	27:1:10:ARG:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:87:MET:CB	30:4:46:ILE:HG21	2.07	0.85
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.57	0.85
1:A:2717:C:C2'	1:A:2718:C:H5''	2.07	0.85
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.21	0.85
1:A:338:C:H4'	5:E:174:ILE:CD1	2.07	0.84
1:A:1116:U:HO2'	1:A:1118:A:H2	0.88	0.84
1:A:2361:A:H5''	37:A:8604:HOH:O	1.78	0.84
9:I:12:ILE:HA	37:I:4499:HOH:O	1.78	0.84
1:A:870:G:C2'	1:A:871:G:H5''	2.07	0.84
1:A:1184:C:H1'	37:A:7001:HOH:O	1.76	0.84
37:A:4509:HOH:O	2:B:3103:A:H4'	1.76	0.84
18:R:25:PRO:HB2	37:R:4350:HOH:O	1.76	0.84
10:J:162:SER:HB2	10:J:163:PRO:CD	2.06	0.84
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.58	0.84
1:A:172:U:OP2	37:A:5755:HOH:O	1.96	0.84
1:A:2420:G:O2'	1:A:2421:G:H5'	1.77	0.83
11:K:99:GLU:HA	37:K:8572:HOH:O	1.77	0.83
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.43	0.83
10:J:139:ASP:N	10:J:140:PRO:HD3	1.93	0.83
14:N:84:LYS:HE2	37:N:8575:HOH:O	1.76	0.83
1:A:541:C:C2'	1:A:542:A:H5''	2.08	0.83
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.77	0.83
1:A:1886:A:N3	37:A:4378:HOH:O	2.12	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.79	0.83
1:A:797:A:C4'	27:1:10:ARG:N	2.42	0.83
1:A:1474:C:H5'	1:A:1474:C:C6	2.14	0.83
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.58	0.83
1:A:962:C:H1'	15:O:5:ARG:HH12	1.43	0.82
22:V:9:CYS:HA	22:V:52:THR:HG23	1.59	0.82
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.08	0.82
14:N:69:LYS:O	14:N:73:ARG:NH2	2.12	0.82
1:A:1666:C:O2'	1:A:1667:A:H5''	1.80	0.82
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.61	0.82
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.60	0.82
1:A:1450:C:H4'	1:A:1451:C:OP2	1.80	0.82
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.62	0.82
5:E:133:ARG:HD2	37:E:8417:HOH:O	1.80	0.82
15:O:113:SER:HB2	37:O:8561:HOH:O	1.80	0.82
10:J:5:MET:HG3	37:J:8366:HOH:O	1.77	0.81
10:J:26:LYS:HG2	10:J:28:ILE:H	1.45	0.81
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:41:THR:HA	37:J:8397:HOH:O	1.80	0.81
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.28	0.81
1:A:645:U:OP2	13:M:4:LYS:HE2	1.81	0.81
1:A:1165:G:H4'	1:A:1174:A:O2'	1.80	0.81
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.63	0.81
18:R:23:THR:HA	37:R:4792:HOH:O	1.80	0.81
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.95	0.81
1:A:2467:A:H2'	37:A:5005:HOH:O	1.80	0.81
1:A:2716:G:H5''	4:D:206:THR:HG21	1.62	0.81
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.63	0.81
27:1:10:ARG:HA	37:1:8415:HOH:O	1.81	0.81
37:A:4134:HOH:O	14:N:83:SER:HA	1.79	0.81
5:E:236:THR:HG22	5:E:239:ALA:N	1.91	0.81
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.16	0.81
1:A:1134:G:C4'	10:J:151:MET:HE1	2.12	0.80
1:A:1353:C:P	37:A:4238:HOH:O	2.40	0.80
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.12	0.80
8:H:96:ALA:HA	37:H:3111:HOH:O	1.81	0.80
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.11	0.80
23:W:1:THR:HG23	23:W:2:VAL:H	1.45	0.80
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.13	0.80
1:A:2468:A:H61	30:4:48:ASN:HD21	1.28	0.80
1:A:1679:C:H5'	37:A:8908:HOH:O	1.82	0.80
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.62	0.80
1:A:1166:A:H1'	1:A:1192:A:C2	2.17	0.80
5:E:2:GLN:HB3	37:E:8336:HOH:O	1.80	0.80
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.63	0.80
15:O:144:GLY:O	15:O:147:ILE:HG22	1.82	0.80
17:Q:143:ALA:HA	37:Q:2178:HOH:O	1.81	0.80
24:X:80:ASP:O	24:X:84:VAL:HG23	1.82	0.80
1:A:2586:U:H3	1:A:2592:G:H22	1.27	0.79
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.81	0.79
8:H:46:GLU:O	8:H:73:PRO:HD2	1.83	0.79
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.63	0.79
5:E:246:ARG:HB3	5:E:246:ARG:NH1	1.96	0.79
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.82	0.79
1:A:1741:U:H5'	1:A:1742:A:OP1	1.81	0.79
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.82	0.79
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.63	0.79
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.80	0.79
37:A:6989:HOH:O	4:D:211:THR:HG21	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.65	0.79
14:N:164:THR:HG23	14:N:165:SER:N	1.96	0.79
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.12	0.79
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.17	0.79
4:D:238:ASN:HD22	4:D:240:GLY:H	1.31	0.79
10:J:137:ASN:O	10:J:139:ASP:N	2.16	0.79
20:T:57:THR:HG22	20:T:59:ASP:N	1.98	0.79
14:N:48:ARG:NH2	37:N:8561:HOH:O	2.14	0.79
1:A:282:C:H1'	1:A:368:C:N4	1.97	0.78
1:A:1834:C:H2'	1:A:1840:A:N6	1.98	0.78
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.46	0.78
1:A:711:G:H1'	37:A:6631:HOH:O	1.83	0.78
37:A:3356:HOH:O	14:N:189:VAL:HG21	1.83	0.78
37:A:4776:HOH:O	12:L:39:GLY:HA2	1.83	0.78
37:A:5341:HOH:O	14:N:170:CYS:SG	2.40	0.78
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.83	0.78
15:O:164:ASP:CG	15:O:167:ASP:HA	2.09	0.78
1:A:1603:A:H5'	1:A:1605:G:O4'	1.82	0.78
8:H:91:VAL:HG12	8:H:92:GLY:N	1.98	0.78
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.83	0.78
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.14	0.78
1:A:1835:U:C5	1:A:1840:A:N7	2.48	0.78
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.19	0.78
1:A:338:C:H4'	5:E:174:ILE:HD11	1.64	0.78
1:A:1372:A:H3'	37:A:6724:HOH:O	1.82	0.78
1:A:545:G:H5'	1:A:545:G:H8	1.49	0.78
11:K:133:GLY:O	11:K:137:GLU:HG3	1.84	0.78
19:S:39:THR:HG22	19:S:42:GLU:H	1.49	0.78
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.23	0.77
1:A:1118:A:H8	1:A:1118:A:H3'	1.49	0.77
2:B:3014:G:H5'	2:B:3014:G:H8	1.49	0.77
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.82	0.77
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.83	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.77
1:A:288:A:H61	1:A:364:C:H42	1.32	0.77
6:F:27:ILE:HG22	6:F:28:GLY:H	1.49	0.77
22:V:20:MET:HE2	22:V:30:HIS:NE2	1.99	0.77
1:A:1058:A:H2'	1:A:1060:C:H5''	1.66	0.77
6:F:154:LYS:H	6:F:154:LYS:HD2	1.49	0.77
1:A:877:G:H5'	1:A:878:G:OP1	1.84	0.77
1:A:2638:G:H1'	37:A:7297:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.20	0.77
29:3:18:ASN:HD21	29:3:40:ARG:H	1.32	0.76
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.55	0.76
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.66	0.76
1:A:236:A:H4'	1:A:237:G:H5'	1.68	0.76
37:A:6410:HOH:O	14:N:178:LYS:HB2	1.84	0.76
20:T:23:LYS:HE2	37:T:3430:HOH:O	1.86	0.76
1:A:1116:U:H3	1:A:1246:A:H62	1.31	0.76
27:1:34:LYS:HE2	37:1:8426:HOH:O	1.85	0.76
10:J:71:TYR:C	10:J:73:GLN:H	1.93	0.76
1:A:31:C:H4'	37:A:6959:HOH:O	1.85	0.76
5:E:139:VAL:HG13	37:E:8455:HOH:O	1.86	0.76
12:L:10:GLN:HE21	12:L:10:GLN:N	1.84	0.76
14:N:164:THR:HG22	14:N:167:GLY:N	1.99	0.76
11:K:76:ASP:HA	37:K:8563:HOH:O	1.85	0.76
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.67	0.76
1:A:560:C:H42	1:A:597:A:H61	1.33	0.76
1:A:2419:U:H5''	1:A:2420:G:H5'	1.68	0.76
1:A:2466:G:OP1	37:A:3220:HOH:O	2.03	0.76
13:M:1:THR:HA	37:M:8525:HOH:O	1.84	0.76
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.66	0.76
1:A:1209:C:H4'	37:A:4834:HOH:O	1.86	0.76
19:S:99:ALA:CB	19:S:109:MET:HE1	2.11	0.76
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.85	0.76
1:A:346:U:H4'	37:A:6380:HOH:O	1.86	0.75
10:J:59:ASN:H	10:J:59:ASN:HD22	1.33	0.75
30:4:65:THR:HG23	30:4:67:LEU:HG	1.68	0.75
1:A:2506:A:O2'	1:A:2507:G:H8	1.67	0.75
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.68	0.75
8:H:91:VAL:HG12	8:H:92:GLY:H	1.49	0.75
25:Y:15:ARG:HB3	25:Y:15:ARG:HH11	1.51	0.75
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.68	0.75
1:A:1164:U:H3	1:A:1192:A:H2	1.33	0.75
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.19	0.75
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.66	0.75
1:A:2274:A:N3	14:N:86:MET:HE1	2.01	0.75
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.68	0.75
1:A:289:G:H22	1:A:363:A:H2	1.35	0.75
10:J:59:ASN:HD22	10:J:59:ASN:N	1.85	0.75
1:A:2812:A:H2	1:A:2814:A:H62	1.29	0.75
37:A:6959:HOH:O	21:U:9:LYS:HB2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.67	0.75
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.27	0.75
1:A:1241:G:N2	11:K:86:MET:HE2	2.02	0.75
3:C:53:ALA:HB3	37:C:8618:HOH:O	1.87	0.74
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.68	0.74
1:A:559:U:H6	1:A:559:U:H5'	1.52	0.74
1:A:1120:U:H6	1:A:1120:U:H5''	1.50	0.74
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.51	0.74
3:C:35:GLY:O	3:C:36:ASP:HB3	1.86	0.74
1:A:2827:A:H2'	1:A:2828:G:O4'	1.87	0.74
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.02	0.74
1:A:31:C:H2'	37:A:7226:HOH:O	1.87	0.74
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.87	0.74
9:I:12:ILE:N	9:I:13:PRO:HD3	2.02	0.74
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.70	0.74
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.69	0.74
1:A:1118:A:H3'	1:A:1118:A:C8	2.22	0.74
1:A:21:G:H5'	19:S:2:ILE:HA	1.69	0.74
1:A:1909:A:N1	1:A:2128:G:H1'	2.02	0.74
7:G:93:MET:HE1	7:G:165:GLY:N	2.03	0.74
10:J:150:LYS:HE2	37:J:8384:HOH:O	1.88	0.74
1:A:2432:C:O2'	1:A:2433:A:H5'	1.87	0.74
15:O:89:GLY:O	15:O:92:ALA:HB3	1.88	0.74
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.70	0.74
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.52	0.74
28:2:10:LYS:HG3	37:2:8433:HOH:O	1.87	0.74
1:A:2054:A:N3	19:S:128:ARG:NH2	2.36	0.73
5:E:25:PRO:HG2	37:E:8325:HOH:O	1.87	0.73
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.70	0.73
30:4:40:ARG:HD2	37:4:8548:HOH:O	1.88	0.73
1:A:450:C:OP1	5:E:184:ARG:NH2	2.21	0.73
37:A:3631:HOH:O	4:D:27:ASN:HB2	1.87	0.73
14:N:85:ARG:HA	14:N:87:MET:HE2	1.70	0.73
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.17	0.73
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.70	0.73
24:X:88:THR:HG22	24:X:89:ASP:N	2.03	0.73
1:A:2710:U:H1'	37:A:7159:HOH:O	1.88	0.73
12:L:55:VAL:HG12	12:L:56:SER:N	2.02	0.73
22:V:14:GLU:O	22:V:17:THR:HB	1.89	0.73
5:E:236:THR:H	5:E:239:ALA:HB3	1.53	0.73
6:F:105:SER:CB	6:F:131:THR:HG23	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.88	0.73
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.16	0.73
13:M:143:THR:HG22	13:M:144:ASP:N	2.01	0.73
14:N:169:ARG:HD2	37:N:8589:HOH:O	1.86	0.73
23:W:4:HIS:HB3	37:W:6622:HOH:O	1.88	0.73
1:A:1120:U:H5''	1:A:1120:U:C6	2.24	0.73
1:A:2421:G:H3'	1:A:2422:U:H5''	1.69	0.73
3:C:194:MET:HE3	3:C:199:HIS:HB2	1.69	0.73
26:Z:235:GLU:H	26:Z:235:GLU:CD	1.95	0.73
1:A:1118:A:H62	1:A:1244:U:H3	1.35	0.73
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.01	0.73
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.69	0.73
1:A:506:G:H22	1:A:509:A:H5'	1.53	0.73
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.70	0.73
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.70	0.73
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.23	0.73
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.71	0.72
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.37	0.72
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.87	0.72
10:J:162:SER:CB	10:J:163:PRO:HD3	2.18	0.72
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.55	0.72
26:Z:212:ARG:HD2	37:Z:8605:HOH:O	1.88	0.72
1:A:1209:C:H2'	1:A:1210:G:H8	1.54	0.72
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.51	0.72
11:K:19:MET:CE	11:K:132:LEU:HD11	2.14	0.72
1:A:1160:G:C5'	1:A:1161:A:H5'	2.16	0.72
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.69	0.72
8:H:99:THR:HA	37:H:3461:HOH:O	1.90	0.72
12:L:81:ARG:HB2	12:L:87:ARG:NH1	2.01	0.72
23:W:39:ALA:N	23:W:40:PRO:HD2	2.05	0.72
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.22	0.72
6:F:19:GLU:O	6:F:20:LYS:HG2	1.90	0.72
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.53	0.72
1:A:1701:A:H4'	1:A:1702:U:H5''	1.72	0.72
4:D:162:MET:HE2	4:D:310:ARG:HD3	1.70	0.72
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.70	0.72
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.90	0.72
1:A:2281:C:H2'	1:A:2282:U:H5'	1.72	0.72
6:F:135:VAL:HG22	6:F:136:ARG:H	1.53	0.72
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.72	0.72
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:TYR:H	10:J:91:HIS:CE1	2.08	0.72
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.20	0.72
1:A:506:G:H22	1:A:509:A:C5'	2.02	0.72
1:A:2432:C:O4'	37:A:9316:HOH:O	2.08	0.72
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.24	0.72
13:M:136:ALA:HB3	37:M:8579:HOH:O	1.89	0.72
14:N:78:ASN:ND2	37:N:8646:HOH:O	2.22	0.72
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.72	0.72
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.72	0.72
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.72	0.72
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.71	0.72
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.54	0.72
1:A:544:G:H2'	1:A:545:G:H5''	1.72	0.71
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.90	0.71
14:N:172:GLY:O	14:N:183:VAL:HG11	1.90	0.71
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.25	0.71
1:A:2281:C:C2'	1:A:2282:U:H5'	2.20	0.71
1:A:2459:G:OP2	30:4:64:LYS:HD2	1.90	0.71
14:N:38:VAL:O	14:N:63:VAL:HG13	1.89	0.71
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.72	0.71
14:N:91:ILE:HA	37:N:8644:HOH:O	1.89	0.71
5:E:76:ARG:HD2	37:E:8440:HOH:O	1.91	0.71
14:N:87:MET:CB	30:4:46:ILE:HD13	2.20	0.71
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.72	0.71
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.24	0.71
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.85	0.71
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.06	0.71
1:A:1485:A:H4'	37:A:9859:HOH:O	1.89	0.71
2:B:3056:A:C2'	2:B:3057:A:H5''	2.20	0.71
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.71	0.71
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.73	0.71
1:A:111:C:O2'	28:2:20:ARG:HG2	1.91	0.71
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.20	0.71
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.73	0.71
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.89	0.71
1:A:1625:U:H4'	37:A:4226:HOH:O	1.90	0.70
37:A:7092:HOH:O	30:4:60:LYS:HG3	1.89	0.70
4:D:62:ARG:HA	4:D:65:MET:CE	2.19	0.70
1:A:263:U:O4'	8:H:59:ILE:HD13	1.90	0.70
1:A:284:C:H4'	1:A:285:A:O5'	1.90	0.70
1:A:541:C:H2'	1:A:542:A:C5'	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:C:H4'	1:A:1081:A:OP1	1.90	0.70
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.06	0.70
1:A:2346:C:O2'	6:F:52:THR:HG21	1.91	0.70
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.91	0.70
1:A:2533:C:H5'	1:A:2533:C:C6	2.23	0.70
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.54	0.70
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.92	0.70
14:N:38:VAL:C	14:N:63:VAL:HG13	2.17	0.70
1:A:1187:U:H2'	37:A:6434:HOH:O	1.91	0.70
7:G:84:MET:HE2	7:G:133:VAL:CG2	2.21	0.70
28:2:8:GLN:HE22	28:2:11:LYS:NZ	1.89	0.70
4:D:62:ARG:CA	4:D:65:MET:HE3	2.22	0.70
10:J:163:PRO:HG2	37:J:8338:HOH:O	1.89	0.70
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.55	0.70
1:A:204:A:H2'	1:A:205:U:H5'	1.72	0.70
1:A:625:U:H5'	37:A:9757:HOH:O	1.92	0.70
1:A:1116:U:O2'	1:A:1118:A:H2	1.70	0.70
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.57	0.70
3:C:200:PRO:HD3	37:C:8520:HOH:O	1.91	0.70
14:N:64:ARG:HD2	37:N:8584:HOH:O	1.91	0.70
22:V:9:CYS:CA	22:V:52:THR:HG23	2.21	0.70
1:A:1334:C:OP2	37:A:3583:HOH:O	2.10	0.70
23:W:12:THR:HG22	23:W:15:GLU:CG	2.21	0.70
1:A:1241:G:H21	11:K:86:MET:HE2	1.57	0.70
11:K:93:ARG:HB3	11:K:93:ARG:HH11	1.55	0.70
7:G:43:ASP:HA	37:G:5864:HOH:O	1.92	0.70
8:H:58:GLU:HG3	8:H:61:MET:HE2	1.74	0.70
8:H:104:ALA:HA	37:H:6617:HOH:O	1.91	0.70
14:N:74:ARG:NH2	37:N:8629:HOH:O	2.23	0.70
1:A:542:A:H5'	1:A:542:A:C8	2.19	0.69
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.22	0.69
1:A:396:U:H4'	37:4:8529:HOH:O	1.92	0.69
14:N:89:ASN:HA	37:N:8554:HOH:O	1.92	0.69
16:P:87:THR:O	16:P:91:GLN:HG3	1.92	0.69
3:C:121:ALA:O	3:C:124:VAL:HG22	1.91	0.69
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.90	0.69
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.75	0.69
28:2:1:THR:HB	37:2:8457:HOH:O	1.90	0.69
1:A:182:G:H4'	14:N:157:LEU:HD13	1.72	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:447:A:OP1	21:U:2:LYS:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.56	0.69
27:1:30:GLU:HA	27:1:33:HIS:CB	2.23	0.69
1:A:1119:G:N2	1:A:1246:A:C2	2.60	0.69
4:D:162:MET:HE2	4:D:310:ARG:CD	2.22	0.69
4:D:175:LEU:HD23	4:D:175:LEU:C	2.17	0.69
14:N:61:ILE:HG13	37:N:8622:HOH:O	1.92	0.69
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.72	0.69
3:C:199:HIS:CD2	3:C:201:PHE:H	2.11	0.69
7:G:84:MET:HE1	7:G:148:ILE:CD1	2.22	0.69
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.69
1:A:1667:A:H5'	1:A:1667:A:C8	2.25	0.69
1:A:1751:G:C2'	1:A:1752:G:H5''	2.22	0.69
1:A:2316:G:H8	37:A:5201:HOH:O	1.76	0.69
5:E:98:ARG:O	37:E:8347:HOH:O	2.09	0.69
1:A:2456:A:H5'	37:A:5241:HOH:O	1.92	0.69
2:B:3013:A:O2'	2:B:3014:G:H5''	1.92	0.69
4:D:258:GLY:H	4:D:260:HIS:CE1	2.10	0.69
11:K:107:ASN:ND2	11:K:109:TYR:H	1.91	0.69
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.92	0.69
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.75	0.69
26:Z:141:THR:HG23	37:Z:8592:HOH:O	1.92	0.69
30:4:31:THR:HB	30:4:33:MET:HE3	1.74	0.69
2:B:3039:U:H1'	2:B:3044:A:H61	1.56	0.69
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.75	0.69
7:G:11:VAL:HG12	7:G:12:ASP:N	2.06	0.69
24:X:65:VAL:HA	24:X:68:THR:HG22	1.75	0.69
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.93	0.68
4:D:141:ARG:HD2	4:D:163:GLU:OE2	1.92	0.68
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.08	0.68
17:Q:58:SER:HB3	37:Q:4744:HOH:O	1.94	0.68
1:A:2271:G:P	37:A:9011:HOH:O	2.50	0.68
1:A:2359:G:O5'	37:A:5237:HOH:O	2.12	0.68
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.08	0.68
1:A:2912:C:OP2	37:A:5101:HOH:O	2.11	0.68
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.75	0.68
14:N:186:SER:O	14:N:189:VAL:HG12	1.93	0.68
1:A:631:A:N3	1:A:2073:G:O2'	2.26	0.68
1:A:2768:A:H2'	1:A:2769:C:O4'	1.92	0.68
1:A:2635:A:O2'	1:A:2636:C:H5'	1.94	0.68
4:D:145:HIS:HD2	4:D:146:THR:O	1.76	0.68
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:A:O2'	37:A:9373:HOH:O	2.11	0.68
1:A:544:G:C2'	1:A:545:G:H5''	2.24	0.68
1:A:951:A:C2'	1:A:952:G:H5'	2.24	0.68
10:J:127:GLY:O	10:J:128:ALA:HB3	1.93	0.68
14:N:139:PRO:O	14:N:140:ALA:HB3	1.92	0.68
1:A:1191:A:H3'	1:A:1192:A:H5''	1.74	0.68
1:A:1249:U:H2'	1:A:1250:C:C6	2.28	0.68
1:A:2506:A:H1'	37:A:5601:HOH:O	1.92	0.68
3:C:192:VAL:HB	37:C:8605:HOH:O	1.92	0.68
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.22	0.68
27:1:29:VAL:O	27:1:33:HIS:HB2	1.94	0.68
27:1:49:ARG:HD2	37:1:8430:HOH:O	1.93	0.68
1:A:656:G:OP2	16:P:37:ARG:HD2	1.93	0.68
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.75	0.68
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.27	0.68
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.29	0.67
1:A:2755:G:H1'	37:A:4242:HOH:O	1.94	0.67
10:J:57:ARG:HG3	37:J:8354:HOH:O	1.94	0.67
1:A:558:C:H5'	37:A:4812:HOH:O	1.92	0.67
24:X:110:GLN:NE2	24:X:110:GLN:HA	2.09	0.67
1:A:516:A:OP2	37:A:5193:HOH:O	2.11	0.67
37:A:4145:HOH:O	14:N:87:MET:HE1	1.95	0.67
14:N:68:ARG:O	14:N:68:ARG:HD3	1.94	0.67
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.76	0.67
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.24	0.67
7:G:93:MET:HE1	7:G:165:GLY:H	1.60	0.67
13:M:21:ARG:N	37:M:8535:HOH:O	2.27	0.67
19:S:39:THR:HB	19:S:42:GLU:HG3	1.75	0.67
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.30	0.67
27:1:75:ALA:HB3	37:1:8439:HOH:O	1.93	0.67
4:D:214:PRO:HD2	37:D:8520:HOH:O	1.95	0.67
24:X:4:LEU:O	24:X:32:CYS:HA	1.94	0.67
6:F:23:VAL:HG23	6:F:23:VAL:O	1.95	0.67
1:A:299:U:H5'	37:A:6872:HOH:O	1.94	0.67
1:A:1878:G:H1'	37:A:5666:HOH:O	1.95	0.67
1:A:2291:A:C8	1:A:2309:C:H5'	2.29	0.67
1:A:2897:C:O2'	1:A:2898:G:H5'	1.95	0.67
11:K:131:THR:HG22	11:K:134:GLU:H	1.60	0.67
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.77	0.67
29:3:41:HIS:N	29:3:45:ASN:HD22	1.90	0.67
1:A:2276:U:H2'	1:A:2277:U:C6	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:ARG:HD3	4:D:9:GLY:O	1.95	0.67
4:D:179:LEU:O	4:D:183:GLU:HG2	1.95	0.67
7:G:79:GLY:HA3	37:G:7046:HOH:O	1.94	0.67
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.94	0.67
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.93	0.67
1:A:2508:C:H2'	37:A:6288:HOH:O	1.95	0.67
23:W:39:ALA:C	23:W:41:GLU:H	2.03	0.67
1:A:383:A:OP2	37:A:9352:HOH:O	2.12	0.66
1:A:941:G:O2'	1:A:942:U:H5'	1.94	0.66
1:A:2466:G:H5''	37:A:3220:HOH:O	1.95	0.66
1:A:1614:G:H2'	37:A:4187:HOH:O	1.94	0.66
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.60	0.66
1:A:2301:A:H5''	1:A:2302:A:H5'	1.76	0.66
14:N:164:THR:CG2	14:N:165:SER:N	2.58	0.66
1:A:204:A:C2'	1:A:205:U:H5'	2.24	0.66
31:A:4000:CAI:H21A	34:A:8523:CL:CL	2.31	0.66
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.95	0.66
8:H:105:ALA:HB2	37:H:5522:HOH:O	1.94	0.66
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.60	0.66
10:J:140:PRO:HB3	37:J:8382:HOH:O	1.95	0.66
14:N:138:HIS:ND1	14:N:139:PRO:O	2.28	0.66
1:A:21:G:C5'	19:S:2:ILE:HA	2.25	0.66
1:A:1159:G:P	37:A:3858:HOH:O	2.53	0.66
5:E:1:MET:HG2	5:E:2:GLN:H	1.60	0.66
1:A:282:C:H1'	1:A:368:C:H42	1.58	0.66
1:A:338:C:H5''	37:E:8427:HOH:O	1.96	0.66
1:A:1735:C:O2'	1:A:1736:A:H5'	1.95	0.66
1:A:2408:A:H2	37:A:9671:HOH:O	1.77	0.66
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.77	0.66
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.26	0.66
27:1:61:GLY:HA3	37:1:8427:HOH:O	1.94	0.66
1:A:1857:A:N6	1:A:2247:C:H1'	2.11	0.66
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.94	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.61	0.66
37:A:3295:HOH:O	14:N:157:LEU:HD11	1.95	0.66
1:A:2064:U:H5'	1:A:2652:U:O3'	1.96	0.66
1:A:2748:G:H2'	37:A:7077:HOH:O	1.96	0.66
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.95	0.66
6:F:69:ILE:HG22	6:F:69:ILE:O	1.95	0.66
6:F:95:THR:C	6:F:97:GLN:H	2.03	0.66
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:71:LYS:HG3	17:Q:71:LYS:O	1.96	0.66
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.96	0.66
1:A:1766:U:O2	1:A:1778:A:H5'	1.96	0.66
1:A:2505:G:O2'	1:A:2506:A:H5'	1.96	0.66
1:A:2851:G:O2'	1:A:2852:A:H5'	1.96	0.66
37:A:4082:HOH:O	14:N:94:LYS:HE3	1.95	0.66
3:C:164:ARG:NE	37:C:8597:HOH:O	2.28	0.66
11:K:103:VAL:HG12	37:K:8563:HOH:O	1.95	0.66
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.78	0.66
1:A:160:A:C4	1:A:177:A:C2	2.84	0.65
1:A:581:G:H5'	37:A:7220:HOH:O	1.96	0.65
1:A:2813:A:OP2	37:A:3849:HOH:O	2.14	0.65
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.76	0.65
6:F:95:THR:O	6:F:97:GLN:N	2.25	0.65
23:W:64:GLY:O	23:W:65:ASP:HB2	1.94	0.65
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.96	0.65
8:H:110:GLU:HG2	37:H:6926:HOH:O	1.95	0.65
10:J:46:VAL:O	10:J:146:TRP:HH2	1.79	0.65
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.45	0.65
1:A:188:C:H5''	14:N:163:LEU:HD21	1.77	0.65
10:J:111:MET:O	10:J:114:PRO:HD3	1.96	0.65
1:A:2064:U:H4'	1:A:2653:A:OP1	1.96	0.65
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
24:X:5:VAL:HG11	24:X:153:MET:HE1	1.79	0.65
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.79	0.65
1:A:871:G:C8	1:A:871:G:C5'	2.65	0.65
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.30	0.65
5:E:178:GLN:OE1	37:E:8473:HOH:O	2.13	0.65
1:A:469:G:O2'	37:A:9628:HOH:O	2.14	0.65
5:E:16:VAL:HG12	5:E:17:ASP:N	2.11	0.65
21:U:48:VAL:HG22	21:U:97:ARG:C	2.20	0.65
1:A:485:A:O2'	1:A:487:G:H5'	1.97	0.65
24:X:130:HIS:O	24:X:136:GLY:HA3	1.97	0.65
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.03	0.65
1:A:2096:A:H2'	1:A:2539:U:H1'	1.77	0.65
1:A:2346:C:O5'	1:A:2346:C:H6	1.79	0.65
6:F:97:GLN:HG2	6:F:97:GLN:O	1.96	0.65
1:A:1160:G:H5'	1:A:1161:A:C5'	2.16	0.65
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.77	0.65
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.95	0.65
14:N:172:GLY:C	14:N:183:VAL:HG11	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27:LYS:N	10:J:58:HIS:HD2	1.93	0.64
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.78	0.64
1:A:134:U:C2	1:A:145:A:C2	2.86	0.64
13:M:143:THR:HG22	13:M:145:LEU:H	1.60	0.64
1:A:820:G:O2'	1:A:856:G:H4'	1.98	0.64
37:A:5232:HOH:O	15:O:21:HIS:HE1	1.81	0.64
2:B:3020:G:H3'	37:B:2984:HOH:O	1.96	0.64
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.77	0.64
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.12	0.64
1:A:2392:C:N3	37:A:4408:HOH:O	2.29	0.64
10:J:136:VAL:HG23	37:J:8343:HOH:O	1.95	0.64
10:J:139:ASP:H	10:J:140:PRO:HD3	1.62	0.64
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.61	0.64
1:A:1187:U:O2'	1:A:1189:A:H2	1.81	0.64
1:A:2421:G:H3'	1:A:2422:U:C5'	2.28	0.64
37:A:3128:HOH:O	14:N:152:ARG:HG3	1.97	0.64
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.62	0.64
19:S:99:ALA:HB1	19:S:109:MET:CE	2.15	0.64
21:U:37:GLN:OE1	21:U:118:SER:HA	1.97	0.64
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.80	0.64
1:A:1256:C:OP2	37:A:6690:HOH:O	2.15	0.64
1:A:1741:U:O2'	1:A:2723:G:H4'	1.97	0.64
1:A:1847:A:OP1	3:C:175:LYS:HG3	1.96	0.64
4:D:221:GLN:HE22	12:L:42:ASN:ND2	1.95	0.64
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.33	0.64
37:A:9768:HOH:O	13:M:4:LYS:HG3	1.96	0.64
2:B:3001:U:O3'	2:B:3003:A:H5''	1.98	0.64
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.79	0.64
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.80	0.64
16:P:44:ASN:OD1	16:P:65:LEU:HB2	1.98	0.64
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.98	0.64
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.64
1:A:1119:G:H22	1:A:1246:A:H2	1.43	0.64
3:C:37:VAL:HG22	37:C:8607:HOH:O	1.98	0.64
13:M:22:ARG:HG2	37:M:8527:HOH:O	1.96	0.64
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.63	0.64
15:O:37:ARG:NE	37:O:8533:HOH:O	2.31	0.64
1:A:2502:C:C2'	1:A:2503:A:H5'	2.28	0.64
2:B:3014:G:H5'	2:B:3014:G:C8	2.31	0.64
3:C:94:LEU:N	3:C:94:LEU:HD23	2.12	0.64
10:J:27:LYS:H	10:J:58:HIS:CD2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:53:GLY:HA2	27:1:67:GLY:O	1.98	0.64
1:A:2094:G:H4'	4:D:245:SER:HB3	1.79	0.63
5:E:115:LEU:O	5:E:118:THR:HB	1.98	0.63
5:E:242:GLU:HG3	37:E:8383:HOH:O	1.97	0.63
9:I:12:ILE:N	9:I:13:PRO:CD	2.61	0.63
21:U:47:THR:HB	21:U:100:ASP:HB3	1.80	0.63
22:V:9:CYS:HA	22:V:52:THR:CG2	2.28	0.63
26:Z:109:LEU:HA	37:Z:8573:HOH:O	1.98	0.63
26:Z:144:ARG:CZ	37:Z:8616:HOH:O	2.45	0.63
1:A:821:U:H2'	1:A:822:C:H6	1.62	0.63
1:A:2361:A:H2'	1:A:2362:A:C8	2.33	0.63
37:A:5791:HOH:O	22:V:56:ARG:HB3	1.97	0.63
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.80	0.63
1:A:873:G:H2'	1:A:875:A:N7	2.14	0.63
3:C:88:ILE:HG22	3:C:88:ILE:O	1.96	0.63
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.80	0.63
12:L:115:ARG:HG3	12:L:116:GLU:N	2.14	0.63
13:M:148:GLU:HA	37:M:8578:HOH:O	1.97	0.63
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.80	0.63
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.29	0.63
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.80	0.63
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.80	0.63
1:A:281:U:H3'	37:A:6740:HOH:O	1.99	0.63
1:A:1311:G:C2	1:A:1312:G:C8	2.87	0.63
1:A:1730:G:H5'	1:A:1731:C:C5	2.34	0.63
7:G:69:ILE:HA	7:G:72:MET:HE2	1.80	0.63
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.98	0.63
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.28	0.63
15:O:12:ARG:HD3	15:O:18:THR:OG1	1.98	0.63
1:A:681:G:H5'	1:A:681:G:N3	2.14	0.63
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.80	0.63
19:S:39:THR:HG23	19:S:107:GLU:O	1.97	0.63
1:A:154:C:H2'	1:A:155:C:H6	1.63	0.63
1:A:2082:G:O2'	1:A:2083:A:H5'	1.98	0.63
2:B:3009:C:OP2	37:B:466:HOH:O	2.16	0.63
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.81	0.63
2:B:3029:C:H2'	2:B:3030:C:H5'	1.79	0.63
15:O:4:PRO:HD2	37:O:8559:HOH:O	1.99	0.63
1:A:168:C:O2'	1:A:169:A:H5'	1.98	0.63
1:A:603:A:H5''	1:A:604:G:OP1	1.97	0.63
1:A:1130:U:H2'	1:A:1131:G:O4'	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:C:H2'	1:A:2503:A:H5'	1.81	0.63
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.14	0.63
1:A:157:G:H4'	14:N:95:LYS:HE3	1.81	0.62
1:A:184:G:H5''	14:N:153:THR:HG22	1.81	0.62
1:A:1834:C:H2'	1:A:1840:A:H62	1.63	0.62
37:A:4392:HOH:O	11:K:47:THR:HB	1.99	0.62
5:E:142:ASP:OD2	5:E:238:SER:OG	2.16	0.62
6:F:35:ALA:N	37:F:5576:HOH:O	2.31	0.62
13:M:114:VAL:HG11	37:M:8579:HOH:O	1.98	0.62
15:O:80:SER:HB2	37:O:8536:HOH:O	1.99	0.62
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.31	0.62
1:A:2613:G:O2'	1:A:2614:C:H5'	2.00	0.62
5:E:84:VAL:O	5:E:85:LYS:HB2	1.99	0.62
12:L:74:VAL:O	12:L:74:VAL:HG12	1.99	0.62
14:N:30:GLU:O	14:N:34:GLU:HG3	1.99	0.62
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.64	0.62
15:O:119:GLN:O	15:O:123:ILE:HG13	1.99	0.62
16:P:39:THR:O	16:P:115:ARG:NH2	2.32	0.62
25:Y:75:ALA:O	25:Y:83:ALA:HA	1.99	0.62
1:A:318:C:O2	37:A:3372:HOH:O	2.13	0.62
1:A:1773:G:C8	27:1:16:PRO:HA	2.34	0.62
4:D:248:ARG:O	4:D:251:VAL:CG1	2.48	0.62
5:E:12:THR:HB	37:E:8448:HOH:O	1.97	0.62
6:F:25:MET:CE	6:F:37:ALA:HB1	2.29	0.62
7:G:6:GLU:HA	7:G:46:THR:HG22	1.81	0.62
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.92	0.62
15:O:169:PRO:O	15:O:172:PHE:HB3	2.00	0.62
1:A:1119:G:H8	11:K:52:GLN:HE22	1.46	0.62
1:A:2433:A:H2'	1:A:2434:A:C8	2.34	0.62
1:A:2472:C:O2'	1:A:2634:G:H4'	1.98	0.62
1:A:2908:A:H2'	1:A:2909:G:O4'	1.99	0.62
2:B:3039:U:H1'	2:B:3044:A:N6	2.13	0.62
4:D:82:VAL:O	4:D:82:VAL:HG12	1.98	0.62
4:D:305:ASP:O	4:D:306:LYS:HB2	1.98	0.62
5:E:118:THR:O	5:E:136:VAL:HG13	1.99	0.62
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.99	0.62
12:L:30:LYS:O	12:L:55:VAL:HG13	1.98	0.62
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.81	0.62
15:O:157:PRO:HA	37:O:8526:HOH:O	1.98	0.62
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.80	0.62
1:A:1700:C:OP2	37:A:5580:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.29	0.62
11:K:74:ARG:O	11:K:78:ILE:HG12	1.98	0.62
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.80	0.62
19:S:82:GLU:HG3	19:S:83:LYS:H	1.65	0.62
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.30	0.62
7:G:69:ILE:HA	7:G:72:MET:CE	2.30	0.62
14:N:47:ASP:CG	14:N:48:ARG:N	2.57	0.62
15:O:73:ALA:N	37:O:8568:HOH:O	2.33	0.62
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.35	0.62
29:3:24:TRP:CD1	37:3:6863:HOH:O	2.52	0.62
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.65	0.62
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.65	0.62
1:A:2047:C:H5'	37:A:9397:HOH:O	1.99	0.62
1:A:2314:G:C2'	1:A:2315:C:H5'	2.30	0.62
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.14	0.62
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.12	0.62
1:A:272:A:H5'	1:A:273:G:OP2	1.99	0.62
1:A:1116:U:O2'	1:A:1118:A:C2	2.49	0.62
1:A:1634:G:H3'	37:A:3463:HOH:O	1.99	0.62
1:A:1819:G:H2'	1:A:1820:G:H4'	1.80	0.62
5:E:61:PHE:HB3	37:E:8451:HOH:O	1.99	0.62
5:E:214:THR:HG21	37:E:8408:HOH:O	1.99	0.62
5:E:246:ARG:NE	37:E:8430:HOH:O	2.32	0.62
6:F:135:VAL:HG22	6:F:136:ARG:N	2.14	0.62
21:U:48:VAL:HG22	21:U:97:ARG:O	1.99	0.62
24:X:81:ASP:OD1	24:X:92:ASP:HB2	1.99	0.62
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.14	0.62
27:1:31:ILE:O	27:1:35:LYS:HG3	1.99	0.62
1:A:2324:G:H4'	1:A:2418:G:O2'	1.99	0.62
1:A:2502:C:H4'	10:J:151:MET:HG2	1.82	0.62
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.15	0.62
1:A:1269:G:O2'	1:A:1270:U:H5'	2.00	0.62
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.80	0.62
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.82	0.62
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.30	0.62
1:A:1923:G:H4'	30:4:31:THR:O	2.00	0.61
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.81	0.61
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.65	0.61
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.65	0.61
3:C:33:GLU:O	3:C:34:ASP:HB2	1.99	0.61
6:F:99:ASP:CB	6:F:103:ASN:H	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:104:ASP:HB3	37:M:8570:HOH:O	2.00	0.61
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.82	0.61
1:A:921:G:H4'	1:A:924:G:C6	2.35	0.61
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.83	0.61
27:1:46:LYS:HB3	37:1:8442:HOH:O	2.00	0.61
1:A:1197:G:N2	37:A:5777:HOH:O	2.33	0.61
1:A:2241:C:O2'	1:A:2242:U:H5'	1.99	0.61
1:A:2414:A:H2'	1:A:2415:A:C8	2.35	0.61
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.97	0.61
1:A:2577:A:H5'	37:A:7289:HOH:O	1.98	0.61
37:A:8976:HOH:O	14:N:94:LYS:HE2	1.99	0.61
5:E:103:ASN:HB3	37:E:8309:HOH:O	2.00	0.61
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.30	0.61
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.65	0.61
14:N:166:ALA:HB1	37:N:8542:HOH:O	2.01	0.61
1:A:272:A:H3'	37:A:7066:HOH:O	2.01	0.61
1:A:1086:A:C6	24:X:11:VAL:HG11	2.35	0.61
1:A:2079:G:O6	37:A:7403:HOH:O	2.12	0.61
1:A:2769:C:H2'	1:A:2770:G:O4'	2.01	0.61
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.82	0.61
6:F:25:MET:HE1	6:F:37:ALA:O	2.00	0.61
14:N:154:ARG:HG3	37:N:8612:HOH:O	1.99	0.61
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.15	0.61
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.98	0.61
1:A:669:G:O2'	1:A:670:G:H5'	2.01	0.61
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.49	0.61
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.83	0.61
19:S:82:GLU:HG3	19:S:83:LYS:N	2.15	0.61
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.01	0.61
1:A:1086:A:N6	24:X:11:VAL:HG11	2.15	0.61
1:A:1205:U:H2'	1:A:1206:U:C5'	2.29	0.61
37:A:5862:HOH:O	6:F:55:LYS:HB2	1.99	0.61
4:D:168:GLY:N	4:D:174:ARG:HD3	2.15	0.61
15:O:86:LEU:O	15:O:90:LEU:HG	2.01	0.61
1:A:20:G:H21	19:S:117:HIS:HD2	1.48	0.61
4:D:248:ARG:NH1	37:D:8619:HOH:O	2.30	0.61
10:J:71:TYR:C	10:J:73:GLN:N	2.56	0.61
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.30	0.61
14:N:139:PRO:O	14:N:140:ALA:CB	2.48	0.61
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.00	0.61
1:A:214:U:H5'	37:A:5686:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2637:A:H5'	37:A:8860:HOH:O	2.01	0.61
1:A:2787:C:H5	37:A:4192:HOH:O	1.84	0.61
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.83	0.61
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.26	0.61
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.83	0.61
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.30	0.61
8:H:53:ASP:OD1	8:H:80:GLN:HB2	2.00	0.61
9:I:63:ARG:N	37:I:2569:HOH:O	2.34	0.61
13:M:143:THR:CG2	13:M:144:ASP:N	2.63	0.61
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.26	0.61
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.33	0.61
1:A:2748:G:H5'	37:A:7077:HOH:O	2.01	0.60
1:A:2878:U:H2'	1:A:2879:A:O4'	2.01	0.60
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.82	0.60
4:D:2:GLN:HA	37:D:8625:HOH:O	2.00	0.60
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.81	0.60
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.01	0.60
5:E:16:VAL:HG12	5:E:17:ASP:H	1.66	0.60
1:A:2096:A:H2'	1:A:2539:U:C1'	2.30	0.60
1:A:2359:G:H3'	37:A:5237:HOH:O	2.01	0.60
5:E:55:ARG:HB2	37:E:8311:HOH:O	1.99	0.60
10:J:75:SER:O	10:J:79:ALA:HB2	2.01	0.60
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.31	0.60
1:A:2587:U:H2'	1:A:2589:U:H5''	1.83	0.60
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.34	0.60
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.31	0.60
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.83	0.60
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.17	0.60
15:O:152:GLU:C	15:O:154:LEU:H	2.07	0.60
22:V:9:CYS:SG	22:V:11:THR:HG23	2.40	0.60
22:V:30:HIS:HB3	37:V:6215:HOH:O	2.01	0.60
24:X:119:HIS:HD2	24:X:120:PRO:O	1.85	0.60
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.33	0.60
1:A:1192:A:O2'	1:A:1193:A:OP1	2.19	0.60
1:A:1713:G:H1'	37:A:4626:HOH:O	2.00	0.60
2:B:3028:U:H2'	2:B:3029:C:C6	2.36	0.60
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.66	0.60
11:K:19:MET:HE2	11:K:79:PHE:HA	1.83	0.60
19:S:44:VAL:O	19:S:48:GLU:HG3	2.01	0.60
23:W:8:ILE:HA	23:W:11:MET:HE3	1.83	0.60
1:A:2766:A:O2'	4:D:265:LEU:O	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.64	0.60
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.83	0.60
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.60
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.14	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.36	0.60
1:A:558:C:C2'	1:A:559:U:H5''	2.32	0.60
1:A:1123:A:C6	1:A:1238:C:H5'	2.37	0.60
37:A:7116:HOH:O	27:1:31:ILE:HG13	2.01	0.60
4:D:140:LEU:HD23	37:D:8583:HOH:O	2.00	0.60
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.32	0.60
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.36	0.60
12:L:9:THR:O	12:L:10:GLN:C	2.44	0.60
1:A:1681:G:H5''	1:A:1682:A:H5'	1.83	0.60
1:A:2453:G:H3'	37:A:5467:HOH:O	2.00	0.60
2:B:3076:G:C3'	2:B:3077:A:H5''	2.31	0.60
5:E:127:ARG:HD2	5:E:229:PRO:O	2.01	0.60
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.83	0.60
6:F:163:VAL:HA	37:F:6326:HOH:O	2.02	0.60
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.83	0.60
23:W:5:VAL:HG23	37:W:2271:HOH:O	2.02	0.60
1:A:816:G:H5'	1:A:1598:A:H4'	1.84	0.60
1:A:1743:G:H1'	37:A:4449:HOH:O	2.00	0.60
1:A:2284:G:H1'	37:A:9149:HOH:O	2.01	0.60
2:B:3049:G:H5''	37:B:4707:HOH:O	2.02	0.60
7:G:84:MET:HE2	7:G:133:VAL:HG21	1.83	0.60
8:H:28:ALA:HB3	8:H:99:THR:O	2.02	0.60
13:M:30:ARG:NH2	37:M:8523:HOH:O	2.26	0.60
14:N:74:ARG:O	14:N:88:VAL:HG13	2.01	0.60
15:O:22:GLN:HG2	15:O:26:LEU:HD22	1.82	0.60
15:O:151:ASP:O	15:O:154:LEU:HB2	2.02	0.60
1:A:513:A:N3	37:A:3234:HOH:O	2.30	0.60
1:A:1474:C:H6	1:A:1474:C:C5'	2.13	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.60
2:B:3003:A:N6	2:B:3022:G:H1'	2.17	0.60
3:C:179:MET:HG2	3:C:186:TRP:CB	2.32	0.60
1:A:2897:C:H2'	1:A:2898:G:H8	1.66	0.60
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.16	0.60
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.37	0.60
14:N:46:LEU:HG	37:N:8621:HOH:O	2.02	0.60
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.17	0.60
14:N:104:ARG:O	14:N:108:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:132:ARG:HG2	19:S:133:ALA:N	2.17	0.60
20:T:43:GLU:HB3	37:T:7106:HOH:O	2.01	0.60
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.60
1:A:1377:C:H6	1:A:1377:C:H5'	1.66	0.59
3:C:131:HIS:O	3:C:132:ASP:HB2	2.00	0.59
7:G:15:GLN:NE2	7:G:40:VAL:O	2.35	0.59
37:A:5067:HOH:O	4:D:298:LYS:HD3	2.01	0.59
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.67	0.59
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.83	0.59
1:A:381:G:H5''	37:A:3882:HOH:O	2.01	0.59
1:A:1641:A:H2'	1:A:1642:A:H5'	1.84	0.59
1:A:2506:A:C1'	37:A:5601:HOH:O	2.50	0.59
6:F:50:VAL:O	6:F:71:ALA:HA	2.02	0.59
10:J:49:VAL:O	10:J:157:ILE:HG23	2.03	0.59
23:W:58:THR:O	23:W:62:GLU:HG3	2.02	0.59
24:X:76:ASP:O	24:X:77:ALA:C	2.46	0.59
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
1:A:739:G:C5	37:A:7079:HOH:O	2.51	0.59
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.66	0.59
3:C:223:ARG:NH1	37:C:8518:HOH:O	2.36	0.59
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.02	0.59
14:N:47:ASP:CG	14:N:48:ARG:H	2.10	0.59
18:R:50:GLY:HA3	18:R:87:THR:OG1	2.02	0.59
20:T:57:THR:C	20:T:59:ASP:H	2.10	0.59
30:4:3:MET:O	30:4:90:PHE:HA	2.02	0.59
1:A:545:G:H5'	1:A:545:G:C8	2.36	0.59
1:A:1810:C:OP1	22:V:44:ARG:NE	2.22	0.59
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.35	0.59
37:E:8357:HOH:O	16:P:3:THR:HG21	2.03	0.59
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.33	0.59
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.85	0.59
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.38	0.59
1:A:189:A:OP1	14:N:171:ARG:NH2	2.36	0.59
1:A:1176:C:H1'	37:A:3499:HOH:O	2.02	0.59
1:A:2064:U:H5'	1:A:2652:U:H4'	1.83	0.59
1:A:2093:G:H5''	37:A:9058:HOH:O	2.00	0.59
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.01	0.59
1:A:2559:C:H4'	37:A:6790:HOH:O	2.02	0.59
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.67	0.59
15:O:154:LEU:O	15:O:155:GLU:HB3	2.01	0.59
27:1:25:ARG:O	27:1:29:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:A:O2'	13:M:41:HIS:HD2	1.86	0.59
1:A:1393:A:H2'	1:A:1394:C:C6	2.38	0.59
1:A:2251:G:H4'	37:A:6944:HOH:O	2.03	0.59
1:A:2433:A:H2'	1:A:2434:A:H8	1.68	0.59
4:D:280:VAL:CG1	4:D:334:SER:HA	2.32	0.59
15:O:58:LEU:HD12	15:O:58:LEU:N	2.17	0.59
28:2:8:GLN:HE22	28:2:11:LYS:HZ1	1.50	0.59
1:A:470:U:O2'	28:2:16:HIS:HD2	1.85	0.59
1:A:1241:G:C2	11:K:86:MET:HE2	2.37	0.59
1:A:1657:A:H2'	1:A:1658:A:C8	2.38	0.59
4:D:146:THR:O	4:D:159:PRO:HB3	2.03	0.59
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.85	0.59
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.01	0.59
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.85	0.59
21:U:75:GLU:O	21:U:76:ASP:HB2	2.02	0.59
24:X:88:THR:CG2	24:X:89:ASP:H	2.11	0.59
1:A:125:U:H2'	37:A:3336:HOH:O	2.02	0.59
1:A:280:C:H2'	1:A:281:U:O4'	2.03	0.59
1:A:661:G:C5	1:A:686:A:C2	2.90	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.03	0.59
11:K:107:ASN:C	11:K:107:ASN:HD22	2.10	0.59
12:L:55:VAL:HG12	12:L:56:SER:H	1.67	0.59
23:W:39:ALA:N	23:W:40:PRO:CD	2.65	0.59
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.38	0.59
27:1:48:LYS:HG2	37:1:8433:HOH:O	2.01	0.59
1:A:182:G:H5'	37:A:4711:HOH:O	2.02	0.59
1:A:285:A:H2'	1:A:286:U:O4'	2.03	0.59
1:A:1204:C:H1'	37:A:4303:HOH:O	2.03	0.59
1:A:1477:C:O2'	1:A:1478:U:H5'	2.02	0.59
1:A:2121:G:O2'	1:A:2122:C:H5'	2.03	0.59
3:C:18:ALA:O	3:C:20:SER:N	2.33	0.59
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.85	0.59
4:D:51:VAL:HG23	4:D:329:TYR:O	2.02	0.59
4:D:79:MET:HE3	4:D:144:THR:HG21	1.83	0.59
5:E:77:ALA:O	5:E:78:ARG:HG3	2.03	0.59
7:G:101:GLU:HB2	7:G:116:THR:O	2.02	0.59
14:N:60:ILE:C	14:N:61:ILE:HD12	2.28	0.59
21:U:71:VAL:CG1	21:U:90:PRO:HB3	2.20	0.59
1:A:1234:U:N3	4:D:244:PRO:HB3	2.18	0.58
4:D:125:GLU:O	4:D:129:ARG:HG3	2.02	0.58
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.02	0.58
14:N:104:ARG:O	14:N:108:LYS:HE2	2.03	0.58
14:N:123:ASP:C	14:N:123:ASP:OD1	2.46	0.58
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.85	0.58
1:A:407:A:H5'	37:A:5570:HOH:O	2.03	0.58
1:A:485:A:N3	1:A:487:G:H5''	2.18	0.58
6:F:55:LYS:HA	37:F:6752:HOH:O	2.04	0.58
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.18	0.58
11:K:74:ARG:HH11	11:K:74:ARG:CB	2.16	0.58
1:A:1265:G:H1'	37:A:4558:HOH:O	2.02	0.58
1:A:1861:C:H4'	3:C:6:GLY:O	2.03	0.58
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.33	0.58
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.33	0.58
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.18	0.58
1:A:553:G:P	26:Z:204:ARG:HH22	2.26	0.58
1:A:960:G:H2'	1:A:960:G:N3	2.19	0.58
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.04	0.58
10:J:112:ARG:O	10:J:113:ALA:C	2.46	0.58
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.18	0.58
1:A:39:G:N2	1:A:444:C:C2	2.72	0.58
4:D:36:PRO:HA	4:D:168:GLY:CA	2.33	0.58
11:K:22:VAL:O	11:K:26:VAL:HG23	2.04	0.58
13:M:148:GLU:HB2	37:M:8594:HOH:O	2.01	0.58
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.39	0.58
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.84	0.58
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.00	0.58
37:B:5851:HOH:O	15:O:113:SER:HB3	2.03	0.58
5:E:236:THR:O	5:E:237:GLU:C	2.46	0.58
1:A:564:G:H1'	37:A:5852:HOH:O	2.04	0.58
1:A:797:A:O4'	27:1:10:ARG:N	2.36	0.58
1:A:958:G:O2'	1:A:959:C:H5'	2.02	0.58
2:B:3055:U:H4'	2:B:3056:A:C8	2.39	0.58
4:D:14:GLY:HA2	4:D:15:PRO:C	2.28	0.58
5:E:79:ARG:O	5:E:87:ARG:HG2	2.03	0.58
6:F:170:TYR:O	6:F:171:ASP:HB3	2.03	0.58
20:T:4:VAL:HG23	37:T:2334:HOH:O	2.01	0.58
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.04	0.58
1:A:21:G:H4'	19:S:2:ILE:HG22	1.86	0.58
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.86	0.58
7:G:15:GLN:HG2	7:G:19:ASP:O	2.04	0.58
15:O:163:PHE:HA	37:O:8519:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:6:LYS:HB2	20:T:27:ALA:O	2.03	0.58
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.85	0.58
1:A:151:A:C2	1:A:442:A:C8	2.92	0.58
1:A:283:U:H5''	1:A:284:C:P	2.44	0.58
1:A:820:G:OP1	27:1:17:ARG:NH2	2.30	0.58
1:A:1406:A:N1	37:A:5580:HOH:O	2.32	0.58
10:J:44:ALA:HA	10:J:163:PRO:O	2.04	0.58
1:A:828:G:N7	37:A:5406:HOH:O	2.32	0.58
1:A:1185:U:H2'	1:A:1186:C:C6	2.39	0.58
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.58
1:A:2634:G:O2'	1:A:2635:A:H5'	2.04	0.58
1:A:2718:C:H6	1:A:2718:C:H5'	1.69	0.58
37:A:6992:HOH:O	5:E:188:ARG:CD	2.52	0.58
23:W:56:ILE:O	23:W:60:GLN:HG3	2.04	0.58
1:A:461:C:H2'	37:A:3568:HOH:O	2.03	0.57
1:A:2506:A:O2'	1:A:2507:G:O5'	2.22	0.57
1:A:2729:C:O2'	1:A:2730:G:H5'	2.03	0.57
4:D:248:ARG:NH2	37:D:8525:HOH:O	2.36	0.57
13:M:145:LEU:O	13:M:148:GLU:HG3	2.04	0.57
15:O:64:SER:C	15:O:66:LEU:H	2.13	0.57
23:W:44:GLY:O	23:W:48:GLU:HG2	2.04	0.57
26:Z:216:ARG:CD	37:Z:8571:HOH:O	2.43	0.57
1:A:113:A:OP2	1:A:114:A:H2'	2.03	0.57
1:A:558:C:O2'	1:A:559:U:H5''	2.05	0.57
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.43	0.57
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.85	0.57
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.86	0.57
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.86	0.57
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.33	0.57
10:J:75:SER:C	10:J:79:ALA:HB2	2.29	0.57
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.03	0.57
1:A:2540:G:O2'	1:A:2541:U:H5''	2.04	0.57
37:A:8711:HOH:O	14:N:82:ARG:HD2	2.05	0.57
4:D:54:VAL:HB	37:D:8615:HOH:O	2.03	0.57
4:D:74:ILE:HG13	37:D:8607:HOH:O	2.04	0.57
4:D:305:ASP:O	4:D:306:LYS:CB	2.51	0.57
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.32	0.57
1:A:1559:A:H1'	37:A:5413:HOH:O	2.04	0.57
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.39	0.57
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.57
3:C:2:ARG:NH1	37:C:8516:HOH:O	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:233:THR:HG22	5:E:234:VAL:N	2.18	0.57
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.86	0.57
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.40	0.57
15:O:141:ARG:N	37:O:8571:HOH:O	2.36	0.57
25:Y:71:ARG:HB2	37:Y:6590:HOH:O	2.04	0.57
1:A:558:C:H2'	1:A:559:U:C5'	2.34	0.57
1:A:1589:G:N2	1:A:1605:G:H1'	2.20	0.57
3:C:105:VAL:HG12	3:C:106:CYS:N	2.19	0.57
4:D:75:GLU:C	4:D:77:PRO:HD3	2.30	0.57
5:E:236:THR:HA	37:E:8457:HOH:O	2.03	0.57
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.39	0.57
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.86	0.57
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.15	0.57
26:Z:186:ARG:HG2	26:Z:186:ARG:HH11	1.70	0.57
1:A:69:A:H5'	1:A:69:A:H8	1.70	0.57
1:A:1041:U:H2'	1:A:1042:U:H5'	1.86	0.57
1:A:1925:G:O2'	1:A:1926:G:H5'	2.05	0.57
1:A:2497:A:OP2	37:A:3560:HOH:O	2.17	0.57
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.86	0.57
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.57
1:A:629:A:C2	1:A:2074:A:C2	2.93	0.57
1:A:1269:G:H2'	1:A:1270:U:C6	2.39	0.57
1:A:1947:G:N2	1:A:1966:U:C2	2.73	0.57
1:A:2443:C:H3'	37:A:3048:HOH:O	2.04	0.57
8:H:100:ASP:O	8:H:101:ALA:O	2.23	0.57
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.33	0.57
1:A:1723:G:H2'	37:A:9203:HOH:O	2.03	0.57
1:A:2507:G:H2'	1:A:2510:C:H42	1.70	0.57
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.53	0.57
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.85	0.57
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.87	0.57
20:T:81:ILE:HG23	37:T:4527:HOH:O	2.05	0.57
24:X:48:VAL:CG1	24:X:48:VAL:O	2.51	0.57
24:X:48:VAL:O	24:X:48:VAL:HG12	2.03	0.57
1:A:2256:G:H2'	1:A:2257:G:H5'	1.87	0.57
1:A:538:C:H5''	1:A:539:G:C8	2.40	0.57
1:A:1329:A:H2	37:A:4243:HOH:O	1.88	0.57
1:A:2001:G:O2'	1:A:2002:C:H5'	2.05	0.57
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.87	0.57
10:J:136:VAL:HG22	10:J:137:ASN:O	2.04	0.57
10:J:139:ASP:N	10:J:140:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.85	0.57
1:A:105:G:O2'	1:A:106:A:H5'	2.05	0.56
1:A:816:G:C6	1:A:817:G:N1	2.73	0.56
37:A:9345:HOH:O	13:M:41:HIS:HE1	1.88	0.56
9:I:12:ILE:HG22	9:I:12:ILE:O	2.04	0.56
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.87	0.56
13:M:138:GLY:HA3	37:M:8558:HOH:O	2.04	0.56
1:A:474:C:O3'	5:E:73:LEU:HD21	2.05	0.56
6:F:37:ALA:O	6:F:40:ILE:HG12	2.06	0.56
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.05	0.56
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.34	0.56
10:J:69:ASN:O	10:J:72:VAL:HG12	2.06	0.56
1:A:183:A:H5'	14:N:157:LEU:HD12	1.87	0.56
1:A:1205:U:C2'	1:A:1206:U:H5'	2.29	0.56
1:A:1523:G:H2'	1:A:1524:U:C6	2.40	0.56
1:A:2405:C:H5'	37:A:6132:HOH:O	2.04	0.56
2:B:3003:A:H2'	37:B:2430:HOH:O	2.04	0.56
2:B:3055:U:H4'	2:B:3056:A:H8	1.70	0.56
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.21	0.56
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.70	0.56
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.56
6:F:59:GLY:C	6:F:61:PHE:H	2.14	0.56
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.86	0.56
30:4:73:GLU:HB2	37:4:8525:HOH:O	2.04	0.56
1:A:12:U:H2'	1:A:13:G:H5'	1.86	0.56
1:A:56:G:H5''	23:W:50:ARG:NH1	2.21	0.56
1:A:383:A:H4'	37:A:4881:HOH:O	2.04	0.56
1:A:1170:U:O2'	1:A:1172:G:N7	2.29	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:2326:U:H4'	1:A:2412:G:H4'	1.86	0.56
1:A:2464:C:H5''	1:A:2465:A:OP1	2.05	0.56
1:A:2906:A:H5'	1:A:2907:C:O4'	2.04	0.56
4:D:16:ARG:NH1	37:D:8620:HOH:O	2.37	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.18	0.56
7:G:7:ILE:HD11	7:G:11:VAL:C	2.30	0.56
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.36	0.56
11:K:45:VAL:HG23	11:K:130:VAL:O	2.04	0.56
27:1:54:ILE:HD12	37:1:8416:HOH:O	2.05	0.56
1:A:1687:C:O2	28:2:9:GLY:HA2	2.05	0.56
1:A:2326:U:H4'	1:A:2412:G:C4'	2.36	0.56
8:H:117:GLU:C	8:H:119:ARG:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:VAL:HG12	13:M:57:VAL:O	2.04	0.56
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.18	0.56
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.26	0.56
1:A:221:G:H2'	1:A:222:A:C8	2.40	0.56
1:A:415:A:O2'	1:A:416:G:H5'	2.06	0.56
1:A:679:G:OP2	37:A:4001:HOH:O	2.17	0.56
1:A:2000:G:O2'	1:A:2001:G:H5'	2.06	0.56
1:A:2896:A:H2'	1:A:2896:A:N3	2.21	0.56
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.20	0.56
4:D:297:VAL:HB	37:D:8607:HOH:O	2.06	0.56
1:A:920:C:H5'	1:A:921:G:C4	2.41	0.56
1:A:2582:G:H4'	37:L:4440:HOH:O	2.06	0.56
2:B:3002:U:OP2	2:B:3002:U:H4'	2.05	0.56
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.06	0.56
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.04	0.56
11:K:126:ASN:O	11:K:129:PHE:HE2	1.89	0.56
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.87	0.56
23:W:64:GLY:O	23:W:65:ASP:CB	2.54	0.56
1:A:251:C:O2'	1:A:252:C:H5'	2.06	0.56
1:A:1029:U:O2'	1:A:1273:C:OP1	2.19	0.56
1:A:2524:G:H21	1:A:2526:C:N4	2.03	0.56
5:E:141:SER:HA	37:E:8381:HOH:O	2.05	0.56
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.35	0.56
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.88	0.56
13:M:149:ARG:O	13:M:150:GLN:HB2	2.06	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
1:A:1441:G:O2'	1:A:1442:A:H5'	2.06	0.56
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.06	0.56
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.04	0.56
1:A:926:A:O2'	13:M:41:HIS:CD2	2.59	0.56
1:A:1057:A:C6	1:A:1058:A:C6	2.94	0.56
1:A:1165:G:OP1	1:A:1165:G:H3'	2.06	0.56
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.56
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.40	0.56
2:B:3107:C:H5	37:B:3167:HOH:O	1.89	0.56
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.69	0.56
7:G:68:HIS:O	7:G:72:MET:HG3	2.06	0.56
11:K:46:ILE:HA	37:K:8527:HOH:O	2.05	0.56
27:I:23:ARG:NH1	37:I:8404:HOH:O	2.39	0.56
1:A:45:A:N6	1:A:147:G:C4	2.74	0.55
1:A:684:G:H2'	1:A:685:C:C6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:A:H1'	1:A:1528:A:C8	2.41	0.55
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.06	0.55
37:A:6979:HOH:O	19:S:132:ARG:NH2	2.39	0.55
37:A:6992:HOH:O	5:E:188:ARG:HD3	2.05	0.55
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.87	0.55
30:4:62:THR:HB	37:4:8550:HOH:O	2.05	0.55
1:A:88:G:H5'	1:A:88:G:H8	1.71	0.55
1:A:2256:G:C2'	1:A:2257:G:H5'	2.36	0.55
5:E:7:ASP:OD1	5:E:11:ASN:O	2.23	0.55
5:E:85:LYS:NZ	37:E:8328:HOH:O	2.13	0.55
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.37	0.55
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.75	0.55
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.55
1:A:542:A:H2'	1:A:543:G:O4'	2.06	0.55
1:A:2791:U:H1'	1:A:2792:A:H5''	1.89	0.55
37:A:9374:HOH:O	12:L:39:GLY:HA3	2.05	0.55
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.88	0.55
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.88	0.55
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.87	0.55
24:X:5:VAL:O	24:X:52:VAL:HG22	2.05	0.55
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.88	0.55
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.41	0.55
1:A:539:G:H2'	1:A:540:A:C8	2.41	0.55
1:A:2429:A:H2'	1:A:2430:A:C8	2.41	0.55
37:A:8806:HOH:O	3:C:11:ARG:HD3	2.05	0.55
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.37	0.55
9:I:12:ILE:HD12	37:I:692:HOH:O	2.05	0.55
9:I:64:ASN:HD22	9:I:64:ASN:N	2.04	0.55
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.88	0.55
10:J:127:GLY:O	10:J:128:ALA:CB	2.54	0.55
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.36	0.55
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.89	0.55
24:X:26:ILE:HG13	24:X:26:ILE:O	2.06	0.55
1:A:2526:C:C2'	1:A:2527:U:H5'	2.36	0.55
10:J:71:TYR:O	10:J:73:GLN:N	2.38	0.55
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.36	0.55
27:1:46:LYS:O	27:1:57:CYS:HA	2.07	0.55
1:A:119:A:H2'	1:A:120:A:H5''	1.88	0.55
1:A:396:U:OP2	30:4:38:ARG:NH1	2.39	0.55
1:A:920:C:H4'	1:A:921:G:C2	2.42	0.55
1:A:1711:A:O2'	1:A:1712:A:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2402:A:H1'	37:A:9731:HOH:O	2.06	0.55
1:A:2769:C:C2'	1:A:2770:G:H5'	2.37	0.55
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.89	0.55
18:R:32:GLU:HA	18:R:71:TYR:OH	2.07	0.55
1:A:212:A:O4'	1:A:214:U:C6	2.60	0.55
1:A:1909:A:H2'	1:A:1910:A:C8	2.41	0.55
34:A:8513:CL:CL	37:A:4243:HOH:O	2.56	0.55
4:D:238:ASN:HD22	4:D:240:GLY:N	2.02	0.55
4:D:248:ARG:O	4:D:251:VAL:HG12	2.06	0.55
6:F:64:ARG:O	6:F:67:ASP:OD2	2.23	0.55
8:H:107:VAL:O	8:H:111:ILE:HG13	2.05	0.55
19:S:39:THR:HB	19:S:42:GLU:CG	2.36	0.55
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.46	0.55
1:A:152:A:O2'	1:A:153:C:H5'	2.07	0.55
1:A:902:G:N7	13:M:18:HIS:HD2	2.04	0.55
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.18	0.55
6:F:101:THR:HG22	37:F:7400:HOH:O	2.07	0.55
10:J:166:ASN:N	10:J:166:ASN:HD22	2.03	0.55
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.22	0.55
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.21	0.55
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.71	0.55
1:A:1003:U:O2	10:J:90:PHE:CZ	2.59	0.55
1:A:1127:C:H2'	1:A:1128:U:H5'	1.88	0.55
1:A:2123:A:H5'	14:N:89:ASN:ND2	2.22	0.55
37:A:4843:HOH:O	24:X:154:ARG:C	2.49	0.55
6:F:136:ARG:HD2	6:F:155:HIS:O	2.07	0.55
7:G:21:THR:HG23	7:G:30:THR:OG1	2.07	0.55
12:L:34:VAL:HB	37:L:7169:HOH:O	2.07	0.55
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.42	0.55
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.65	0.55
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.07	0.55
1:A:2459:G:P	30:4:64:LYS:HB2	2.47	0.55
1:A:2729:C:H2'	1:A:2730:G:H8	1.72	0.55
31:A:4000:CAI:H2B1	31:A:4000:CAI:H6A3	1.89	0.55
3:C:164:ARG:CZ	37:C:8597:HOH:O	2.55	0.55
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.89	0.55
10:J:65:ARG:CZ	37:J:8386:HOH:O	2.55	0.55
24:X:38:THR:HG22	24:X:39:ASP:N	2.22	0.55
1:A:155:C:OP2	14:N:188:ARG:HD3	2.07	0.54
1:A:182:G:O2'	1:A:183:A:H5'	2.07	0.54
4:D:204:GLY:C	37:D:8660:HOH:O	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ARG:NH1	37:E:8356:HOH:O	2.39	0.54
7:G:23:GLU:HG2	7:G:28:SER:CB	2.37	0.54
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.72	0.54
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.37	0.54
1:A:289:G:N2	1:A:363:A:H2	2.03	0.54
1:A:559:U:H5'	1:A:559:U:C6	2.40	0.54
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.72	0.54
1:A:1308:A:H5'	37:A:6473:HOH:O	2.07	0.54
1:A:1894:C:C2	1:A:1939:U:C4	2.94	0.54
2:B:3035:C:H5''	37:B:4078:HOH:O	2.07	0.54
3:C:93:THR:C	3:C:94:LEU:HD23	2.32	0.54
24:X:13:MET:HE2	24:X:18:GLN:HA	1.89	0.54
1:A:306:A:P	21:U:38:ARG:HH21	2.30	0.54
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.43	0.54
1:A:1753:C:O2	4:D:229:ARG:NH2	2.40	0.54
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.39	0.54
9:I:64:ASN:O	9:I:68:GLU:HG3	2.07	0.54
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.89	0.54
11:K:142:ASN:O	11:K:144:THR:N	2.40	0.54
12:L:55:VAL:CG1	12:L:56:SER:N	2.71	0.54
14:N:155:HIS:O	14:N:158:ARG:HG2	2.07	0.54
24:X:122:ARG:NH2	24:X:154:ARG:CD	2.62	0.54
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.22	0.54
29:3:41:HIS:H	29:3:45:ASN:ND2	1.97	0.54
30:4:48:ASN:ND2	30:4:50:GLY:H	2.05	0.54
1:A:1174:A:C5	1:A:1201:C:H4'	2.42	0.54
1:A:1434:A:H2'	1:A:1436:C:C5	2.42	0.54
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.89	0.54
8:H:99:THR:O	8:H:99:THR:HG23	2.07	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
16:P:25:VAL:HG23	16:P:26:TRP:N	2.22	0.54
23:W:49:LEU:O	23:W:53:ILE:HG13	2.07	0.54
27:1:77:LYS:HA	27:1:80:MET:HE2	1.89	0.54
28:2:25:LYS:HG2	28:2:25:LYS:O	2.07	0.54
30:4:55:VAL:HG22	37:4:8509:HOH:O	2.07	0.54
1:A:921:G:H4'	1:A:924:G:N1	2.23	0.54
1:A:929:A:C8	1:A:930:C:C5	2.96	0.54
1:A:1134:G:C5'	10:J:151:MET:HE1	2.36	0.54
1:A:1659:A:H2'	1:A:1660:G:O4'	2.08	0.54
1:A:1669:A:H2'	1:A:1670:G:C8	2.43	0.54
1:A:2100:A:C2	31:A:4000:CAI:H201	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2445:U:H2'	1:A:2446:G:C8	2.42	0.54
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.90	0.54
14:N:59:GLY:C	14:N:141:ILE:HD11	2.33	0.54
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.88	0.54
28:2:2:GLY:O	28:2:6:PRO:HG2	2.08	0.54
1:A:394:G:H1	14:N:181:GLU:CD	2.16	0.54
1:A:541:C:O2'	1:A:542:A:H5''	2.07	0.54
1:A:951:A:H2'	1:A:952:G:H5'	1.88	0.54
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.71	0.54
1:A:1209:C:H2'	1:A:1210:G:C8	2.39	0.54
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.35	0.54
1:A:2638:G:H5'	37:A:4487:HOH:O	2.07	0.54
1:A:2860:G:H1'	37:A:6337:HOH:O	2.08	0.54
2:B:3020:G:O2'	2:B:3021:G:H5'	2.07	0.54
4:D:85:ARG:NH1	37:D:8641:HOH:O	2.40	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.37	0.54
6:F:84:LEU:C	6:F:86:THR:H	2.15	0.54
13:M:65:ASP:HA	13:M:109:LEU:O	2.07	0.54
16:P:35:LYS:O	16:P:40:HIS:NE2	2.41	0.54
1:A:1504:A:OP2	37:A:7351:HOH:O	2.18	0.54
1:A:2779:G:H21	7:G:143:GLN:NE2	2.05	0.54
2:B:3054:A:O2'	2:B:3055:U:H5'	2.08	0.54
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.89	0.54
6:F:99:ASP:HB3	6:F:103:ASN:H	1.72	0.54
14:N:52:LEU:HD21	37:N:8615:HOH:O	2.08	0.54
14:N:81:ARG:O	14:N:86:MET:HE2	2.08	0.54
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.26	0.54
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.22	0.54
26:Z:235:GLU:CD	26:Z:235:GLU:N	2.66	0.54
29:3:18:ASN:ND2	29:3:40:ARG:H	2.01	0.54
1:A:534:C:N4	37:A:7113:HOH:O	2.31	0.54
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.54
1:A:1182:C:H1'	1:A:1192:A:H8	1.73	0.54
1:A:1768:C:H2'	1:A:1769:C:O4'	2.07	0.54
1:A:1972:U:H2'	1:A:1973:A:H5'	1.89	0.54
1:A:2089:A:C2'	1:A:2090:G:H5'	2.37	0.54
1:A:2314:G:O2'	1:A:2315:C:H5'	2.07	0.54
2:B:3023:U:H5''	2:B:3024:U:OP2	2.07	0.54
8:H:46:GLU:N	37:H:3461:HOH:O	2.41	0.54
11:K:107:ASN:HD22	11:K:109:TYR:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.90	0.54
14:N:72:SER:OG	14:N:74:ARG:HB2	2.08	0.54
14:N:164:THR:HB	37:N:8520:HOH:O	2.07	0.54
26:Z:144:ARG:NE	37:Z:8616:HOH:O	2.41	0.54
30:4:75:GLY:HA2	37:4:8558:HOH:O	2.08	0.54
1:A:240:C:H4'	14:N:146:GLN:NE2	2.22	0.54
1:A:918:G:C2	1:A:926:A:C2	2.96	0.54
4:D:251:VAL:HG23	4:D:252:PRO:HD2	1.89	0.54
6:F:86:THR:O	6:F:90:LEU:HG	2.08	0.54
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.54	0.54
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.89	0.54
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.06	0.54
21:U:48:VAL:CG2	21:U:98:VAL:HA	2.37	0.54
1:A:652:G:H8	37:A:9583:HOH:O	1.90	0.54
1:A:1333:U:H2'	1:A:1334:C:C6	2.43	0.54
1:A:1878:G:C1'	37:A:5666:HOH:O	2.55	0.54
10:J:117:LYS:O	10:J:119:VAL:HG13	2.08	0.54
13:M:104:ASP:O	13:M:105:TYR:HB3	2.07	0.54
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.37	0.54
1:A:1391:G:H2'	1:A:1392:A:H5'	1.91	0.53
5:E:219:ASN:O	5:E:222:ASP:OD1	2.26	0.53
7:G:81:GLU:HG2	7:G:134:SER:CB	2.35	0.53
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.36	0.53
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.38	0.53
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.40	0.53
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.91	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.08	0.53
1:A:738:G:H3'	37:A:6584:HOH:O	2.07	0.53
1:A:778:C:C4	1:A:779:U:C4	2.96	0.53
1:A:877:G:H3'	37:A:9683:HOH:O	2.07	0.53
1:A:1119:G:H8	11:K:52:GLN:NE2	2.06	0.53
1:A:2862:G:H4'	4:D:336:GLN:O	2.08	0.53
2:B:3031:C:O2'	2:B:3032:G:H5'	2.08	0.53
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.90	0.53
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.21	0.53
10:J:57:ARG:O	10:J:61:LEU:HD22	2.07	0.53
12:L:125:ALA:C	12:L:127:ALA:H	2.16	0.53
13:M:143:THR:HG22	13:M:144:ASP:H	1.73	0.53
1:A:1299:G:O6	13:M:6:ARG:HD3	2.09	0.53
1:A:1551:C:O2	1:A:1634:G:N2	2.36	0.53
1:A:2251:G:H2'	1:A:2252:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2630:G:O6	3:C:206:ARG:NH2	2.42	0.53
1:A:2649:A:H5'	1:A:2649:A:H8	1.73	0.53
3:C:24:LYS:NZ	3:C:47:HIS:O	2.39	0.53
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.44	0.53
11:K:6:PHE:O	11:K:8:ALA:N	2.41	0.53
11:K:130:VAL:HG12	11:K:131:THR:N	2.22	0.53
1:A:25:A:H5'	37:A:8713:HOH:O	2.09	0.53
1:A:281:U:O2'	1:A:282:C:H5'	2.09	0.53
1:A:820:G:C6	3:C:171:LYS:HB2	2.44	0.53
1:A:1636:G:O2'	1:A:1637:A:H5'	2.08	0.53
1:A:2371:G:H5'	37:A:4565:HOH:O	2.07	0.53
2:B:3064:C:H2'	2:B:3065:A:H5'	1.90	0.53
3:C:173:GLY:O	3:C:176:HIS:HB3	2.08	0.53
6:F:10:PHE:CG	6:F:11:HIS:N	2.76	0.53
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.90	0.53
8:H:34:ASN:O	8:H:38:LYS:HG3	2.08	0.53
12:L:74:VAL:O	12:L:74:VAL:CG1	2.54	0.53
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.90	0.53
15:O:151:ASP:HB3	37:O:8528:HOH:O	2.07	0.53
1:A:2266:A:P	37:A:5407:HOH:O	2.65	0.53
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.53
37:A:9275:HOH:O	4:D:254:GLN:HG3	2.08	0.53
2:B:3059:C:H5'	37:B:5233:HOH:O	2.08	0.53
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.89	0.53
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.40	0.53
8:H:21:GLU:O	8:H:24:ARG:HG3	2.07	0.53
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.24	0.53
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.91	0.53
1:A:766:A:H5'	37:A:4212:HOH:O	2.09	0.53
1:A:1066:U:H2'	1:A:1067:A:C8	2.43	0.53
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.53
1:A:1183:C:N4	37:A:3962:HOH:O	2.38	0.53
1:A:2379:G:H4'	1:A:2380:A:H5''	1.91	0.53
1:A:2467:A:H3'	37:A:5005:HOH:O	2.08	0.53
4:D:240:GLY:HA3	37:D:8529:HOH:O	2.07	0.53
11:K:77:GLY:O	11:K:78:ILE:C	2.50	0.53
1:A:175:G:H2'	14:N:192:ALA:HB3	1.90	0.53
1:A:390:G:N7	37:A:9613:HOH:O	2.34	0.53
1:A:585:C:H6	37:A:5640:HOH:O	1.90	0.53
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.53
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.90	0.53
1:A:2089:A:O2'	1:A:2090:G:H5'	2.09	0.53
1:A:2719:A:C2	4:D:70:PRO:HG3	2.44	0.53
37:A:3236:HOH:O	14:N:79:LYS:HD2	2.09	0.53
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.73	0.53
4:D:138:GLY:O	4:D:139:ASP:O	2.26	0.53
10:J:53:PRO:HG3	10:J:127:GLY:H	1.73	0.53
10:J:59:ASN:H	10:J:59:ASN:ND2	2.06	0.53
12:L:101:ASN:O	12:L:102:GLU:HB2	2.08	0.53
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.39	0.53
1:A:1349:G:H5''	37:A:3359:HOH:O	2.08	0.53
1:A:1697:G:H1'	37:A:6813:HOH:O	2.08	0.53
1:A:2720:C:O2	12:L:87:ARG:NH2	2.41	0.53
4:D:7:ARG:CD	4:D:9:GLY:O	2.56	0.53
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.44	0.53
10:J:163:PRO:O	10:J:164:ALA:HB2	2.08	0.53
14:N:115:LEU:O	14:N:116:ASN:HB2	2.08	0.53
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.08	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.09	0.53
1:A:1951:G:N2	37:A:5804:HOH:O	2.42	0.53
1:A:2382:A:H5'	37:A:4302:HOH:O	2.08	0.53
1:A:2421:G:H4'	37:A:4339:HOH:O	2.08	0.53
1:A:2760:C:H5''	37:A:4880:HOH:O	2.08	0.53
4:D:162:MET:CE	4:D:308:LEU:HD21	2.26	0.53
13:M:146:GLY:C	13:M:148:GLU:H	2.17	0.53
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.39	0.53
27:1:19:GLY:O	27:1:23:ARG:HG2	2.09	0.53
27:1:58:GLY:HA3	37:1:8442:HOH:O	2.08	0.53
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.44	0.53
1:A:371:U:H2'	1:A:372:A:H8	1.74	0.53
1:A:514:G:OP1	1:A:514:G:H2'	2.09	0.53
1:A:1166:A:H1'	1:A:1192:A:N1	2.23	0.53
1:A:2502:C:C4'	10:J:151:MET:HG2	2.38	0.53
2:B:3103:A:O2'	2:B:3104:A:H5'	2.08	0.53
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.91	0.53
3:C:194:MET:HE3	3:C:199:HIS:CB	2.39	0.53
4:D:2:GLN:CD	37:D:8625:HOH:O	2.50	0.53
4:D:254:GLN:HG2	4:D:255:GLY:N	2.23	0.53
5:E:162:VAL:HG12	5:E:162:VAL:O	2.09	0.53
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.90	0.53
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:41:TYR:O	24:X:45:VAL:HG13	2.09	0.53
27:1:59:HIS:CE1	37:1:8441:HOH:O	2.62	0.53
1:A:453:A:H4'	1:A:455:A:N7	2.24	0.52
1:A:646:G:H2'	1:A:647:U:C6	2.44	0.52
1:A:1058:A:H2'	1:A:1060:C:C5'	2.38	0.52
1:A:1213:C:O2'	1:A:1214:G:H5'	2.09	0.52
1:A:2405:C:C5'	37:A:6132:HOH:O	2.56	0.52
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.21	0.52
19:S:114:VAL:O	19:S:114:VAL:HG13	2.08	0.52
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.43	0.52
24:X:149:LEU:CG	24:X:153:MET:HE2	2.33	0.52
2:B:3006:C:P	15:O:37:ARG:NH1	2.82	0.52
4:D:168:GLY:H	4:D:174:ARG:HD3	1.73	0.52
6:F:58:VAL:HG12	6:F:59:GLY:N	2.24	0.52
7:G:143:GLN:CG	37:G:2113:HOH:O	2.57	0.52
7:G:143:GLN:HG2	37:G:2113:HOH:O	2.08	0.52
13:M:73:VAL:HG23	13:M:74:THR:H	1.73	0.52
15:O:34:LEU:HD13	15:O:47:LEU:HD21	1.91	0.52
1:A:111:C:OP1	37:A:3446:HOH:O	2.19	0.52
1:A:834:G:H5''	1:A:835:U:O5'	2.09	0.52
37:A:5737:HOH:O	29:3:44:ARG:HG2	2.09	0.52
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.22	0.52
4:D:55:ASN:HB3	4:D:64:GLY:H	1.74	0.52
7:G:77:THR:OG1	7:G:78:GLU:N	2.41	0.52
11:K:77:GLY:O	11:K:80:LYS:N	2.42	0.52
14:N:134:ILE:O	14:N:136:PRO:HD3	2.10	0.52
15:O:80:SER:CB	37:O:8536:HOH:O	2.57	0.52
19:S:29:LYS:HB3	37:S:8533:HOH:O	2.09	0.52
26:Z:122:ARG:NH2	37:Z:8533:HOH:O	2.42	0.52
1:A:159:G:H2'	1:A:175:G:H22	1.73	0.52
1:A:1164:U:C4'	1:A:1165:G:OP1	2.51	0.52
1:A:1497:G:H4'	1:A:1627:G:O2'	2.09	0.52
1:A:2269:C:C2'	1:A:2270:G:H5'	2.39	0.52
1:A:2435:U:H1'	37:A:4978:HOH:O	2.10	0.52
1:A:2724:U:H2'	1:A:2725:G:O4'	2.09	0.52
4:D:243:ASN:HA	4:D:244:PRO:C	2.34	0.52
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.09	0.52
8:H:110:GLU:O	8:H:114:LYS:HG3	2.09	0.52
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.84	0.52
10:J:57:ARG:C	10:J:59:ASN:N	2.66	0.52
17:Q:115:SER:O	17:Q:117:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:14:GLU:OE1	22:V:15:PRO:HD2	2.09	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.09	0.52
1:A:219:G:O5'	1:A:220:C:H5''	2.09	0.52
1:A:660:A:H4'	1:A:661:G:O5'	2.10	0.52
1:A:812:A:H1'	37:A:3527:HOH:O	2.09	0.52
1:A:1701:A:H4'	1:A:1702:U:C5'	2.39	0.52
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.75	0.52
5:E:111:VAL:HB	37:E:8324:HOH:O	2.09	0.52
10:J:13:ALA:HA	10:J:91:HIS:HE1	1.74	0.52
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.25	0.52
24:X:110:GLN:HE21	24:X:110:GLN:HA	1.72	0.52
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.45	0.52
1:A:1969:A:O2'	1:A:1970:G:H5'	2.08	0.52
1:A:2119:C:O2'	1:A:2120:U:H5'	2.10	0.52
4:D:54:VAL:O	4:D:55:ASN:C	2.52	0.52
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.09	0.52
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.25	0.52
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.44	0.52
18:R:28:ARG:HD3	37:R:6206:HOH:O	2.10	0.52
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.74	0.52
1:A:201:G:N2	1:A:202:U:C2	2.78	0.52
1:A:558:C:H2'	1:A:559:U:H5'	1.92	0.52
1:A:1701:A:H5''	1:A:1702:U:H3'	1.92	0.52
2:B:3008:G:P	37:B:5071:HOH:O	2.67	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.71	0.52
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.90	0.52
15:O:182:GLY:N	37:O:8572:HOH:O	2.43	0.52
17:Q:115:SER:C	17:Q:117:SER:H	2.18	0.52
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.39	0.52
1:A:1003:U:O2	10:J:90:PHE:HZ	1.92	0.52
1:A:1067:A:OP1	24:X:15:THR:OG1	2.26	0.52
1:A:1477:C:H5'	1:A:1868:G:C5'	2.40	0.52
1:A:2540:G:H2'	1:A:2541:U:H5'	1.91	0.52
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.91	0.52
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.23	0.52
18:R:33:PHE:N	18:R:71:TYR:OH	2.38	0.52
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.91	0.52
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.09	0.52
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.09	0.52
24:X:122:ARG:HH22	24:X:154:ARG:C	2.18	0.52
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1666:C:C2'	1:A:1667:A:C5'	2.88	0.52
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.92	0.52
3:C:55:VAL:HG22	3:C:68:ILE:O	2.10	0.52
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.91	0.52
5:E:160:LEU:O	5:E:162:VAL:HG23	2.09	0.52
8:H:91:VAL:CG1	8:H:92:GLY:N	2.69	0.52
28:2:1:THR:HA	37:2:8411:HOH:O	2.10	0.52
1:A:849:C:O2'	1:A:850:U:H5'	2.10	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.10	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
1:A:2487:C:H2'	1:A:2488:A:H5'	1.90	0.52
1:A:2563:U:H2'	1:A:2565:C:O5'	2.10	0.52
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.91	0.52
5:E:76:ARG:HD3	37:E:8367:HOH:O	2.10	0.52
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.92	0.52
13:M:143:THR:CG2	13:M:144:ASP:H	2.23	0.52
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.37	0.52
1:A:1778:A:H2'	1:A:1779:A:H5'	1.91	0.51
1:A:1996:U:O2'	1:A:1997:A:H5'	2.10	0.51
3:C:199:HIS:HD2	3:C:201:PHE:H	1.59	0.51
5:E:139:VAL:CG1	37:E:8455:HOH:O	2.54	0.51
6:F:86:THR:C	6:F:89:PRO:HD2	2.35	0.51
6:F:86:THR:HG23	37:F:7477:HOH:O	2.08	0.51
6:F:153:THR:HG22	37:F:5234:HOH:O	2.10	0.51
8:H:105:ALA:CB	37:H:5522:HOH:O	2.56	0.51
10:J:62:GLU:O	10:J:66:VAL:HG23	2.10	0.51
15:O:5:ARG:HG3	18:R:18:PRO:HB3	1.92	0.51
19:S:119:VAL:O	19:S:119:VAL:HG12	2.09	0.51
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.91	0.51
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.92	0.51
25:Y:15:ARG:HB3	25:Y:15:ARG:NH1	2.21	0.51
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.51
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.94	0.51
1:A:952:G:H4'	37:A:3596:HOH:O	2.09	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.91	0.51
1:A:1593:C:OP1	17:Q:117:SER:CB	2.58	0.51
1:A:2055:A:H5'	19:S:134:SER:HB2	1.92	0.51
1:A:2570:G:H5''	37:A:4472:HOH:O	2.11	0.51
1:A:2851:G:C2'	1:A:2852:A:H5'	2.40	0.51
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.91	0.51
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.56	0.51
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.44	0.51
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.75	0.51
1:A:1332:C:O2'	1:A:1333:U:H5'	2.10	0.51
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.91	0.51
11:K:45:VAL:HG22	11:K:46:ILE:N	2.24	0.51
14:N:39:ARG:NE	37:N:8622:HOH:O	2.43	0.51
15:O:170:GLU:O	15:O:174:GLU:HG3	2.10	0.51
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.92	0.51
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.57	0.51
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.24	0.51
26:Z:144:ARG:NH2	37:Z:8616:HOH:O	2.42	0.51
1:A:724:G:O2'	1:A:725:C:H5'	2.11	0.51
1:A:1422:U:H2'	1:A:1423:C:C6	2.45	0.51
1:A:1500:U:P	17:Q:41:ARG:HH22	2.33	0.51
1:A:2269:C:H2'	1:A:2270:G:H5'	1.91	0.51
37:A:9534:HOH:O	30:4:84:ARG:HB2	2.09	0.51
3:C:132:ASP:OD1	3:C:133:ARG:N	2.41	0.51
5:E:39:GLN:O	5:E:43:LYS:HD3	2.11	0.51
8:H:19:ALA:O	8:H:22:VAL:HG22	2.10	0.51
21:U:28:SER:O	21:U:32:ARG:HG3	2.10	0.51
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.11	0.51
3:C:171:LYS:NZ	37:C:8526:HOH:O	2.18	0.51
8:H:58:GLU:HA	8:H:61:MET:HE2	1.92	0.51
8:H:58:GLU:HA	8:H:61:MET:HG3	1.93	0.51
10:J:154:THR:HB	10:J:155:PRO:HD3	1.93	0.51
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.10	0.51
15:O:32:PRO:HD2	15:O:99:GLU:O	2.11	0.51
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.45	0.51
1:A:1262:C:H1'	24:X:120:PRO:HG3	1.92	0.51
1:A:1719:G:H1'	37:A:3297:HOH:O	2.10	0.51
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.26	0.51
6:F:19:GLU:O	6:F:133:ASN:HB3	2.11	0.51
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.09	0.51
8:H:91:VAL:CG1	8:H:92:GLY:H	2.19	0.51
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.93	0.51
14:N:52:LEU:HD13	14:N:116:ASN:CG	2.36	0.51
15:O:82:TYR:C	15:O:82:TYR:CD2	2.88	0.51
16:P:47:ARG:NH2	37:P:510:HOH:O	2.43	0.51
20:T:73:ASP:O	20:T:77:VAL:HG23	2.10	0.51
26:Z:187:VAL:HB	37:Z:8572:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:G:OP2	37:A:9059:HOH:O	2.19	0.51
1:A:440:C:H2'	1:A:441:A:C8	2.46	0.51
1:A:516:A:P	37:A:5193:HOH:O	2.67	0.51
1:A:535:G:H8	37:A:4691:HOH:O	1.92	0.51
3:C:109:GLU:HG2	3:C:116:GLY:H	1.76	0.51
3:C:109:GLU:HG2	3:C:116:GLY:N	2.26	0.51
6:F:25:MET:HE3	6:F:37:ALA:HB1	1.91	0.51
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.79	0.51
8:H:28:ALA:CB	8:H:99:THR:HG23	2.40	0.51
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.92	0.51
13:M:34:GLY:C	13:M:36:ASP:H	2.18	0.51
14:N:27:ARG:O	14:N:30:GLU:N	2.44	0.51
14:N:87:MET:SD	37:N:8532:HOH:O	2.59	0.51
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.93	0.51
17:Q:98:ILE:HD12	17:Q:102:ARG:CZ	2.40	0.51
19:S:39:THR:HB	19:S:42:GLU:CD	2.34	0.51
24:X:13:MET:HE2	24:X:18:GLN:CA	2.41	0.51
1:A:875:A:C2	3:C:194:MET:SD	3.04	0.51
1:A:1130:U:H5'	37:A:7209:HOH:O	2.10	0.51
1:A:1882:C:O2'	1:A:2012:U:OP2	2.27	0.51
37:A:5409:HOH:O	11:K:74:ARG:HD3	2.10	0.51
6:F:35:ALA:C	6:F:37:ALA:N	2.67	0.51
7:G:32:ARG:O	7:G:33:LEU:HD23	2.10	0.51
8:H:79:GLN:HB2	37:H:5498:HOH:O	2.10	0.51
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.23	0.51
12:L:101:ASN:O	12:L:102:GLU:CB	2.59	0.51
15:O:50:LEU:HB2	37:O:8523:HOH:O	2.11	0.51
22:V:52:THR:HG22	22:V:54:THR:HB	1.93	0.51
1:A:283:U:H5''	1:A:284:C:OP2	2.11	0.51
1:A:303:C:O2'	1:A:304:G:H5'	2.11	0.51
1:A:449:A:N7	5:E:43:LYS:HG2	2.26	0.51
1:A:929:A:H8	1:A:929:A:O5'	1.93	0.51
1:A:1166:A:H61	1:A:1180:U:H3	1.58	0.51
1:A:1189:A:H1'	1:A:1209:C:C1'	2.41	0.51
1:A:1850:U:H2'	1:A:1851:G:H8	1.75	0.51
1:A:2256:G:H2'	1:A:2257:G:C5'	2.41	0.51
5:E:1:MET:HG2	5:E:2:GLN:N	2.24	0.51
10:J:129:ASN:HD22	10:J:129:ASN:N	2.09	0.51
13:M:134:GLU:HA	13:M:138:GLY:O	2.11	0.51
24:X:26:ILE:O	24:X:26:ILE:CG1	2.58	0.51
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:C:H5'	37:A:4768:HOH:O	2.10	0.51
1:A:402:U:H2'	1:A:403:C:C6	2.45	0.51
1:A:962:C:C1'	15:O:5:ARG:NH1	2.66	0.51
1:A:2459:G:C8	37:A:6544:HOH:O	2.54	0.51
3:C:129:LEU:CD1	3:C:145:MET:HE1	2.41	0.51
10:J:81:TYR:CD1	10:J:81:TYR:C	2.88	0.51
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.45	0.51
10:J:139:ASP:OD2	37:J:8394:HOH:O	2.19	0.51
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.92	0.51
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.69	0.51
1:A:138:U:H5''	1:A:139:C:OP2	2.11	0.50
1:A:894:A:C2	5:E:87:ARG:NH2	2.79	0.50
1:A:1044:C:H5''	37:A:8623:HOH:O	2.10	0.50
1:A:1921:A:C6	1:A:1922:A:C2	2.99	0.50
1:A:2623:G:O2'	1:A:2624:A:H5'	2.10	0.50
1:A:2866:U:H4'	1:A:2867:G:H5'	1.93	0.50
1:A:2909:G:O2'	1:A:2910:A:H5'	2.12	0.50
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.50
5:E:246:ARG:NH2	37:E:8430:HOH:O	2.43	0.50
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.74	0.50
10:J:112:ARG:C	10:J:114:PRO:HD3	2.35	0.50
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.46	0.50
15:O:176:ARG:O	15:O:180:LEU:HG	2.11	0.50
1:A:820:G:C5	3:C:171:LYS:HB2	2.47	0.50
1:A:1483:C:O2'	1:A:1484:G:H5'	2.11	0.50
1:A:1495:C:H1'	1:A:1573:A:H1'	1.93	0.50
1:A:2314:G:H2'	1:A:2315:C:H5'	1.92	0.50
5:E:132:ASP:HB3	37:E:8363:HOH:O	2.09	0.50
5:E:150:THR:HA	5:E:203:ALA:O	2.11	0.50
1:A:1250:C:O2'	1:A:1251:C:H5'	2.12	0.50
1:A:1444:G:O2'	1:A:1445:G:H5'	2.11	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.93	0.50
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.40	0.50
1:A:317:A:H5''	21:U:52:ARG:HD2	1.92	0.50
1:A:2598:U:H5''	12:L:36:GLY:HA2	1.93	0.50
1:A:2815:G:H2'	37:A:5264:HOH:O	2.09	0.50
37:A:7083:HOH:O	4:D:2:GLN:HG3	2.10	0.50
37:B:7568:HOH:O	15:O:107:ASN:HB3	2.11	0.50
13:M:72:ASN:O	13:M:76:LEU:HG	2.11	0.50
16:P:44:ASN:HA	16:P:65:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.90	0.50
21:U:32:ARG:NH1	21:U:38:ARG:HH12	2.10	0.50
21:U:77:VAL:HB	37:U:4584:HOH:O	2.11	0.50
1:A:135:G:O2'	14:N:135:ASP:OD2	2.24	0.50
1:A:702:G:O2'	1:A:703:G:H5'	2.12	0.50
1:A:1172:G:H1'	37:A:4531:HOH:O	2.11	0.50
1:A:2004:U:O2	1:A:2004:U:H2'	2.11	0.50
1:A:2368:A:N6	15:O:18:THR:O	2.45	0.50
1:A:2911:C:H2'	1:A:2912:C:C6	2.47	0.50
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.26	0.50
4:D:8:LYS:HG3	4:D:220:VAL:HG12	1.92	0.50
5:E:178:GLN:C	5:E:180:SER:N	2.66	0.50
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.94	0.50
14:N:154:ARG:CZ	37:N:8642:HOH:O	2.59	0.50
19:S:96:VAL:HG13	19:S:106:GLY:HA3	1.93	0.50
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.30	0.50
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.75	0.50
29:3:49:GLU:O	37:3:131:HOH:O	2.19	0.50
1:A:431:G:P	14:N:48:ARG:HH12	2.34	0.50
1:A:643:A:N1	1:A:902:G:O2'	2.41	0.50
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.26	0.50
5:E:168:ARG:NH2	5:E:190:ALA:O	2.44	0.50
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.40	0.50
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.92	0.50
19:S:132:ARG:NH1	37:S:8558:HOH:O	2.43	0.50
24:X:90:TYR:N	24:X:90:TYR:CD1	2.79	0.50
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.12	0.50
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.41	0.50
1:A:338:C:H4'	5:E:174:ILE:HD12	1.92	0.50
1:A:661:G:C4	1:A:686:A:C2	3.00	0.50
1:A:677:C:H4'	5:E:246:ARG:NH2	2.27	0.50
1:A:1205:U:C2'	1:A:1206:U:C5'	2.89	0.50
1:A:1525:G:H5'	1:A:1526:A:OP2	2.12	0.50
1:A:1804:A:H2'	1:A:1805:G:C8	2.45	0.50
1:A:2036:C:OP1	37:A:6235:HOH:O	2.20	0.50
1:A:2467:A:P	37:A:8640:HOH:O	2.63	0.50
2:B:3091:C:H2'	2:B:3092:G:O4'	2.11	0.50
4:D:234:ARG:NH1	37:D:8623:HOH:O	2.44	0.50
5:E:237:GLU:HB2	37:E:8437:HOH:O	2.11	0.50
14:N:63:VAL:O	14:N:130:GLU:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.12	0.50
1:A:514:G:H8	1:A:514:G:O5'	1.95	0.50
1:A:797:A:H5'	27:1:10:ARG:HG2	1.94	0.50
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.47	0.50
1:A:1828:G:H2'	1:A:1829:A:H5'	1.92	0.50
1:A:1942:A:O2'	1:A:1943:C:H5'	2.12	0.50
2:B:3008:G:O6	15:O:11:ARG:NH1	2.44	0.50
3:C:13:THR:HB	37:C:8543:HOH:O	2.12	0.50
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.93	0.50
6:F:11:HIS:O	6:F:12:GLU:HB3	2.11	0.50
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.42	0.50
10:J:132:PHE:O	10:J:133:ILE:HD13	2.11	0.50
14:N:35:PRO:CG	14:N:38:VAL:CG2	2.81	0.50
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.41	0.50
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.41	0.50
27:1:50:ALA:HB3	27:1:54:ILE:HG22	1.93	0.50
1:A:168:C:C2'	1:A:169:A:H5'	2.41	0.50
1:A:710:G:OP1	16:P:24:ALA:HB3	2.12	0.50
1:A:1056:U:H2'	1:A:1057:A:O4'	2.12	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50
37:A:4634:HOH:O	4:D:216:LYS:HA	2.11	0.50
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.11	0.50
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.41	0.50
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.75	0.50
14:N:80:GLY:O	14:N:81:ARG:HD3	2.12	0.50
16:P:32:ARG:HD3	16:P:32:ARG:C	2.37	0.50
1:A:78:G:C6	1:A:79:G:C6	3.00	0.49
37:A:3328:HOH:O	21:U:9:LYS:CD	2.59	0.49
2:B:3029:C:C2'	2:B:3030:C:H5'	2.42	0.49
2:B:3042:C:H2'	37:B:6700:HOH:O	2.12	0.49
5:E:25:PRO:HD2	37:E:8435:HOH:O	2.11	0.49
5:E:246:ARG:HH11	5:E:246:ARG:CB	2.24	0.49
14:N:61:ILE:HD12	14:N:61:ILE:N	2.27	0.49
14:N:68:ARG:O	14:N:68:ARG:CD	2.59	0.49
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.36	0.49
21:U:38:ARG:HH11	21:U:38:ARG:HG3	1.76	0.49
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.93	0.49
22:V:52:THR:HG22	22:V:54:THR:H	1.77	0.49
1:A:1896:G:H1'	37:A:3823:HOH:O	2.11	0.49
1:A:2321:A:O2'	1:A:2322:U:H3'	2.12	0.49
3:C:36:ASP:O	3:C:38:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:141:ASN:CA	37:J:8367:HOH:O	2.45	0.49
14:N:62:VAL:C	14:N:63:VAL:HG23	2.37	0.49
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.42	0.49
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.41	0.49
22:V:33:SER:O	22:V:37:GLU:HG3	2.12	0.49
27:1:30:GLU:O	27:1:33:HIS:HB3	2.12	0.49
1:A:95:A:H5''	1:A:97:G:O4'	2.12	0.49
1:A:159:G:H2'	1:A:175:G:N2	2.26	0.49
1:A:220:C:P	37:A:5602:HOH:O	2.69	0.49
1:A:371:U:H2'	1:A:372:A:C8	2.48	0.49
1:A:1268:C:H2'	1:A:1269:G:H8	1.77	0.49
1:A:2756:U:H3	1:A:2896:A:H2	1.56	0.49
2:B:3096:C:H2'	2:B:3097:U:C6	2.47	0.49
4:D:175:LEU:C	4:D:175:LEU:CD2	2.84	0.49
4:D:240:GLY:HA3	37:D:8662:HOH:O	2.12	0.49
6:F:27:ILE:HG22	6:F:28:GLY:N	2.21	0.49
6:F:57:THR:HG23	6:F:63:ILE:CB	2.42	0.49
30:4:17:HIS:O	30:4:18:GLN:HG3	2.12	0.49
1:A:1052:G:N3	1:A:1052:G:H2'	2.26	0.49
1:A:1127:C:C5	1:A:1128:U:C4	2.99	0.49
1:A:2763:G:OP1	12:L:9:THR:OG1	2.19	0.49
5:E:20:ASP:O	5:E:23:GLU:HB2	2.13	0.49
5:E:84:VAL:O	5:E:85:LYS:CB	2.59	0.49
14:N:52:LEU:HD13	14:N:116:ASN:CB	2.42	0.49
14:N:114:VAL:HB	14:N:159:THR:HG23	1.95	0.49
15:O:11:ARG:O	15:O:15:GLU:HG3	2.12	0.49
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.56	0.49
24:X:142:ASP:HB3	24:X:145:GLY:H	1.76	0.49
27:1:59:HIS:HA	37:1:8444:HOH:O	2.12	0.49
1:A:737:A:H2'	1:A:738:G:O4'	2.12	0.49
1:A:1717:A:H5''	17:Q:54:LYS:HB2	1.94	0.49
1:A:2064:U:H2'	1:A:2065:C:H6	1.78	0.49
1:A:2271:G:H2'	1:A:2271:G:N3	2.27	0.49
2:B:3042:C:O2	6:F:76:ARG:NH1	2.45	0.49
2:B:3092:G:H2'	2:B:3093:A:C8	2.47	0.49
4:D:1:PRO:O	4:D:2:GLN:HB2	2.12	0.49
4:D:43:GLY:O	4:D:308:LEU:HD12	2.12	0.49
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.95	0.49
5:E:104:ASP:O	5:E:108:GLN:HG3	2.13	0.49
6:F:23:VAL:O	6:F:23:VAL:CG2	2.59	0.49
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:45:ARG:C	23:W:47:LYS:N	2.69	0.49
25:Y:30:MET:HE3	25:Y:55:ASN:OD1	2.11	0.49
1:A:88:G:N7	29:3:28:LYS:HD2	2.27	0.49
1:A:432:G:O2'	1:A:433:C:H5'	2.12	0.49
1:A:952:G:OP1	18:R:42:LYS:HE2	2.12	0.49
1:A:1334:C:H2'	1:A:1335:C:H6	1.76	0.49
1:A:2777:G:O2'	1:A:2778:A:H5'	2.12	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.12	0.49
12:L:76:GLN:HB2	37:L:1433:HOH:O	2.13	0.49
14:N:39:ARG:NH2	37:N:8622:HOH:O	2.46	0.49
17:Q:27:ARG:HA	37:Q:3969:HOH:O	2.12	0.49
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.42	0.49
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	0.49
26:Z:115:ARG:CZ	37:Z:8556:HOH:O	2.61	0.49
30:4:73:GLU:HB3	37:4:8559:HOH:O	2.12	0.49
1:A:418:C:OP2	37:A:5329:HOH:O	2.19	0.49
1:A:544:G:H2'	1:A:545:G:C5'	2.43	0.49
1:A:1644:C:C2	1:A:1645:U:C6	3.01	0.49
1:A:1730:G:H5'	1:A:1731:C:C6	2.47	0.49
1:A:2533:C:H6	1:A:2533:C:C5'	2.18	0.49
4:D:60:SER:C	4:D:62:ARG:H	2.20	0.49
14:N:138:HIS:C	14:N:139:PRO:O	2.49	0.49
1:A:775:G:OP1	28:2:16:HIS:HE1	1.96	0.49
1:A:1592:G:O2'	1:A:1593:C:O4'	2.29	0.49
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.49
1:A:2276:U:H2'	1:A:2277:U:H6	1.78	0.49
1:A:2403:C:H5'	37:A:5571:HOH:O	2.13	0.49
1:A:2812:A:C2	1:A:2814:A:N6	2.74	0.49
37:A:7217:HOH:O	14:N:154:ARG:HB2	2.12	0.49
2:B:3041:C:C6	6:F:50:VAL:HG21	2.48	0.49
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.95	0.49
6:F:65:GLU:HA	37:F:6752:HOH:O	2.11	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.12	0.49
14:N:68:ARG:O	14:N:68:ARG:CG	2.58	0.49
16:P:88:LYS:HB3	37:P:7061:HOH:O	2.12	0.49
17:Q:38:GLU:N	37:Q:3178:HOH:O	2.43	0.49
17:Q:83:LYS:NZ	37:Q:6315:HOH:O	2.45	0.49
24:X:139:GLY:O	24:X:141:HIS:HD2	1.95	0.49
30:4:81:GLU:HB2	37:4:8540:HOH:O	2.11	0.49
30:4:91:GLN:O	30:4:92:GLU:HB2	2.12	0.49
1:A:84:G:O2'	1:A:85:C:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:U:H5''	1:A:1044:C:N4	2.27	0.49
1:A:903:U:C2	13:M:11:ARG:O	2.66	0.49
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.46	0.49
1:A:1773:G:O2'	27:1:15:GLY:HA2	2.12	0.49
1:A:1825:U:O2'	1:A:1826:C:H5'	2.13	0.49
1:A:2115:U:H2'	1:A:2116:U:C6	2.48	0.49
1:A:2121:G:C2'	1:A:2122:C:H5'	2.42	0.49
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.12	0.49
10:J:151:MET:HA	10:J:151:MET:HE3	1.94	0.49
19:S:39:THR:CB	19:S:42:GLU:HG3	2.43	0.49
26:Z:136:LYS:HE2	26:Z:138:ARG:NH1	2.28	0.49
1:A:644:G:N3	1:A:644:G:H5'	2.28	0.49
1:A:1594:C:O2'	1:A:1607:A:H4'	2.13	0.49
1:A:1618:G:H5'	37:A:3540:HOH:O	2.12	0.49
1:A:2488:A:H2	37:A:6812:HOH:O	1.96	0.49
3:C:186:TRP:CG	3:C:187:PRO:HA	2.48	0.49
6:F:36:ASN:HA	37:F:7500:HOH:O	2.13	0.49
6:F:95:THR:C	6:F:97:GLN:N	2.68	0.49
6:F:99:ASP:HB2	6:F:103:ASN:H	1.78	0.49
13:M:101:ASP:C	13:M:103:ALA:H	2.18	0.49
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.78	0.49
1:A:224:U:H1'	37:A:9469:HOH:O	2.12	0.48
1:A:558:C:H2'	1:A:559:U:H5''	1.94	0.48
1:A:760:G:C6	1:A:894:A:N6	2.81	0.48
1:A:858:U:H2'	1:A:859:C:C6	2.47	0.48
10:J:166:ASN:N	10:J:166:ASN:ND2	2.61	0.48
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.60	0.48
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.94	0.48
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.48	0.48
27:1:38:LYS:HG3	37:1:8431:HOH:O	2.11	0.48
1:A:739:G:N7	37:A:7079:HOH:O	2.45	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.30	0.48
1:A:1249:U:H2'	1:A:1250:C:H6	1.76	0.48
1:A:1819:G:H2'	1:A:1820:G:C5'	2.43	0.48
1:A:2015:A:H2'	1:A:2016:U:O4'	2.13	0.48
1:A:2672:C:O2'	1:A:2673:U:H5'	2.13	0.48
4:D:119:HIS:O	4:D:121:PRO:HD3	2.12	0.48
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.26	0.48
5:E:154:VAL:O	5:E:158:GLU:HG3	2.13	0.48
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.94	0.48
14:N:137:ASP:C	14:N:142:LYS:HE3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:98:ILE:CD1	17:Q:102:ARG:NE	2.76	0.48
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.21	0.48
27:1:51:GLY:HA3	37:1:8416:HOH:O	2.12	0.48
1:A:164:G:N7	37:A:3207:HOH:O	2.35	0.48
1:A:506:G:H22	1:A:509:A:H5''	1.75	0.48
1:A:821:U:O2'	1:A:822:C:H5'	2.13	0.48
1:A:1306:U:OP1	5:E:184:ARG:HD2	2.14	0.48
1:A:2649:A:H5'	1:A:2649:A:C8	2.48	0.48
1:A:2713:G:O2'	1:A:2714:U:H5'	2.12	0.48
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.13	0.48
1:A:2898:G:O2'	1:A:2899:A:H5'	2.13	0.48
37:A:5165:HOH:O	17:Q:55:LYS:HA	2.12	0.48
4:D:205:VAL:O	4:D:307:ARG:NE	2.46	0.48
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.95	0.48
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.97	0.48
10:J:144:GLU:OE1	10:J:144:GLU:HA	2.13	0.48
12:L:30:LYS:C	12:L:55:VAL:HG13	2.38	0.48
13:M:148:GLU:CG	37:M:8556:HOH:O	2.60	0.48
16:P:77:ALA:HA	16:P:96:VAL:O	2.13	0.48
24:X:58:SER:OG	24:X:147:ASP:OD2	2.28	0.48
24:X:119:HIS:CD2	24:X:120:PRO:O	2.65	0.48
1:A:251:C:H1'	14:N:58:GLN:HE22	1.77	0.48
1:A:920:C:H4'	1:A:921:G:N2	2.28	0.48
1:A:2432:C:C1'	37:A:3646:HOH:O	2.62	0.48
1:A:2594:C:O2'	1:A:2595:U:H5'	2.13	0.48
1:A:2598:U:O2	1:A:2600:A:H8	1.96	0.48
1:A:2672:C:H1'	37:D:8641:HOH:O	2.13	0.48
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.94	0.48
5:E:76:ARG:HG2	5:E:78:ARG:NH1	2.27	0.48
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.14	0.48
9:I:63:ARG:O	9:I:67:LEU:HG	2.13	0.48
11:K:131:THR:HG22	11:K:133:GLY:N	2.28	0.48
14:N:174:ARG:HG3	37:N:8522:HOH:O	2.13	0.48
20:T:37:VAL:O	20:T:41:VAL:HG23	2.13	0.48
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.78	0.48
1:A:92:G:H4'	23:W:44:GLY:HA3	1.95	0.48
1:A:305:A:C5	1:A:329:A:C2	3.01	0.48
1:A:1653:A:N6	37:A:3828:HOH:O	2.46	0.48
1:A:1982:C:OP2	37:A:3844:HOH:O	2.20	0.48
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.96	0.48
1:A:2084:C:O2'	1:A:2085:A:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4843:HOH:O	24:X:122:ARG:NH2	2.46	0.48
2:B:3057:A:C8	6:F:141:VAL:HG21	2.49	0.48
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.60	0.48
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.96	0.48
15:O:141:ARG:HB3	37:O:8571:HOH:O	2.13	0.48
22:V:52:THR:CG2	22:V:54:THR:HB	2.44	0.48
1:A:317:A:C2	1:A:337:A:C5	3.01	0.48
1:A:1241:G:N3	11:K:86:MET:HE2	2.28	0.48
1:A:1862:C:H1'	37:A:6753:HOH:O	2.14	0.48
5:E:133:ARG:NH2	37:E:8432:HOH:O	2.47	0.48
6:F:59:GLY:O	6:F:61:PHE:N	2.36	0.48
14:N:55:LYS:O	14:N:60:ILE:HD12	2.13	0.48
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.42	0.48
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.28	0.48
27:1:10:ARG:HG3	27:1:11:THR:N	2.29	0.48
1:A:1592:G:O2'	1:A:1593:C:O5'	2.31	0.48
1:A:1666:C:O2'	1:A:1667:A:C5'	2.57	0.48
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.46	0.48
1:A:1862:C:C2'	1:A:1863:G:H5'	2.44	0.48
1:A:2783:A:H3'	37:A:4786:HOH:O	2.12	0.48
4:D:76:THR:N	4:D:77:PRO:HD3	2.29	0.48
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.48	0.48
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.13	0.48
21:U:48:VAL:HG11	21:U:96:VAL:CG1	2.44	0.48
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.49	0.48
26:Z:117:LEU:HD12	26:Z:174:VAL:CG1	2.44	0.48
1:A:128:A:H3'	1:A:128:A:C8	2.48	0.48
1:A:512:G:O3'	1:A:513:A:H8	1.97	0.48
1:A:870:G:C3'	1:A:871:G:H5''	2.44	0.48
1:A:1173:A:H2'	37:A:3911:HOH:O	2.14	0.48
1:A:1189:A:H1'	1:A:1209:C:H1'	1.96	0.48
1:A:1669:A:H2'	1:A:1670:G:H8	1.79	0.48
37:A:3328:HOH:O	21:U:9:LYS:HD2	2.11	0.48
2:B:3051:A:H5'	15:O:160:SER:HB3	1.96	0.48
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.95	0.48
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.96	0.48
20:T:29:ASP:OD2	20:T:31:ARG:NH1	2.46	0.48
24:X:38:THR:HG22	24:X:39:ASP:H	1.79	0.48
24:X:76:ASP:O	24:X:77:ALA:O	2.32	0.48
1:A:379:G:OP1	37:A:9129:HOH:O	2.20	0.48
1:A:1407:A:O2'	1:A:1408:U:H3'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2118:A:O2'	1:A:2119:C:H5'	2.14	0.48
3:C:168:PRO:O	3:C:170:VAL:HG23	2.14	0.48
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.44	0.48
10:J:118:PRO:HD2	37:J:8339:HOH:O	2.14	0.48
16:P:32:ARG:HB2	37:P:4656:HOH:O	2.13	0.48
1:A:177:A:H2'	1:A:178:U:O4'	2.14	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
1:A:837:U:H4'	37:A:9970:HOH:O	2.12	0.48
1:A:1269:G:H2'	1:A:1270:U:H6	1.78	0.48
1:A:1333:U:H2'	1:A:1334:C:H6	1.79	0.48
1:A:1666:C:C2'	1:A:1667:A:H5'	2.42	0.48
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.96	0.48
1:A:2780:C:H2'	1:A:2781:U:C6	2.49	0.48
1:A:2781:U:H2'	1:A:2782:G:H5'	1.95	0.48
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.44	0.48
5:E:107:ARG:CB	5:E:107:ARG:HH11	2.27	0.48
6:F:128:LEU:HD23	6:F:128:LEU:C	2.39	0.48
7:G:11:VAL:HG12	7:G:12:ASP:H	1.79	0.48
7:G:93:MET:HE2	7:G:107:PHE:CD1	2.49	0.48
10:J:46:VAL:O	10:J:146:TRP:CH2	2.63	0.48
13:M:140:VAL:O	13:M:140:VAL:HG12	2.13	0.48
15:O:58:LEU:N	15:O:58:LEU:CD1	2.77	0.48
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.96	0.48
24:X:13:MET:CE	24:X:17:ILE:HG22	2.43	0.48
1:A:21:G:H5''	19:S:1:GLY:O	2.14	0.47
1:A:220:C:O5'	37:A:5602:HOH:O	2.20	0.47
1:A:542:A:H1'	37:A:4236:HOH:O	2.13	0.47
1:A:1733:A:H4'	4:D:212:GLN:HA	1.95	0.47
1:A:1907:U:O2	1:A:1933:G:C2	2.67	0.47
1:A:2781:U:C2'	1:A:2782:G:H5'	2.44	0.47
6:F:95:THR:OG1	6:F:174:VAL:HG22	2.14	0.47
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.43	0.47
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.62	0.47
16:P:80:ASP:OD1	16:P:81:PHE:N	2.46	0.47
19:S:22:GLN:HA	19:S:139:PRO:O	2.14	0.47
1:A:187:A:H3'	1:A:188:C:H6	1.79	0.47
1:A:417:G:P	37:A:6953:HOH:O	2.71	0.47
1:A:907:A:H4'	1:A:1328:A:C2	2.49	0.47
1:A:920:C:H5''	1:A:921:G:O5'	2.13	0.47
1:A:1060:C:H6	1:A:1060:C:H5'	1.79	0.47
1:A:1555:G:H4'	1:A:1630:A:H2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2830:U:H3'	37:A:4782:HOH:O	2.12	0.47
5:E:95:GLU:OE1	5:E:95:GLU:N	2.44	0.47
10:J:157:ILE:CG2	10:J:158:ASN:N	2.76	0.47
13:M:149:ARG:N	37:M:8575:HOH:O	2.47	0.47
14:N:173:LEU:HD23	14:N:183:VAL:CG1	2.43	0.47
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.43	0.47
15:O:154:LEU:O	15:O:155:GLU:CB	2.63	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.79	0.47
16:P:25:VAL:HG23	16:P:26:TRP:H	1.79	0.47
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.14	0.47
1:A:10:U:H5'	37:A:5583:HOH:O	2.14	0.47
1:A:278:A:H2'	1:A:279:C:O4'	2.15	0.47
1:A:445:U:H1'	37:A:6872:HOH:O	2.14	0.47
1:A:1242:A:H5'	11:K:82:THR:CG2	2.33	0.47
1:A:2004:U:H5''	1:A:2005:G:C8	2.49	0.47
1:A:2079:G:C6	1:A:2080:G:C6	3.02	0.47
1:A:2445:U:H2'	1:A:2446:G:H8	1.76	0.47
37:A:6563:HOH:O	3:C:211:LYS:HG2	2.13	0.47
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.14	0.47
3:C:194:MET:HE1	37:C:8517:HOH:O	2.14	0.47
5:E:147:LEU:HA	37:E:8421:HOH:O	2.15	0.47
6:F:35:ALA:O	6:F:37:ALA:N	2.47	0.47
7:G:7:ILE:HG22	7:G:45:ASP:O	2.14	0.47
8:H:60:VAL:O	8:H:61:MET:C	2.57	0.47
10:J:149:ALA:C	10:J:151:MET:H	2.20	0.47
12:L:14:LYS:HB2	12:L:45:PRO:CG	2.37	0.47
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.96	0.47
13:M:143:THR:HG21	37:M:8543:HOH:O	2.14	0.47
14:N:55:LYS:O	14:N:57:LYS:N	2.47	0.47
14:N:149:TRP:O	14:N:152:ARG:HG2	2.13	0.47
14:N:186:SER:OG	14:N:189:VAL:HG12	2.14	0.47
17:Q:115:SER:C	17:Q:117:SER:N	2.72	0.47
19:S:40:ALA:O	19:S:44:VAL:HG23	2.14	0.47
1:A:154:C:H2'	1:A:155:C:C6	2.45	0.47
1:A:814:G:H4'	37:A:9704:HOH:O	2.14	0.47
1:A:1545:C:H2'	1:A:1546:G:O4'	2.14	0.47
1:A:2435:U:P	30:4:28:GLY:HA3	2.54	0.47
1:A:2459:G:OP1	30:4:64:LYS:N	2.25	0.47
1:A:2831:C:H2'	1:A:2832:C:H5'	1.97	0.47
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.44	0.47
4:D:53:LEU:HD21	4:D:270:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:59:GLY:C	6:F:61:PHE:N	2.71	0.47
7:G:9:GLU:HG3	7:G:10:ASP:N	2.29	0.47
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.15	0.47
12:L:118:ALA:C	12:L:120:ARG:H	2.23	0.47
29:3:39:ARG:NH1	37:3:6391:HOH:O	2.48	0.47
1:A:328:U:O4'	5:E:202:THR:HG22	2.14	0.47
1:A:840:U:H2'	19:S:128:ARG:NH1	2.30	0.47
1:A:1819:G:H2'	1:A:1820:G:C4'	2.45	0.47
1:A:2103:A:H5'	37:A:5551:HOH:O	2.14	0.47
1:A:2112:A:H2'	1:A:2113:G:C8	2.50	0.47
1:A:2420:G:H4'	37:A:3662:HOH:O	2.15	0.47
1:A:2499:U:H1'	37:A:9007:HOH:O	2.14	0.47
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.14	0.47
37:A:3579:HOH:O	4:D:48:MET:N	2.45	0.47
37:A:8906:HOH:O	27:1:16:PRO:HG3	2.14	0.47
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.38	0.47
4:D:108:GLU:HB3	4:D:111:ARG:HD2	1.96	0.47
10:J:26:LYS:CD	10:J:28:ILE:HB	2.44	0.47
11:K:52:GLN:HG3	11:K:53:ILE:N	2.29	0.47
13:M:78:ALA:N	37:M:8534:HOH:O	2.47	0.47
14:N:12:TRP:HB2	37:N:8601:HOH:O	2.14	0.47
15:O:132:ASN:O	15:O:135:VAL:HG12	2.15	0.47
24:X:1:MET:HE3	24:X:101:LEU:HA	1.95	0.47
26:Z:186:ARG:HG2	26:Z:186:ARG:NH1	2.30	0.47
1:A:380:A:OP2	14:N:9:ARG:HD2	2.15	0.47
1:A:2032:U:O2'	1:A:2033:G:H5''	2.14	0.47
37:A:8973:HOH:O	27:1:34:LYS:HD3	2.14	0.47
4:D:162:MET:HE2	4:D:310:ARG:CG	2.44	0.47
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.46	0.47
5:E:55:ARG:N	37:E:8311:HOH:O	2.37	0.47
14:N:49:ALA:C	14:N:54:TYR:HB3	2.39	0.47
1:A:56:G:H5''	23:W:50:ARG:HH12	1.80	0.47
1:A:106:A:H1'	37:A:9077:HOH:O	2.15	0.47
1:A:120:A:H2'	1:A:120:A:N3	2.29	0.47
1:A:303:C:H2'	1:A:304:G:O4'	2.14	0.47
1:A:324:G:O2'	1:A:325:U:H5'	2.15	0.47
1:A:426:G:C2	1:A:427:C:C2	3.02	0.47
1:A:450:C:H4'	5:E:46:TYR:CE1	2.50	0.47
1:A:639:A:H2'	1:A:640:G:C8	2.48	0.47
1:A:1055:G:OP2	10:J:94:ARG:NH1	2.48	0.47
1:A:1189:A:H1'	1:A:1209:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:A:H4'	37:A:6783:HOH:O	2.14	0.47
1:A:1592:G:HO2'	1:A:1593:C:C4'	2.28	0.47
1:A:1992:U:H2'	1:A:1994:A:OP2	2.14	0.47
1:A:2079:G:C6	1:A:2080:G:C5	3.03	0.47
1:A:2415:A:N3	15:O:26:LEU:HD13	2.29	0.47
1:A:2769:C:O2'	1:A:2770:G:H5'	2.15	0.47
1:A:2819:C:H2'	1:A:2820:A:C8	2.49	0.47
1:A:2894:C:O2'	1:A:2895:C:H5'	2.14	0.47
37:A:4784:HOH:O	16:P:38:ARG:HG2	2.14	0.47
37:A:6979:HOH:O	19:S:132:ARG:CZ	2.62	0.47
3:C:169:PHE:O	3:C:170:VAL:HB	2.15	0.47
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.40	0.47
4:D:123:ALA:O	37:D:8650:HOH:O	2.21	0.47
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.97	0.47
5:E:178:GLN:O	5:E:179:GLY:C	2.58	0.47
5:E:246:ARG:CZ	37:E:8430:HOH:O	2.61	0.47
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.15	0.47
7:G:20:ILE:CD1	7:G:33:LEU:HD12	2.45	0.47
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.96	0.47
10:J:39:GLY:O	10:J:41:THR:N	2.48	0.47
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.49	0.47
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.97	0.47
21:U:74:VAL:HB	21:U:77:VAL:HG21	1.97	0.47
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.63	0.47
27:1:26:VAL:O	27:1:30:GLU:HG3	2.15	0.47
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.49	0.47
1:A:316:A:H5'	21:U:54:ASP:OD2	2.13	0.47
1:A:603:A:H4'	1:A:604:G:O5'	2.14	0.47
1:A:816:G:OP1	17:Q:91:LYS:NZ	2.44	0.47
1:A:929:A:N7	1:A:930:C:C5	2.82	0.47
1:A:1450:C:O2'	1:A:1494:A:H5'	2.14	0.47
1:A:1473:U:C2	28:2:42:SER:HB2	2.50	0.47
1:A:2088:C:H1'	1:A:2841:A:N1	2.29	0.47
1:A:2100:A:N3	31:A:4000:CAI:H201	2.29	0.47
1:A:2453:G:H4'	13:M:50:GLY:C	2.40	0.47
2:B:3047:A:C2	2:B:3048:C:C2	3.02	0.47
2:B:3049:G:H2'	2:B:3050:G:O4'	2.15	0.47
1:A:407:A:C2	1:A:408:A:C4	3.03	0.47
1:A:1132:A:N6	1:A:1229:C:H2'	2.30	0.47
1:A:1634:G:H2'	1:A:1635:U:C6	2.50	0.47
1:A:2416:G:H2'	1:A:2417:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2426:G:H5'	37:A:8817:HOH:O	2.14	0.47
1:A:2533:C:O2'	1:A:2534:C:H5'	2.15	0.47
6:F:35:ALA:C	6:F:37:ALA:H	2.22	0.47
6:F:49:PRO:HA	6:F:73:VAL:HG22	1.97	0.47
9:I:66:LEU:O	9:I:69:ARG:HB3	2.14	0.47
9:I:71:LEU:C	9:I:73:ASP:H	2.22	0.47
15:O:110:THR:HB	15:O:113:SER:OG	2.15	0.47
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.78	0.47
1:A:120:A:C6	28:2:17:THR:HG21	2.50	0.47
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.47
1:A:288:A:H2'	1:A:289:G:C8	2.50	0.47
1:A:470:U:O2'	28:2:16:HIS:CD2	2.66	0.47
1:A:558:C:C2'	1:A:559:U:C5'	2.92	0.47
1:A:1218:U:H2'	1:A:1219:U:C6	2.50	0.47
1:A:1829:A:H2'	1:A:1830:C:H5'	1.97	0.47
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.15	0.47
1:A:2795:C:O2'	1:A:2796:U:H5'	2.15	0.47
37:A:3923:HOH:O	16:P:37:ARG:HG3	2.15	0.47
4:D:175:LEU:HD23	4:D:175:LEU:O	2.14	0.47
16:P:7:LEU:HD22	37:P:5650:HOH:O	2.14	0.47
16:P:49:GLU:HG2	37:P:5191:HOH:O	2.14	0.47
1:A:858:U:H2'	1:A:859:C:H6	1.80	0.46
1:A:920:C:N4	1:A:2467:A:C4	2.83	0.46
1:A:1667:A:H2'	1:A:1668:U:C6	2.50	0.46
1:A:1850:U:H2'	1:A:1851:G:C8	2.50	0.46
1:A:2011:A:P	37:A:5505:HOH:O	2.73	0.46
1:A:2293:G:C5	1:A:2294:C:C5	3.04	0.46
1:A:2473:U:O3'	1:A:2474:A:H3'	2.14	0.46
1:A:2501:G:H1'	37:A:4103:HOH:O	2.14	0.46
4:D:148:PRO:HD2	37:D:8584:HOH:O	2.14	0.46
6:F:25:MET:SD	6:F:40:ILE:HD11	2.55	0.46
11:K:19:MET:HE1	11:K:78:ILE:HG22	1.98	0.46
13:M:73:VAL:HG23	13:M:74:THR:N	2.30	0.46
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.15	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.14	0.46
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.50	0.46
24:X:65:VAL:HA	24:X:68:THR:CG2	2.44	0.46
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.46
1:A:202:U:O2'	1:A:203:G:H5'	2.15	0.46
1:A:731:U:O2'	1:A:732:C:H5'	2.16	0.46
1:A:1116:U:H3	1:A:1246:A:N6	2.05	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:G:C1'	37:A:4558:HOH:O	2.62	0.46
1:A:2271:G:OP2	37:A:9011:HOH:O	2.21	0.46
2:B:3064:C:C2'	2:B:3065:A:H5'	2.45	0.46
2:B:3117:G:C2'	37:B:2118:HOH:O	2.63	0.46
4:D:248:ARG:O	4:D:251:VAL:HG13	2.16	0.46
10:J:26:LYS:HG2	10:J:28:ILE:N	2.24	0.46
10:J:35:ASN:ND2	10:J:79:ALA:O	2.48	0.46
14:N:108:LYS:N	14:N:108:LYS:HD3	2.30	0.46
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.46
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.15	0.46
1:A:710:G:P	16:P:24:ALA:HB3	2.56	0.46
1:A:1562:C:O2	1:A:1562:C:H2'	2.15	0.46
1:A:2107:U:O2'	1:A:2108:A:H5'	2.15	0.46
1:A:2133:U:H4'	1:A:2134:G:H5'	1.97	0.46
1:A:2134:G:C6	1:A:2258:A:C8	3.04	0.46
37:A:6839:HOH:O	14:N:39:ARG:CD	2.64	0.46
4:D:177:HIS:O	4:D:181:ILE:HG13	2.16	0.46
7:G:95:VAL:O	7:G:126:ILE:HD13	2.16	0.46
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.50	0.46
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.31	0.46
1:A:88:G:H2'	1:A:89:G:C8	2.50	0.46
1:A:2111:G:C2	1:A:2477:C:C2	3.04	0.46
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.16	0.46
4:D:144:THR:HG22	4:D:145:HIS:N	2.30	0.46
5:E:216:SER:OG	37:E:8408:HOH:O	2.20	0.46
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.45	0.46
8:H:62:HIS:O	8:H:63:ILE:C	2.58	0.46
10:J:45:GLN:HE21	10:J:135:TRP:NE1	2.13	0.46
37:L:408:HOH:O	22:V:37:GLU:HB3	2.16	0.46
19:S:35:ILE:O	19:S:38:LYS:HB2	2.14	0.46
19:S:61:GLN:CD	37:S:8541:HOH:O	2.57	0.46
24:X:28:HIS:CD2	24:X:31:HIS:CE1	3.04	0.46
26:Z:129:ASN:CG	26:Z:141:THR:OG1	2.58	0.46
1:A:464:G:N7	37:A:5000:HOH:O	2.36	0.46
1:A:682:A:H3'	1:A:683:G:H8	1.80	0.46
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.16	0.46
1:A:1699:C:H4'	37:A:5982:HOH:O	2.16	0.46
1:A:2826:G:C6	1:A:2913:A:N6	2.84	0.46
2:B:3030:C:OP1	6:F:137:PRO:O	2.33	0.46
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.46
3:C:93:THR:HG23	3:C:154:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ASN:HB3	4:D:64:GLY:N	2.30	0.46
6:F:52:THR:N	6:F:70:GLY:O	2.48	0.46
10:J:53:PRO:HA	10:J:125:VAL:O	2.15	0.46
14:N:113:ARG:NH1	14:N:152:ARG:O	2.47	0.46
15:O:19:ASP:C	15:O:19:ASP:OD1	2.57	0.46
15:O:154:LEU:HG	15:O:155:GLU:N	2.30	0.46
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.63	0.46
22:V:9:CYS:O	22:V:52:THR:HG23	2.14	0.46
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.97	0.46
26:Z:189:ASN:C	26:Z:189:ASN:ND2	2.73	0.46
1:A:458:G:H5'	37:E:8372:HOH:O	2.15	0.46
1:A:765:G:O3'	5:E:69:HIS:HB3	2.15	0.46
1:A:790:A:H1'	1:A:1710:A:H2'	1.97	0.46
1:A:1023:C:H2'	1:A:1024:G:O4'	2.15	0.46
1:A:1041:U:H2'	1:A:1042:U:C5'	2.46	0.46
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.14	0.46
4:D:60:SER:C	4:D:62:ARG:N	2.73	0.46
4:D:275:GLY:O	4:D:291:ASP:HA	2.16	0.46
4:D:280:VAL:HG13	4:D:334:SER:HA	1.97	0.46
9:I:12:ILE:O	9:I:13:PRO:C	2.58	0.46
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.48	0.46
10:J:165:GLY:C	10:J:166:ASN:HD22	2.24	0.46
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.51	0.46
11:K:46:ILE:HG12	11:K:53:ILE:HD13	1.96	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.96	0.46
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.51	0.46
16:P:60:VAL:O	16:P:62:GLY:N	2.38	0.46
18:R:93:ARG:HG3	18:R:93:ARG:NH1	2.31	0.46
1:A:113:A:H3'	1:A:114:A:H5''	1.98	0.46
1:A:1535:G:H2'	1:A:1536:C:C6	2.51	0.46
1:A:1785:G:OP1	17:Q:76:GLY:HA3	2.16	0.46
1:A:2296:C:H5	37:R:5998:HOH:O	1.98	0.46
1:A:2365:G:H4'	18:R:45:PRO:O	2.15	0.46
1:A:2467:A:C2'	37:A:5005:HOH:O	2.50	0.46
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.24	0.46
6:F:81:GLU:C	6:F:83:PHE:N	2.74	0.46
6:F:173:GLU:O	6:F:174:VAL:C	2.59	0.46
7:G:84:MET:HE1	7:G:148:ILE:HD13	1.95	0.46
10:J:65:ARG:HB3	37:J:8386:HOH:O	2.15	0.46
13:M:126:SER:O	13:M:127:GLU:C	2.57	0.46
15:O:5:ARG:O	37:O:8555:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:48:VAL:HG13	21:U:49:GLU:N	2.29	0.46
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.97	0.46
27:1:28:ASP:O	27:1:31:ILE:HG22	2.16	0.46
29:3:24:TRP:NE1	37:3:6863:HOH:O	2.47	0.46
1:A:319:A:H4'	1:A:338:C:C4	2.50	0.46
1:A:392:U:O2'	1:A:394:G:N7	2.41	0.46
1:A:524:A:H5'	19:S:29:LYS:HE2	1.98	0.46
1:A:818:A:C2	27:1:13:ARG:HA	2.51	0.46
1:A:1773:G:H8	27:1:16:PRO:HA	1.81	0.46
1:A:1862:C:O2'	1:A:1863:G:H5'	2.16	0.46
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.81	0.46
6:F:41:LEU:O	6:F:44:ILE:HG22	2.16	0.46
11:K:54:VAL:HG11	11:K:138:THR:HG21	1.98	0.46
11:K:79:PHE:O	11:K:79:PHE:HD2	1.97	0.46
13:M:148:GLU:HG3	37:M:8556:HOH:O	2.15	0.46
20:T:58:MET:SD	29:3:8:LYS:HE3	2.56	0.46
1:A:257:G:O2'	1:A:258:G:H5'	2.16	0.46
1:A:382:U:C5	1:A:406:G:N2	2.84	0.46
1:A:2910:A:H5''	37:A:3697:HOH:O	2.15	0.46
37:A:4103:HOH:O	10:J:151:MET:HE2	2.15	0.46
2:B:3049:G:O2'	2:B:3050:G:H5'	2.16	0.46
3:C:3:ARG:HB2	3:C:8:ARG:HE	1.81	0.46
4:D:88:GLU:O	4:D:88:GLU:HG3	2.15	0.46
4:D:217:ARG:CG	4:D:257:THR:HG22	2.43	0.46
4:D:279:THR:CG2	4:D:280:VAL:N	2.78	0.46
6:F:10:PHE:CD1	6:F:11:HIS:N	2.84	0.46
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.16	0.46
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.45	0.46
10:J:33:MET:SD	10:J:65:ARG:HD2	2.56	0.46
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.46	0.46
14:N:91:ILE:HG23	37:N:8644:HOH:O	2.15	0.46
19:S:75:TRP:CG	19:S:76:ASP:H	2.34	0.46
30:4:57:GLY:HA2	37:4:8524:HOH:O	2.16	0.46
1:A:269:G:C2	1:A:270:U:O4	2.69	0.46
1:A:451:C:N4	1:A:452:G:C6	2.84	0.46
1:A:949:U:O2'	18:R:40:HIS:HE1	1.99	0.46
1:A:960:G:N3	1:A:960:G:C2'	2.78	0.46
1:A:1947:G:N2	1:A:1966:U:O2	2.48	0.46
2:B:3057:A:H8	6:F:141:VAL:HG21	1.80	0.46
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.98	0.46
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:4:LEU:HD21	24:X:52:VAL:HG11	1.98	0.46
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.15	0.46
30:4:69:TYR:O	30:4:77:ALA:HA	2.16	0.46
1:A:182:G:O3'	14:N:157:LEU:CD1	2.64	0.45
1:A:653:C:H2'	1:A:654:A:C8	2.50	0.45
1:A:825:U:H5''	1:A:826:U:OP1	2.15	0.45
1:A:1079:A:N1	1:A:2068:G:O2'	2.45	0.45
1:A:1159:G:H1	1:A:1208:C:H42	1.64	0.45
1:A:1423:C:O2'	1:A:1424:A:H5'	2.16	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.16	0.45
4:D:36:PRO:HA	4:D:168:GLY:HA2	1.98	0.45
4:D:81:ALA:O	4:D:186:GLY:HA3	2.16	0.45
7:G:80:TRP:O	7:G:134:SER:HA	2.15	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.45	0.45
15:O:37:ARG:HA	15:O:37:ARG:HD3	1.81	0.45
19:S:84:ALA:O	19:S:88:PHE:HD1	1.99	0.45
1:A:413:G:N2	1:A:428:G:C4	2.84	0.45
1:A:500:G:H21	19:S:98:ASN:HD21	1.63	0.45
1:A:2064:U:H2'	1:A:2065:C:C6	2.52	0.45
1:A:2430:A:O5'	1:A:2430:A:H8	1.99	0.45
3:C:192:VAL:HG12	3:C:192:VAL:O	2.16	0.45
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.98	0.45
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.84	0.45
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.46	0.45
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.45
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.45	0.45
10:J:95:GLU:HB3	10:J:119:VAL:HG11	1.98	0.45
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.45
13:M:35:ARG:NH1	13:M:35:ARG:O	2.48	0.45
13:M:98:GLU:O	13:M:99:GLU:CB	2.64	0.45
15:O:21:HIS:HB3	37:O:8566:HOH:O	2.16	0.45
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.51	0.45
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.45
24:X:139:GLY:O	24:X:141:HIS:CD2	2.69	0.45
1:A:424:C:H2'	1:A:425:U:C6	2.50	0.45
1:A:1463:A:C6	1:A:1464:U:C4	3.04	0.45
1:A:1506:U:H6	1:A:1506:U:H5'	1.81	0.45
1:A:2094:G:C2	1:A:2652:U:O2	2.69	0.45
1:A:2820:A:H2'	1:A:2821:C:C6	2.52	0.45
5:E:76:ARG:HG2	5:E:78:ARG:HH12	1.82	0.45
5:E:203:ALA:C	37:E:8423:HOH:O	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.99	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.99	0.45
9:I:16:LYS:O	9:I:20:VAL:HG23	2.17	0.45
13:M:91:VAL:HG13	13:M:91:VAL:O	2.16	0.45
14:N:147:LEU:O	14:N:148:SER:C	2.60	0.45
24:X:4:LEU:HD22	24:X:52:VAL:HG22	1.96	0.45
24:X:41:TYR:HA	24:X:44:MET:HE3	1.98	0.45
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.45
1:A:86:A:C2	29:3:25:VAL:HG13	2.52	0.45
1:A:202:U:C2'	1:A:203:G:H5'	2.47	0.45
1:A:283:U:H5	1:A:284:C:N4	2.14	0.45
1:A:962:C:H5''	37:A:4474:HOH:O	2.17	0.45
1:A:1268:C:O2'	1:A:1269:G:H5'	2.16	0.45
1:A:1471:A:H5''	37:N:8577:HOH:O	2.15	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
1:A:2580:G:H4'	37:A:6303:HOH:O	2.17	0.45
4:D:139:ASP:HB3	37:D:8550:HOH:O	2.16	0.45
5:E:25:PRO:HA	37:E:8355:HOH:O	2.17	0.45
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.46	0.45
11:K:79:PHE:O	11:K:83:ILE:HG13	2.16	0.45
13:M:54:PRO:HG2	13:M:57:VAL:HG21	1.97	0.45
15:O:75:THR:CG2	37:O:8538:HOH:O	2.64	0.45
21:U:96:VAL:HG13	21:U:97:ARG:N	2.31	0.45
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.44	0.45
1:A:1706:G:C5	1:A:1707:G:C6	3.05	0.45
1:A:1878:G:C4'	37:A:5666:HOH:O	2.64	0.45
1:A:2073:G:OP2	1:A:2490:A:H5'	2.16	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
1:A:2428:G:HO2'	1:A:2429:A:P	2.40	0.45
1:A:2488:A:OP1	37:A:4244:HOH:O	2.20	0.45
1:A:2501:G:O2'	10:J:151:MET:HE2	2.16	0.45
1:A:2541:U:O2'	1:A:2542:C:H5'	2.16	0.45
1:A:2832:C:H5	37:A:6747:HOH:O	1.98	0.45
5:E:95:GLU:H	5:E:95:GLU:CD	2.24	0.45
5:E:97:ASP:OD2	5:E:99:SER:OG	2.26	0.45
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.99	0.45
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.85	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
15:O:152:GLU:C	15:O:154:LEU:N	2.74	0.45
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.82	0.45
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:21:LEU:HB3	24:X:26:ILE:CG1	2.47	0.45
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.17	0.45
1:A:24:G:N2	1:A:518:G:H1'	2.31	0.45
1:A:329:A:OP2	5:E:206:ASN:HB2	2.17	0.45
1:A:424:C:H2'	1:A:425:U:H6	1.82	0.45
1:A:820:G:H5'	1:A:821:U:H5'	1.98	0.45
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.81	0.45
1:A:1594:C:C2	1:A:1601:G:C2	3.05	0.45
1:A:1682:A:H5''	37:A:9032:HOH:O	2.17	0.45
1:A:2621:U:H5	37:A:9557:HOH:O	2.00	0.45
1:A:2723:G:H1'	37:A:4397:HOH:O	2.15	0.45
37:A:7070:HOH:O	30:4:79:LEU:HD22	2.16	0.45
5:E:104:ASP:N	37:E:8309:HOH:O	2.49	0.45
5:E:180:SER:HB2	37:E:8452:HOH:O	2.17	0.45
5:E:185:LYS:HD3	5:E:186:TYR:CE1	2.52	0.45
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.46	0.45
12:L:10:GLN:NE2	12:L:10:GLN:N	2.47	0.45
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.32	0.45
20:T:38:ALA:O	20:T:42:GLU:HG3	2.16	0.45
22:V:44:ARG:CB	37:V:3805:HOH:O	2.64	0.45
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.17	0.45
1:A:255:A:H2'	1:A:256:C:C6	2.52	0.45
1:A:883:U:O2	1:A:883:U:C2'	2.65	0.45
1:A:1135:G:H5'	37:A:5475:HOH:O	2.17	0.45
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.17	0.45
1:A:2769:C:H2'	1:A:2770:G:C5'	2.46	0.45
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.82	0.45
2:B:3078:G:O2'	2:B:3079:U:P	2.75	0.45
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.98	0.45
3:C:102:GLY:C	3:C:127:GLN:HE22	2.25	0.45
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.98	0.45
4:D:322:ARG:HB2	37:D:8609:HOH:O	2.17	0.45
7:G:7:ILE:HD11	7:G:11:VAL:O	2.17	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.35	0.45
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.17	0.45
10:J:29:ALA:N	10:J:62:GLU:OE1	2.47	0.45
10:J:30:GLN:H	10:J:65:ARG:NH1	2.15	0.45
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.65	0.45
14:N:18:GLY:O	14:N:21:ALA:HB3	2.17	0.45
16:P:32:ARG:NH1	37:P:2336:HOH:O	2.49	0.45
17:Q:7:LYS:CD	17:Q:21:VAL:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.17	0.45
22:V:20:MET:CG	22:V:28:THR:HG23	2.47	0.45
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.31	0.45
24:X:28:HIS:HD2	24:X:31:HIS:CE1	2.34	0.45
26:Z:133:HIS:HD2	37:Z:8585:HOH:O	2.00	0.45
1:A:682:A:H2'	1:A:683:G:O4'	2.17	0.45
1:A:812:A:H2'	1:A:813:C:O4'	2.17	0.45
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.45
1:A:1185:U:H5'	37:A:7001:HOH:O	2.17	0.45
1:A:2011:A:H4'	1:A:2012:U:O5'	2.17	0.45
1:A:2453:G:H5'	37:A:4251:HOH:O	2.17	0.45
1:A:2505:G:C2'	1:A:2506:A:H5'	2.47	0.45
1:A:2852:A:H5''	37:A:4787:HOH:O	2.16	0.45
37:A:5571:HOH:O	18:R:50:GLY:HA2	2.17	0.45
3:C:30:ARG:HE	3:C:30:ARG:HB3	1.61	0.45
3:C:111:SER:O	3:C:112:PRO:C	2.59	0.45
3:C:123:GLY:HA3	3:C:162:GLY:HA2	1.99	0.45
5:E:107:ARG:NH1	5:E:107:ARG:CB	2.79	0.45
6:F:140:ARG:O	6:F:144:ARG:HG2	2.16	0.45
14:N:14:ARG:HB3	37:N:8593:HOH:O	2.16	0.45
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.47	0.45
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.45	0.45
19:S:104:PHE:CB	19:S:109:MET:HE2	2.47	0.45
28:2:28:HIS:HD2	28:2:30:LYS:H	1.65	0.45
1:A:183:A:C5'	14:N:157:LEU:HD12	2.47	0.45
1:A:241:A:C2	1:A:378:A:H4'	2.52	0.45
1:A:324:G:C6	1:A:325:U:C5	3.05	0.45
1:A:524:A:C5'	19:S:29:LYS:HE2	2.46	0.45
1:A:667:C:H5'	37:A:9605:HOH:O	2.16	0.45
1:A:1119:G:N2	1:A:1246:A:H2	2.10	0.45
1:A:1362:U:H5'	37:A:9838:HOH:O	2.17	0.45
1:A:1409:G:H5'	37:A:3297:HOH:O	2.16	0.45
1:A:1845:A:P	3:C:190:ARG:HH11	2.39	0.45
1:A:2269:C:H2'	1:A:2270:G:C5'	2.47	0.45
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.82	0.45
5:E:21:VAL:C	5:E:23:GLU:H	2.24	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.35	0.45
7:G:101:GLU:OE2	7:G:115:ARG:NH1	2.49	0.45
8:H:21:GLU:HA	8:H:24:ARG:HE	1.81	0.45
8:H:78:GLU:CB	37:H:2750:HOH:O	2.64	0.45
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1:ALA:HB3	37:O:8576:HOH:O	2.16	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.31	0.45
15:O:163:PHE:O	15:O:164:ASP:O	2.34	0.45
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.98	0.45
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.52	0.45
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.65	0.45
1:A:567:U:H5''	37:X:5817:HOH:O	2.17	0.45
1:A:1583:U:H1'	37:A:9552:HOH:O	2.16	0.45
1:A:2679:G:H2'	1:A:2681:A:OP2	2.17	0.45
3:C:3:ARG:HB2	3:C:8:ARG:NE	2.32	0.45
4:D:11:LEU:C	37:D:8620:HOH:O	2.60	0.45
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.99	0.45
10:J:137:ASN:O	10:J:138:PRO:C	2.58	0.45
10:J:139:ASP:CG	10:J:139:ASP:O	2.60	0.45
15:O:161:GLY:O	15:O:162:ASP:C	2.59	0.45
19:S:28:SER:O	19:S:29:LYS:C	2.59	0.45
21:U:19:ARG:NH1	21:U:68:ASP:O	2.50	0.45
22:V:52:THR:HG22	22:V:54:THR:N	2.32	0.45
1:A:486:A:H1'	37:A:6311:HOH:O	2.17	0.44
1:A:657:G:OP1	5:E:27:ARG:NH2	2.40	0.44
1:A:963:C:O5'	1:A:963:C:H6	2.00	0.44
1:A:1375:A:C2'	1:A:1376:G:H5'	2.47	0.44
1:A:1609:C:H2'	1:A:1610:G:H8	1.81	0.44
1:A:2123:A:OP1	14:N:89:ASN:ND2	2.50	0.44
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.52	0.44
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.79	0.44
10:J:4:ALA:HB3	37:J:8366:HOH:O	2.17	0.44
12:L:37:TYR:HE2	12:L:45:PRO:HA	1.81	0.44
17:Q:13:VAL:HG11	17:Q:40:VAL:HG11	1.98	0.44
19:S:145:LEU:HD12	19:S:146:ILE:H	1.82	0.44
24:X:108:ARG:O	24:X:111:GLY:N	2.41	0.44
28:2:52:SER:HA	37:2:8443:HOH:O	2.17	0.44
1:A:777:U:O2'	28:2:11:LYS:HG2	2.17	0.44
1:A:779:U:H5'	1:A:1836:A:C2	2.52	0.44
1:A:814:G:H8	37:A:6743:HOH:O	2.00	0.44
1:A:911:G:H5'	1:A:932:U:OP1	2.17	0.44
1:A:1302:G:C5'	1:A:1331:A:O3'	2.65	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.82	0.44
37:A:5827:HOH:O	26:Z:158:LYS:HD3	2.17	0.44
3:C:51:ARG:HB2	37:C:8618:HOH:O	2.15	0.44
3:C:217:ARG:CG	3:C:217:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.52	0.44
5:E:129:HIS:CE1	5:E:232:LEU:H	2.35	0.44
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.18	0.44
8:H:117:GLU:C	8:H:119:ARG:N	2.75	0.44
9:I:23:ILE:O	9:I:27:ILE:HG13	2.16	0.44
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.17	0.44
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.47	0.44
24:X:11:VAL:O	24:X:12:ASN:HB2	2.17	0.44
1:A:121:U:OP2	29:3:10:ARG:NH2	2.47	0.44
1:A:128:A:O2'	1:A:129:A:H5'	2.17	0.44
1:A:553:G:O4'	1:A:1325:G:H5'	2.18	0.44
1:A:815:U:OP1	37:A:9239:HOH:O	2.20	0.44
1:A:926:A:H1'	13:M:38:HIS:O	2.18	0.44
1:A:1743:G:N7	37:A:8844:HOH:O	2.36	0.44
1:A:2727:A:H2'	1:A:2728:C:H5'	1.99	0.44
1:A:2840:A:OP1	4:D:211:THR:HG23	2.18	0.44
3:C:43:VAL:O	3:C:44:ASP:HB2	2.17	0.44
12:L:22:ASP:C	12:L:22:ASP:OD1	2.61	0.44
13:M:34:GLY:C	13:M:36:ASP:N	2.74	0.44
15:O:67:ALA:C	15:O:69:TYR:H	2.25	0.44
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.16	0.44
1:A:158:A:O2'	1:A:159:G:H5'	2.18	0.44
1:A:1414:A:H2'	1:A:1415:G:O4'	2.18	0.44
1:A:1512:G:N2	1:A:1513:C:H1'	2.31	0.44
1:A:1543:G:N1	1:A:1641:A:OP2	2.39	0.44
1:A:1786:C:O2'	37:A:6875:HOH:O	2.21	0.44
1:A:1878:G:O2'	1:A:1879:U:C6	2.67	0.44
1:A:2012:U:H6	37:A:3110:HOH:O	2.00	0.44
1:A:2715:G:N2	4:D:264:GLU:OE1	2.51	0.44
1:A:2791:U:C1'	1:A:2792:A:H5''	2.47	0.44
3:C:105:VAL:HG13	3:C:155:THR:O	2.18	0.44
4:D:279:THR:OG1	4:D:290:VAL:HB	2.18	0.44
5:E:141:SER:HB3	37:E:8424:HOH:O	2.18	0.44
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.17	0.44
6:F:154:LYS:H	6:F:154:LYS:CD	2.24	0.44
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.48	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.47	0.44
9:I:12:ILE:HB	37:I:4714:HOH:O	2.17	0.44
10:J:31:PHE:HE2	10:J:87:LYS:O	2.00	0.44
15:O:182:GLY:O	15:O:183:ASP:O	2.36	0.44
17:Q:7:LYS:HD3	17:Q:21:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:141:ILE:C	17:Q:143:ALA:H	2.25	0.44
21:U:19:ARG:HD3	21:U:67:LEU:O	2.18	0.44
21:U:65:VAL:HG22	21:U:72:ILE:HG22	2.00	0.44
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.53	0.44
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.80	0.44
26:Z:130:ARG:HB2	26:Z:142:SER:O	2.18	0.44
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.53	0.44
1:A:204:A:H2'	1:A:205:U:C5'	2.45	0.44
1:A:282:C:H2'	1:A:283:U:O4'	2.17	0.44
1:A:563:C:H2'	1:A:564:G:O4'	2.18	0.44
1:A:1050:G:C6	1:A:1051:C:C4	3.06	0.44
1:A:1302:G:H5'	1:A:1331:A:O3'	2.18	0.44
1:A:1386:G:N3	37:A:9760:HOH:O	2.36	0.44
1:A:1523:G:C6	1:A:1524:U:O4	2.70	0.44
1:A:1730:G:C5'	1:A:1731:C:C6	3.00	0.44
1:A:1871:U:O4'	1:A:1873:G:C8	2.71	0.44
1:A:2045:G:H2'	1:A:2046:G:O4'	2.17	0.44
1:A:2317:C:C4	1:A:2318:C:C4	3.05	0.44
1:A:2467:A:C3'	37:A:5005:HOH:O	2.65	0.44
37:A:9465:HOH:O	8:H:34:ASN:HB2	2.17	0.44
4:D:62:ARG:CB	4:D:65:MET:HE3	2.47	0.44
8:H:21:GLU:O	8:H:24:ARG:CG	2.65	0.44
26:Z:102:LEU:HA	37:Z:8525:HOH:O	2.18	0.44
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.17	0.44
1:A:420:U:H2'	1:A:421:C:C6	2.52	0.44
1:A:645:U:H4'	37:E:8335:HOH:O	2.16	0.44
1:A:1307:A:H1'	37:A:4452:HOH:O	2.17	0.44
1:A:1494:A:C4	1:A:1495:C:C5	3.06	0.44
1:A:2779:G:O2'	1:A:2780:C:H5'	2.18	0.44
2:B:3104:A:O2'	2:B:3105:A:H5'	2.18	0.44
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.47	0.44
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.17	0.44
4:D:82:VAL:O	4:D:82:VAL:CG1	2.63	0.44
4:D:225:GLY:HA3	37:D:8571:HOH:O	2.17	0.44
6:F:81:GLU:O	6:F:83:PHE:N	2.51	0.44
22:V:49:LEU:O	22:V:55:ALA:CB	2.66	0.44
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.46	0.44
29:3:40:ARG:HG2	29:3:40:ARG:NH1	2.32	0.44
1:A:148:A:H5''	28:2:44:LYS:HG2	2.00	0.44
1:A:793:A:H5''	17:Q:83:LYS:HG2	2.00	0.44
1:A:1940:C:H4'	37:A:6881:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:G:O2'	1:A:2657:G:H5'	2.17	0.44
1:A:2898:G:H4'	4:D:288:GLY:HA2	1.99	0.44
3:C:36:ASP:O	3:C:37:VAL:C	2.61	0.44
4:D:102:THR:HG22	37:D:8617:HOH:O	2.17	0.44
5:E:187:ARG:O	5:E:187:ARG:HG3	2.17	0.44
10:J:136:VAL:HA	37:J:8343:HOH:O	2.18	0.44
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.48	0.44
15:O:167:ASP:O	15:O:168:LEU:HD23	2.18	0.44
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.18	0.44
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.52	0.44
19:S:33:ARG:HG3	37:S:8565:HOH:O	2.17	0.44
20:T:80:ARG:NH1	37:T:7263:HOH:O	2.50	0.44
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.76	0.44
1:A:135:G:H1'	14:N:135:ASP:OD2	2.18	0.44
1:A:160:A:C5	1:A:177:A:C2	3.05	0.44
1:A:183:A:O2'	1:A:184:G:H5'	2.17	0.44
1:A:639:A:C2	1:A:1363:G:C2	3.06	0.44
1:A:795:G:N3	1:A:817:G:C2	2.86	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
1:A:1098:A:H2'	1:A:1099:G:O4'	2.18	0.44
1:A:1644:C:H2'	1:A:1645:U:H6	1.83	0.44
1:A:2409:C:O2'	1:A:2410:G:H5'	2.18	0.44
37:A:9809:HOH:O	3:C:221:PRO:HA	2.18	0.44
3:C:51:ARG:NH1	3:C:120:ARG:O	2.50	0.44
3:C:110:SER:N	3:C:114:ASP:OD2	2.51	0.44
4:D:41:PHE:HB3	4:D:190:MET:CE	2.47	0.44
4:D:97:LEU:HD21	37:D:8648:HOH:O	2.18	0.44
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.99	0.44
5:E:34:ALA:HB3	5:E:220:THR:HG21	2.00	0.44
5:E:219:ASN:O	5:E:223:LEU:HB2	2.18	0.44
6:F:94:ALA:O	6:F:95:THR:O	2.36	0.44
6:F:140:ARG:HH11	6:F:140:ARG:HG3	1.83	0.44
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.48	0.44
10:J:150:LYS:HE2	37:J:8380:HOH:O	2.18	0.44
15:O:72:GLU:H	15:O:171:HIS:CE1	2.35	0.44
16:P:26:TRP:N	37:P:3062:HOH:O	2.49	0.44
1:A:392:U:C5'	14:N:193:LYS:HB3	2.48	0.44
1:A:596:C:H2'	1:A:597:A:C8	2.53	0.44
1:A:1014:A:H5''	2:B:3101:G:O2'	2.17	0.44
1:A:1057:A:N6	1:A:1058:A:N6	2.65	0.44
1:A:1119:G:C8	11:K:52:GLN:NE2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:U:C1'	1:A:1165:G:OP1	2.66	0.44
1:A:1268:C:O2'	26:Z:169:ARG:HB2	2.18	0.44
1:A:1335:C:OP2	26:Z:207:SER:CB	2.66	0.44
1:A:1609:C:H2'	1:A:1610:G:C8	2.53	0.44
1:A:1823:G:C6	1:A:1824:C:C4	3.06	0.44
4:D:23:THR:HA	4:D:24:PRO:HD3	1.84	0.44
5:E:19:PRO:HG2	5:E:22:PHE:CD1	2.53	0.44
5:E:103:ASN:O	5:E:104:ASP:C	2.61	0.44
5:E:129:HIS:HD2	5:E:165:ASP:OD2	2.00	0.44
6:F:173:GLU:HG3	6:F:174:VAL:N	2.33	0.44
7:G:118:ILE:HG23	7:G:144:THR:HG21	2.00	0.44
7:G:139:GLU:CG	37:G:5919:HOH:O	2.65	0.44
15:O:175:LEU:HD12	15:O:175:LEU:HA	1.87	0.44
16:P:4:ASN:HB3	16:P:7:LEU:HB3	2.00	0.44
19:S:141:VAL:HG12	19:S:142:ASP:O	2.18	0.44
22:V:38:ASN:O	22:V:42:LEU:HG	2.17	0.44
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.98	0.44
1:A:222:A:H2'	1:A:223:G:O4'	2.18	0.43
1:A:537:G:C6	1:A:620:A:C8	3.06	0.43
1:A:1301:C:O2'	1:A:1331:A:H4'	2.18	0.43
1:A:1589:G:H22	1:A:1605:G:H1'	1.82	0.43
1:A:1912:A:O5'	1:A:1912:A:H8	2.01	0.43
1:A:2293:G:H1'	1:A:2464:C:C2	2.53	0.43
1:A:2526:C:C6	1:A:2526:C:H5'	2.52	0.43
1:A:2584:G:C2	1:A:2585:G:N7	2.86	0.43
37:A:6992:HOH:O	5:E:188:ARG:HD2	2.17	0.43
3:C:69:LEU:C	3:C:69:LEU:HD12	2.42	0.43
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.33	0.43
5:E:107:ARG:HB3	5:E:107:ARG:HH11	1.79	0.43
5:E:114:ALA:HB1	5:E:223:LEU:HB3	2.00	0.43
5:E:140:VAL:HG12	5:E:141:SER:N	2.33	0.43
7:G:20:ILE:HD12	7:G:33:LEU:HD12	2.00	0.43
7:G:34:TRP:O	11:K:127:ILE:HD11	2.17	0.43
7:G:36:PRO:HD3	11:K:127:ILE:HD12	2.00	0.43
10:J:57:ARG:C	10:J:59:ASN:H	2.26	0.43
13:M:34:GLY:O	13:M:36:ASP:N	2.51	0.43
13:M:48:LYS:NZ	37:M:8532:HOH:O	2.35	0.43
13:M:64:ILE:O	13:M:64:ILE:HG23	2.17	0.43
15:O:108:SER:HA	15:O:109:PRO:HD3	1.78	0.43
15:O:154:LEU:C	15:O:156:GLU:H	2.24	0.43
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:42:GLU:HG2	20:T:49:VAL:HG23	1.99	0.43
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.64	0.43
1:A:40:C:H6	1:A:40:C:O5'	2.01	0.43
1:A:154:C:O2'	1:A:155:C:H5'	2.18	0.43
1:A:485:A:OP2	37:A:3543:HOH:O	2.21	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.52	0.43
1:A:1161:A:H8	1:A:1161:A:O5'	2.01	0.43
1:A:1211:G:O2'	1:A:1212:C:H5'	2.18	0.43
1:A:1246:A:O2'	1:A:1247:A:H3'	2.19	0.43
1:A:1336:U:C2	1:A:1337:A:C8	3.05	0.43
1:A:1562:C:H42	1:A:2738:G:H1	1.65	0.43
1:A:2455:A:H2'	1:A:2456:A:O4'	2.18	0.43
2:B:3114:G:H2'	2:B:3115:C:C6	2.54	0.43
3:C:8:ARG:HG2	37:C:8554:HOH:O	2.18	0.43
3:C:192:VAL:CG1	3:C:192:VAL:O	2.66	0.43
4:D:223:ARG:HG3	4:D:232:TRP:O	2.18	0.43
5:E:153:VAL:O	5:E:157:LEU:HG	2.18	0.43
8:H:111:ILE:O	8:H:115:VAL:HG23	2.17	0.43
10:J:47:GLU:HG2	10:J:133:ILE:HD12	1.99	0.43
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.33	0.43
11:K:46:ILE:HG12	11:K:46:ILE:O	2.18	0.43
14:N:97:ILE:HD13	14:N:127:LYS:HD2	1.98	0.43
15:O:171:HIS:CE1	37:O:8568:HOH:O	2.70	0.43
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.43
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.18	0.43
27:1:11:THR:HG23	27:1:23:ARG:HB2	1.97	0.43
1:A:344:C:H2'	1:A:345:G:O4'	2.17	0.43
1:A:426:G:O2'	1:A:427:C:H5'	2.18	0.43
1:A:1943:C:O4'	3:C:212:PRO:HA	2.17	0.43
1:A:2317:C:C5	1:A:2318:C:C4	3.06	0.43
2:B:3006:C:P	15:O:37:ARG:HH11	2.40	0.43
6:F:84:LEU:HA	6:F:87:ALA:HB3	2.01	0.43
7:G:107:PHE:CZ	7:G:108:LEU:HD13	2.51	0.43
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.01	0.43
12:L:65:ARG:O	12:L:66:ARG:HB2	2.18	0.43
15:O:184:ILE:HG22	15:O:185:GLU:N	2.32	0.43
21:U:26:THR:HA	21:U:39:ASN:HB3	1.99	0.43
23:W:1:THR:C	23:W:3:LEU:N	2.76	0.43
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.49	0.43
30:4:43:ASN:ND2	37:4:8506:HOH:O	2.29	0.43
1:A:113:A:OP2	1:A:114:A:H5''	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:U:H2'	1:A:124:C:H6	1.84	0.43
1:A:134:U:O2	1:A:145:A:C2	2.70	0.43
1:A:236:A:H2'	1:A:236:A:O5'	2.18	0.43
1:A:396:U:O2'	1:A:418:C:H4'	2.18	0.43
1:A:832:U:H2'	1:A:833:G:C8	2.54	0.43
1:A:1044:C:C5'	37:A:8623:HOH:O	2.67	0.43
1:A:1773:G:H2'	1:A:1774:G:H5'	2.00	0.43
1:A:1969:A:N7	1:A:1970:G:C6	2.86	0.43
1:A:2325:C:H1'	37:A:3713:HOH:O	2.17	0.43
4:D:7:ARG:NH2	4:D:250:THR:O	2.52	0.43
7:G:102:VAL:HG11	7:G:148:ILE:HD11	2.00	0.43
7:G:132:THR:HB	37:G:2227:HOH:O	2.18	0.43
8:H:99:THR:O	8:H:100:ASP:HB2	2.18	0.43
10:J:117:LYS:HB2	37:J:8339:HOH:O	2.19	0.43
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.34	0.43
11:K:70:PHE:CD2	11:K:70:PHE:O	2.71	0.43
17:Q:16:VAL:CG1	17:Q:20:ARG:HB2	2.48	0.43
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.43
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.24	0.43
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.48	0.43
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.32	0.43
27:1:33:HIS:HE1	27:1:49:ARG:NE	2.17	0.43
1:A:244:C:O5'	1:A:244:C:H6	2.01	0.43
1:A:251:C:H4'	14:N:140:ALA:HB2	2.01	0.43
1:A:821:U:H2'	1:A:822:C:C6	2.47	0.43
1:A:1238:C:H4'	37:A:5565:HOH:O	2.17	0.43
1:A:1593:C:H5'	17:Q:116:SER:O	2.18	0.43
1:A:2123:A:P	14:N:89:ASN:HD22	2.41	0.43
1:A:2265:U:H2'	1:A:2266:A:C8	2.54	0.43
1:A:2432:C:H4'	30:4:36:ILE:HG12	2.00	0.43
1:A:2481:G:H3'	1:A:2482:G:H5''	2.00	0.43
1:A:2745:C:H5	37:A:5432:HOH:O	2.01	0.43
1:A:2769:C:H2'	1:A:2770:G:H5'	2.01	0.43
37:A:4024:HOH:O	14:N:146:GLN:HG2	2.17	0.43
2:B:3078:G:N2	2:B:3103:A:OP2	2.49	0.43
3:C:99:ILE:O	3:C:131:HIS:CE1	2.71	0.43
4:D:316:ARG:N	4:D:317:PRO:HD3	2.34	0.43
8:H:12:LEU:HD23	8:H:12:LEU:O	2.18	0.43
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.01	0.43
11:K:93:ARG:HH11	11:K:93:ARG:CB	2.26	0.43
12:L:55:VAL:CG1	12:L:56:SER:H	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:54:GLU:HG2	16:P:73:ASP:O	2.19	0.43
18:R:77:ASP:N	18:R:80:LYS:O	2.52	0.43
19:S:15:LYS:HE3	37:S:8577:HOH:O	2.18	0.43
24:X:5:VAL:O	24:X:52:VAL:CG2	2.66	0.43
1:A:1246:A:C4	1:A:1248:A:C8	3.07	0.43
1:A:1398:G:H2'	1:A:1399:A:C8	2.54	0.43
1:A:1461:U:H2'	1:A:1462:C:C6	2.54	0.43
1:A:1574:C:H6	1:A:1574:C:O5'	2.01	0.43
1:A:1890:U:H4'	1:A:2010:A:C6	2.54	0.43
1:A:2730:G:O2'	1:A:2731:G:H5'	2.19	0.43
1:A:2883:A:H2'	1:A:2884:G:O4'	2.19	0.43
37:A:4287:HOH:O	15:O:21:HIS:HD2	2.01	0.43
4:D:16:ARG:NE	37:D:8556:HOH:O	2.28	0.43
5:E:3:ALA:HA	37:E:8459:HOH:O	2.19	0.43
10:J:114:PRO:O	10:J:115:PHE:C	2.62	0.43
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.66	0.43
14:N:87:MET:H	14:N:87:MET:HG3	1.48	0.43
15:O:120:GLU:HG3	15:O:136:LEU:HD13	2.00	0.43
16:P:59:VAL:CG2	16:P:111:VAL:HG23	2.49	0.43
19:S:39:THR:O	19:S:40:ALA:C	2.61	0.43
24:X:21:LEU:HD13	24:X:26:ILE:HD11	2.00	0.43
27:1:42:CYS:SG	27:1:44:PHE:N	2.81	0.43
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.80	0.43
1:A:107:U:H2'	1:A:108:U:H5'	2.00	0.43
1:A:123:U:O2'	1:A:124:C:H5'	2.19	0.43
1:A:308:U:C4	1:A:342:C:H1'	2.53	0.43
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.43
1:A:745:G:O6	16:P:68:GLY:HA3	2.19	0.43
1:A:1041:U:C2'	1:A:1042:U:H5'	2.49	0.43
1:A:1189:A:N3	37:A:7218:HOH:O	2.48	0.43
1:A:1191:A:C3'	1:A:1192:A:H5''	2.44	0.43
1:A:1191:A:N1	1:A:1206:U:O4	2.51	0.43
1:A:1586:G:O2'	1:A:1587:U:H5'	2.18	0.43
1:A:1970:G:C5'	37:A:6606:HOH:O	2.66	0.43
1:A:2064:U:H4'	1:A:2653:A:P	2.59	0.43
1:A:2681:A:N6	1:A:2714:U:H4'	2.33	0.43
1:A:2911:C:H2'	1:A:2912:C:H6	1.83	0.43
37:A:3701:HOH:O	25:Y:59:TRP:HB2	2.18	0.43
4:D:274:GLU:HA	4:D:292:GLY:O	2.18	0.43
10:J:113:ALA:N	10:J:114:PRO:CD	2.82	0.43
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:130:VAL:CG1	11:K:131:THR:N	2.82	0.43
12:L:37:TYR:HD2	37:L:7169:HOH:O	1.92	0.43
14:N:76:ARG:HG2	14:N:76:ARG:HH11	1.82	0.43
15:O:154:LEU:HD12	15:O:156:GLU:O	2.19	0.43
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.18	0.43
1:A:155:C:OP1	14:N:186:SER:OG	2.31	0.43
1:A:236:A:O5'	1:A:236:A:C2'	2.66	0.43
1:A:922:A:N7	1:A:2281:C:H5'	2.33	0.43
1:A:941:G:C5	1:A:942:U:C4	3.06	0.43
1:A:1706:G:C6	1:A:1707:G:C6	3.06	0.43
1:A:1730:G:H5'	1:A:1731:C:H5	1.80	0.43
1:A:1937:U:O2'	1:A:1938:G:H5'	2.18	0.43
1:A:2428:G:C6	1:A:2464:C:H1'	2.54	0.43
1:A:2526:C:H5''	37:A:7143:HOH:O	2.17	0.43
2:B:3007:G:OP1	15:O:23:ARG:HD2	2.17	0.43
2:B:3078:G:O2'	2:B:3079:U:OP2	2.35	0.43
3:C:105:VAL:CG1	3:C:106:CYS:N	2.81	0.43
10:J:48:LEU:CG	10:J:157:ILE:HG21	2.47	0.43
15:O:115:VAL:O	15:O:118:ILE:HB	2.18	0.43
17:Q:64:GLU:HG2	37:Q:2495:HOH:O	2.18	0.43
21:U:48:VAL:HG13	21:U:96:VAL:HG13	2.01	0.43
23:W:12:THR:HG23	23:W:14:ALA:N	2.34	0.43
25:Y:8:ARG:NH1	37:Y:2479:HOH:O	2.51	0.43
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.54	0.43
1:A:220:C:OP2	1:A:2431:C:H1'	2.19	0.43
1:A:466:A:H2'	1:A:467:G:O4'	2.19	0.43
1:A:1221:G:N7	37:A:3410:HOH:O	2.37	0.43
1:A:1299:G:N7	13:M:6:ARG:NH1	2.66	0.43
1:A:1572:A:H2'	1:A:1573:A:C8	2.53	0.43
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.45	0.43
1:A:2073:G:C6	1:A:2607:U:C2	3.06	0.43
1:A:2488:A:O2'	1:A:2489:G:H5'	2.19	0.43
4:D:248:ARG:HG2	37:K:8540:HOH:O	2.19	0.43
5:E:200:PRO:HB3	5:E:212:VAL:HG23	2.01	0.43
7:G:20:ILE:HD12	7:G:33:LEU:CD1	2.49	0.43
7:G:137:ASP:O	7:G:141:VAL:HG23	2.19	0.43
9:I:20:VAL:O	9:I:24:VAL:HG23	2.19	0.43
12:L:99:ASP:OD1	12:L:101:ASN:N	2.51	0.43
14:N:137:ASP:O	14:N:142:LYS:HE3	2.19	0.43
19:S:79:ARG:C	19:S:81:PRO:HD3	2.44	0.43
22:V:20:MET:HE1	37:V:7438:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:G:H2'	1:A:65:C:O4'	2.19	0.43
1:A:1167:G:O2'	1:A:1168:C:H5'	2.19	0.43
1:A:1596:U:H2'	1:A:1598:A:OP2	2.19	0.43
1:A:1869:A:H2'	1:A:1870:C:O4'	2.18	0.43
1:A:1925:G:OP1	30:4:29:ARG:NH2	2.52	0.43
1:A:2262:C:O5'	1:A:2262:C:H6	2.02	0.43
1:A:2290:U:H4'	1:A:2291:A:OP1	2.17	0.43
1:A:2468:A:H1'	37:A:3402:HOH:O	2.18	0.43
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.81	0.43
4:D:104:GLU:HG3	37:D:8594:HOH:O	2.19	0.43
7:G:11:VAL:HG13	7:G:23:GLU:O	2.18	0.43
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.36	0.43
8:H:63:ILE:HB	8:H:64:PRO:CD	2.45	0.43
15:O:149:GLU:O	15:O:152:GLU:HB2	2.18	0.43
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.49	0.43
19:S:113:HIS:O	19:S:145:LEU:HD12	2.19	0.43
23:W:38:GLY:C	23:W:40:PRO:HD2	2.44	0.43
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.34	0.43
1:A:161:A:H3'	37:A:8917:HOH:O	2.18	0.42
1:A:221:G:C6	1:A:222:A:C6	3.07	0.42
1:A:686:A:O2'	1:A:747:G:H4'	2.19	0.42
1:A:1199:A:C5	1:A:1200:A:C5	3.07	0.42
1:A:1268:C:H2'	1:A:1269:G:C8	2.54	0.42
1:A:1278:A:H4'	1:A:1279:U:C4	2.54	0.42
1:A:1504:A:O2'	1:A:1506:U:OP2	2.33	0.42
1:A:2812:A:N7	37:A:7054:HOH:O	2.36	0.42
1:A:2821:C:H4'	4:D:116:PRO:CB	2.49	0.42
2:B:3092:G:C6	2:B:3093:A:C6	3.08	0.42
3:C:39:ALA:HB3	3:C:61:GLU:OE2	2.19	0.42
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.48	0.42
4:D:51:VAL:HG13	4:D:53:LEU:HD13	2.01	0.42
4:D:204:GLY:HA3	37:D:8660:HOH:O	2.18	0.42
7:G:11:VAL:CG1	7:G:12:ASP:H	2.32	0.42
7:G:162:PHE:CD1	7:G:162:PHE:N	2.86	0.42
10:J:167:ALA:HA	37:J:8373:HOH:O	2.19	0.42
13:M:125:PHE:CE1	13:M:140:VAL:HG13	2.54	0.42
13:M:145:LEU:HB2	37:M:8543:HOH:O	2.18	0.42
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.49	0.42
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.54	0.42
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.49	0.42
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.81	0.42
25:Y:70:ILE:O	25:Y:70:ILE:HG23	2.19	0.42
29:3:19:SER:HB3	37:3:4479:HOH:O	2.18	0.42
1:A:123:U:H2'	1:A:124:C:C6	2.54	0.42
1:A:419:A:H1'	1:A:1921:A:C2	2.54	0.42
1:A:492:C:C2	1:A:501:G:N2	2.87	0.42
1:A:1123:A:C2	1:A:1129:C:H4'	2.54	0.42
1:A:1634:G:H2'	1:A:1635:U:H6	1.84	0.42
1:A:1707:G:N2	1:A:1709:G:H3'	2.34	0.42
1:A:2108:A:O2'	1:A:2110:G:H5''	2.19	0.42
1:A:2569:A:H2'	1:A:2570:G:O5'	2.19	0.42
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.42
1:A:2846:C:H2'	1:A:2847:G:H8	1.83	0.42
1:A:2890:A:H2'	37:A:4745:HOH:O	2.19	0.42
37:A:9642:HOH:O	19:S:83:LYS:HB3	2.19	0.42
3:C:192:VAL:O	3:C:207:GLN:HG2	2.19	0.42
4:D:4:SER:O	4:D:5:ARG:HB2	2.20	0.42
4:D:98:THR:O	4:D:99:GLU:HG3	2.19	0.42
4:D:260:HIS:HA	37:D:8633:HOH:O	2.18	0.42
6:F:76:ARG:O	6:F:77:ASP:HB2	2.19	0.42
8:H:26:THR:HB	8:H:102:GLY:HA3	2.01	0.42
13:M:145:LEU:O	13:M:145:LEU:HD23	2.18	0.42
14:N:62:VAL:C	14:N:63:VAL:CG2	2.92	0.42
15:O:71:TRP:CE3	15:O:175:LEU:CD2	2.96	0.42
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.82	0.42
20:T:57:THR:HG22	20:T:59:ASP:CB	2.49	0.42
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.18	0.42
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.42
1:A:470:U:H2'	1:A:471:G:O4'	2.19	0.42
1:A:816:G:C5	1:A:817:G:C6	3.08	0.42
1:A:951:A:O2'	1:A:952:G:H5'	2.19	0.42
1:A:1500:U:OP2	17:Q:41:ARG:NH2	2.52	0.42
1:A:1592:G:C5	1:A:1593:C:C4	3.06	0.42
1:A:1754:A:H2'	1:A:1755:A:O4'	2.20	0.42
1:A:1790:C:H2'	1:A:1791:U:H6	1.84	0.42
1:A:1825:U:O4'	1:A:1999:C:H5''	2.18	0.42
1:A:2016:U:O5'	1:A:2016:U:H6	2.02	0.42
37:A:3971:HOH:O	3:C:11:ARG:NE	2.52	0.42
2:B:3008:G:C6	2:B:3009:C:C4	3.07	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.29	0.42
3:C:179:MET:HG2	3:C:186:TRP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:304:PRO:HA	37:D:8536:HOH:O	2.19	0.42
6:F:167:GLU:C	6:F:169:THR:H	2.27	0.42
10:J:150:LYS:NZ	37:J:8380:HOH:O	2.48	0.42
12:L:58:THR:HG22	12:L:59:LYS:HG3	2.01	0.42
14:N:71:SER:O	14:N:73:ARG:NH1	2.49	0.42
23:W:42:ASN:O	23:W:44:GLY:N	2.52	0.42
24:X:122:ARG:HG2	24:X:152:ALA:O	2.18	0.42
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.45	0.42
29:3:40:ARG:HG3	29:3:45:ASN:CB	2.49	0.42
1:A:182:G:O3'	14:N:157:LEU:HD13	2.18	0.42
1:A:236:A:H4'	1:A:237:G:OP1	2.19	0.42
1:A:392:U:H4'	14:N:193:LYS:HB3	2.02	0.42
1:A:407:A:H2'	1:A:408:A:C8	2.55	0.42
1:A:716:G:H2'	1:A:717:C:O5'	2.20	0.42
1:A:929:A:N7	1:A:930:C:C4	2.87	0.42
1:A:1338:U:H2'	1:A:1339:G:O4'	2.19	0.42
1:A:1524:U:O2'	1:A:1525:G:P	2.77	0.42
1:A:1931:A:H8	1:A:1931:A:O5'	2.02	0.42
1:A:2096:A:H2'	1:A:2539:U:O4'	2.20	0.42
1:A:2356:A:H2'	1:A:2357:G:O4'	2.19	0.42
37:A:5786:HOH:O	3:C:22:ARG:HG2	2.19	0.42
4:D:53:LEU:HD11	4:D:327:VAL:HG22	2.02	0.42
4:D:57:GLU:HA	4:D:58:PRO:HD2	1.91	0.42
4:D:221:GLN:NE2	12:L:42:ASN:HD22	2.10	0.42
14:N:19:GLN:N	37:N:8563:HOH:O	2.52	0.42
15:O:127:LEU:HD12	15:O:127:LEU:HA	1.85	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.47	0.42
17:Q:11:ALA:HB2	17:Q:18:LYS:HA	2.01	0.42
20:T:53:ASN:ND2	37:T:2190:HOH:O	2.53	0.42
1:A:154:C:P	14:N:188:ARG:HH12	2.42	0.42
1:A:515:C:H3'	37:A:5193:HOH:O	2.18	0.42
1:A:1069:C:H4'	1:A:1081:A:O2'	2.19	0.42
1:A:1236:A:H2'	1:A:1237:U:O4'	2.19	0.42
1:A:1471:A:H2'	1:A:1472:C:C6	2.54	0.42
1:A:2107:U:O5'	1:A:2107:U:H6	2.02	0.42
1:A:2431:C:O2'	1:A:2432:C:H5'	2.19	0.42
5:E:173:LYS:HB3	5:E:187:ARG:HG3	2.01	0.42
6:F:63:ILE:C	37:F:5728:HOH:O	2.62	0.42
7:G:22:VAL:O	7:G:28:SER:HA	2.19	0.42
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.55	0.42
24:X:38:THR:O	24:X:42:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:76:ARG:HA	25:Y:82:GLU:O	2.19	0.42
30:4:65:THR:HG23	30:4:67:LEU:CG	2.42	0.42
1:A:690:G:H4'	1:A:741:C:O2	2.20	0.42
1:A:844:A:C6	1:A:882:A:C5	3.07	0.42
1:A:1189:A:H3'	37:A:7218:HOH:O	2.20	0.42
1:A:1450:C:O2'	1:A:1493:A:H2'	2.20	0.42
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.02	0.42
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.19	0.42
1:A:2560:C:O2	37:A:9455:HOH:O	2.22	0.42
1:A:2670:G:O2'	1:A:2671:U:H5'	2.20	0.42
3:C:199:HIS:HD2	3:C:201:PHE:CB	2.22	0.42
6:F:35:ALA:HB2	37:F:5858:HOH:O	2.20	0.42
6:F:55:LYS:C	37:F:4069:HOH:O	2.63	0.42
8:H:53:ASP:CG	8:H:80:GLN:HB2	2.45	0.42
9:I:71:LEU:C	9:I:73:ASP:N	2.78	0.42
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.38	0.42
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.19	0.42
18:R:47:VAL:HA	18:R:48:PRO:HD3	1.82	0.42
1:A:226:A:H1'	1:A:393:G:C5	2.54	0.42
1:A:413:G:N3	1:A:428:G:C2	2.88	0.42
1:A:711:G:C2	1:A:718:C:C2	3.07	0.42
1:A:1209:C:C2	1:A:1210:G:C8	3.07	0.42
1:A:1973:A:H5'	1:A:1973:A:H8	1.85	0.42
1:A:2090:G:H2'	1:A:2091:G:C8	2.55	0.42
1:A:2118:A:H2'	1:A:2119:C:H6	1.85	0.42
1:A:2263:G:C6	1:A:2264:A:C5	3.08	0.42
1:A:2377:U:O5'	1:A:2377:U:H6	2.02	0.42
1:A:2779:G:H1'	37:A:5650:HOH:O	2.19	0.42
2:B:3038:A:H2	2:B:3043:G:H5''	1.84	0.42
3:C:153:ARG:HH11	3:C:153:ARG:CB	2.32	0.42
4:D:279:THR:HG22	4:D:280:VAL:N	2.34	0.42
5:E:57:PRO:HA	37:E:8317:HOH:O	2.19	0.42
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.54	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
14:N:100:ILE:O	14:N:101:ALA:C	2.63	0.42
14:N:115:LEU:HD13	14:N:116:ASN:HB2	2.00	0.42
15:O:93:GLN:HG2	37:O:8558:HOH:O	2.19	0.42
20:T:57:THR:C	20:T:59:ASP:N	2.74	0.42
24:X:101:LEU:C	24:X:103:GLU:H	2.28	0.42
1:A:31:C:C2	37:A:5697:HOH:O	2.56	0.42
1:A:218:C:OP2	1:A:220:C:N4	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:A:O4'	1:A:774:C:H4'	2.19	0.42
1:A:657:G:H2'	1:A:658:C:C6	2.55	0.42
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.19	0.42
1:A:1456:C:H2'	1:A:1457:U:C6	2.55	0.42
1:A:1501:A:C6	1:A:1502:A:C6	3.07	0.42
1:A:1934:A:C8	1:A:1935:C:C5	3.08	0.42
1:A:1973:A:H2'	1:A:1974:G:O4'	2.20	0.42
1:A:2758:G:H2'	1:A:2759:C:C6	2.55	0.42
3:C:161:GLY:O	3:C:162:GLY:C	2.62	0.42
5:E:127:ARG:NE	5:E:228:ALA:O	2.42	0.42
10:J:46:VAL:C	10:J:146:TRP:CZ3	2.98	0.42
12:L:66:ARG:HG2	12:L:66:ARG:HH11	1.85	0.42
13:M:73:VAL:HG11	13:M:118:LEU:HD21	2.01	0.42
14:N:45:ARG:HB3	14:N:48:ARG:HB2	2.02	0.42
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.42	0.42
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.20	0.42
23:W:11:MET:HB3	23:W:15:GLU:HB2	2.00	0.42
29:3:25:VAL:O	29:3:29:THR:HG23	2.20	0.42
1:A:213:G:N2	1:A:225:G:H2'	2.35	0.42
1:A:217:C:OP1	1:A:395:A:O2'	2.30	0.42
1:A:332:G:H4'	21:U:2:LYS:O	2.19	0.42
1:A:400:C:O2'	1:A:401:C:H5'	2.20	0.42
1:A:1015:C:H2'	1:A:1016:U:C6	2.55	0.42
1:A:1158:G:O2'	1:A:1159:G:H5'	2.20	0.42
1:A:1589:G:H4'	37:A:6394:HOH:O	2.20	0.42
1:A:1730:G:C5'	1:A:1731:C:H6	2.32	0.42
1:A:1820:G:C6	1:A:2030:A:C2	3.08	0.42
1:A:2564:G:OP2	1:A:2565:C:H5''	2.20	0.42
1:A:2712:G:P	37:A:4776:HOH:O	2.78	0.42
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.48	0.42
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.50	0.42
6:F:169:THR:O	6:F:170:TYR:HB2	2.19	0.42
7:G:126:ILE:HB	7:G:131:LEU:HD23	2.01	0.42
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.19	0.42
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.50	0.42
15:O:49:THR:CG2	15:O:58:LEU:HD11	2.50	0.42
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	2.01	0.42
20:T:33:SER:OG	20:T:36:GLU:HG3	2.20	0.42
21:U:6:LYS:NZ	37:U:644:HOH:O	2.49	0.42
21:U:105:ASP:OD1	21:U:107:LYS:N	2.52	0.42
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:G:C6	1:A:316:A:C6	3.08	0.42
1:A:840:U:H2'	19:S:128:ARG:HH12	1.83	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.35	0.42
1:A:1549:C:N3	1:A:1637:A:C2	2.88	0.42
1:A:1634:G:C6	1:A:1635:U:C4	3.07	0.42
1:A:1804:A:H2'	1:A:1805:G:H8	1.85	0.42
1:A:2428:G:O6	1:A:2464:C:H1'	2.20	0.42
1:A:2623:G:C2'	1:A:2624:A:H5'	2.50	0.42
1:A:2737:C:H2'	37:A:5688:HOH:O	2.19	0.42
5:E:55:ARG:NH2	28:2:56:GLU:OE2	2.34	0.42
6:F:48:MET:HA	6:F:49:PRO:HD3	1.77	0.42
6:F:93:LEU:HG	37:F:3862:HOH:O	2.20	0.42
7:G:69:ILE:HA	7:G:72:MET:HE3	2.02	0.42
16:P:105:ASN:O	16:P:105:ASN:CG	2.63	0.42
17:Q:37:ARG:O	17:Q:41:ARG:HG3	2.20	0.42
26:Z:185:VAL:HG12	37:Z:8572:HOH:O	2.19	0.42
1:A:60:A:O2'	1:A:61:G:H5'	2.20	0.41
1:A:97:G:C2	21:U:107:LYS:HD2	2.55	0.41
1:A:177:A:C8	1:A:178:U:C5	3.08	0.41
1:A:331:A:C6	1:A:332:G:C4	3.07	0.41
1:A:397:A:P	37:A:3908:HOH:O	2.77	0.41
1:A:573:A:P	37:A:6582:HOH:O	2.78	0.41
1:A:671:A:O2'	1:A:672:G:H2'	2.19	0.41
1:A:790:A:H2'	1:A:791:A:O4'	2.20	0.41
1:A:920:C:C4	1:A:2467:A:C5	3.07	0.41
1:A:1788:U:C2	1:A:1805:G:N2	2.87	0.41
1:A:1815:A:H4'	1:A:2751:C:O4'	2.20	0.41
37:A:3971:HOH:O	3:C:11:ARG:CZ	2.68	0.41
37:A:5739:HOH:O	14:N:174:ARG:HD3	2.20	0.41
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.84	0.41
5:E:109:LEU:HD12	5:E:109:LEU:O	2.20	0.41
6:F:67:ASP:O	6:F:69:ILE:HG13	2.19	0.41
6:F:77:ASP:HB3	6:F:78:GLU:H	1.59	0.41
6:F:92:GLU:O	6:F:93:LEU:O	2.38	0.41
6:F:159:PRO:O	6:F:163:VAL:HG23	2.19	0.41
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.20	0.41
13:M:63:THR:HA	13:M:107:LYS:O	2.20	0.41
14:N:62:VAL:O	14:N:63:VAL:CG2	2.68	0.41
14:N:98:GLN:NE2	14:N:117:SER:O	2.52	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.02	0.41
20:T:23:LYS:HD3	20:T:65:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:U:C1'	37:A:6872:HOH:O	2.67	0.41
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.21	0.41
1:A:1339:G:C6	1:A:1340:G:N1	2.88	0.41
1:A:1384:C:H5'	25:Y:30:MET:HG2	2.02	0.41
1:A:1593:C:OP1	17:Q:117:SER:HB2	2.21	0.41
1:A:1759:A:N3	1:A:1818:C:H2'	2.35	0.41
1:A:2300:A:H4'	1:A:2301:A:O5'	2.20	0.41
1:A:2415:A:H2'	1:A:2416:G:H5'	2.01	0.41
1:A:2502:C:H2'	1:A:2503:A:C5'	2.49	0.41
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.53	0.41
1:A:2697:A:H2'	1:A:2698:G:O4'	2.19	0.41
2:B:3116:C:O2'	2:B:3117:G:H5'	2.21	0.41
5:E:57:PRO:O	5:E:58:ALA:C	2.63	0.41
7:G:132:THR:O	7:G:132:THR:HG23	2.20	0.41
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.44	0.41
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.02	0.41
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.20	0.41
1:A:195:C:H2'	1:A:196:G:H5'	2.02	0.41
1:A:319:A:H4'	1:A:338:C:C5	2.54	0.41
1:A:380:A:H5''	14:N:48:ARG:NH2	2.35	0.41
1:A:482:G:H4'	1:A:508:A:N1	2.35	0.41
1:A:734:U:O2'	1:A:737:A:N6	2.53	0.41
1:A:1654:U:OP1	37:A:6956:HOH:O	2.22	0.41
1:A:2025:G:C6	1:A:2026:C:C4	3.08	0.41
1:A:2424:U:H4'	18:R:6:PRO:HD2	2.02	0.41
1:A:2721:U:C4	1:A:2722:G:N7	2.89	0.41
1:A:2911:C:H3'	37:A:5101:HOH:O	2.20	0.41
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.01	0.41
10:J:85:ILE:HG23	10:J:85:ILE:O	2.20	0.41
10:J:86:ARG:H	10:J:86:ARG:HG2	1.44	0.41
11:K:135:ILE:O	11:K:139:LEU:HG	2.20	0.41
13:M:68:GLU:O	13:M:69:ILE:C	2.62	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.19	0.41
14:N:115:LEU:HD13	14:N:115:LEU:C	2.45	0.41
15:O:67:ALA:HA	15:O:71:TRP:H	1.85	0.41
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.53	0.41
30:4:74:CYS:SG	30:4:76:LYS:CB	3.05	0.41
1:A:263:U:C2	8:H:59:ILE:HD12	2.55	0.41
1:A:655:U:O2'	16:P:3:THR:HB	2.20	0.41
1:A:757:C:H2'	1:A:758:A:C8	2.56	0.41
1:A:912:A:C4	1:A:1294:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:G:C2	1:A:2072:G:N7	2.89	0.41
1:A:1275:C:C2'	1:A:1276:U:H5'	2.50	0.41
1:A:2385:G:H2'	1:A:2386:U:C6	2.56	0.41
1:A:2405:C:P	37:A:6132:HOH:O	2.77	0.41
1:A:2481:G:C3'	1:A:2482:G:H5''	2.51	0.41
1:A:2781:U:H2'	1:A:2782:G:C5'	2.50	0.41
37:A:3328:HOH:O	21:U:9:LYS:HD3	2.21	0.41
37:A:9345:HOH:O	13:M:41:HIS:CE1	2.66	0.41
2:B:3093:A:C5	2:B:3094:G:H1'	2.56	0.41
4:D:238:ASN:ND2	4:D:240:GLY:H	2.09	0.41
8:H:26:THR:HB	8:H:102:GLY:C	2.45	0.41
14:N:131:VAL:O	14:N:133:LEU:HD12	2.20	0.41
15:O:34:LEU:HD22	15:O:129:ILE:CD1	2.50	0.41
17:Q:2:ASP:OD1	17:Q:2:ASP:C	2.62	0.41
21:U:96:VAL:CG1	21:U:97:ARG:N	2.80	0.41
24:X:13:MET:HE3	24:X:17:ILE:HG22	2.02	0.41
27:1:22:ILE:O	27:1:26:VAL:HG23	2.21	0.41
28:2:28:HIS:O	28:2:32:LYS:N	2.49	0.41
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.41
1:A:290:C:O2'	1:A:291:C:H5'	2.20	0.41
1:A:638:C:H2'	1:A:639:A:C8	2.55	0.41
1:A:696:C:C2'	1:A:697:G:H5'	2.50	0.41
1:A:772:G:H2'	1:A:773:A:O4'	2.21	0.41
1:A:920:C:H5'	1:A:921:G:N3	2.35	0.41
1:A:1019:C:P	37:A:3516:HOH:O	2.78	0.41
1:A:1187:U:C3'	37:A:6434:HOH:O	2.68	0.41
1:A:2083:A:N6	11:K:90:LYS:HE2	2.35	0.41
1:A:2362:A:H2'	1:A:2363:G:C8	2.55	0.41
1:A:2488:A:H61	1:A:2534:C:H42	1.69	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.79	0.41
1:A:2549:C:H1'	4:D:248:ARG:NH2	2.35	0.41
1:A:2646:G:H1'	34:A:8523:CL:CL	2.57	0.41
1:A:2833:C:C2	1:A:2848:G:N2	2.89	0.41
10:J:26:LYS:HD2	10:J:28:ILE:CB	2.50	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
11:K:46:ILE:O	11:K:46:ILE:CG1	2.65	0.41
11:K:56:LYS:HE2	11:K:60:ARG:NH2	2.36	0.41
14:N:85:ARG:NE	37:N:8519:HOH:O	2.47	0.41
14:N:185:PRO:CG	14:N:189:VAL:HG11	2.49	0.41
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	2.03	0.41
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:11:CYS:HB2	30:4:20:HIS:HE1	1.84	0.41
30:4:40:ARG:HG3	30:4:52:PHE:CD2	2.55	0.41
1:A:134:U:N3	1:A:145:A:N1	2.68	0.41
1:A:244:C:OP2	8:H:38:LYS:HE3	2.21	0.41
1:A:245:C:H2'	1:A:246:G:H5'	2.01	0.41
1:A:1019:C:O2	18:R:94:GLN:NE2	2.54	0.41
1:A:1391:G:C5	1:A:1435:U:C4	3.08	0.41
1:A:1494:A:C2	1:A:1495:C:C4	3.08	0.41
1:A:1656:A:H2'	1:A:1657:A:O4'	2.21	0.41
1:A:1829:A:C2'	1:A:1830:C:H5'	2.50	0.41
1:A:2346:C:H4'	6:F:52:THR:HG22	2.03	0.41
1:A:2467:A:O2'	1:A:2468:A:H2'	2.20	0.41
1:A:2750:G:H8	1:A:2750:G:O5'	2.04	0.41
1:A:2868:C:H2'	1:A:2869:G:O4'	2.21	0.41
5:E:16:VAL:CG1	5:E:17:ASP:N	2.80	0.41
5:E:214:THR:HG23	37:E:8443:HOH:O	2.21	0.41
6:F:67:ASP:OD1	6:F:67:ASP:N	2.53	0.41
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.56	0.41
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.19	0.41
12:L:19:THR:HG22	12:L:20:CYS:N	2.35	0.41
14:N:81:ARG:HB3	14:N:86:MET:HG2	2.02	0.41
14:N:173:LEU:HA	14:N:183:VAL:HG11	2.03	0.41
15:O:33:ARG:NH2	37:O:8554:HOH:O	2.41	0.41
16:P:21:SER:OG	16:P:106:PRO:HB2	2.20	0.41
21:U:55:PHE:O	21:U:56:ALA:C	2.63	0.41
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.69	0.41
1:A:240:C:O2	1:A:240:C:H2'	2.21	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.51	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.35	0.41
1:A:383:A:C2	1:A:407:A:C4	3.08	0.41
1:A:567:U:O2'	1:A:568:G:H5'	2.20	0.41
1:A:661:G:C6	1:A:686:A:C2	3.09	0.41
1:A:1440:U:P	37:A:4027:HOH:O	2.79	0.41
1:A:2241:C:H2'	1:A:2242:U:C6	2.55	0.41
1:A:2346:C:H4'	6:F:52:THR:CG2	2.50	0.41
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.55	0.41
1:A:2690:U:H4'	7:G:111:LYS:NZ	2.35	0.41
37:A:3756:HOH:O	26:Z:186:ARG:HD2	2.20	0.41
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.41
5:E:236:THR:C	37:E:8455:HOH:O	2.64	0.41
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.51	0.41
6:F:60:GLU:C	6:F:62:ASP:N	2.75	0.41
10:J:56:ILE:HG21	10:J:61:LEU:CD1	2.51	0.41
10:J:73:GLN:OE1	10:J:73:GLN:CA	2.68	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.89	0.41
12:L:99:ASP:OD1	12:L:99:ASP:C	2.63	0.41
13:M:148:GLU:HG2	37:M:8556:HOH:O	2.20	0.41
15:O:25:ARG:HA	15:O:28:LYS:HG3	2.02	0.41
17:Q:83:LYS:O	17:Q:86:ALA:HB3	2.21	0.41
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.20	0.41
1:A:198:A:H2'	37:A:5442:HOH:O	2.20	0.41
1:A:391:U:OP2	14:N:84:LYS:NZ	2.49	0.41
1:A:492:C:O2'	1:A:493:U:H5'	2.21	0.41
1:A:566:A:H2'	1:A:567:U:O4'	2.21	0.41
1:A:582:C:N4	37:A:5985:HOH:O	2.54	0.41
1:A:1051:C:H2'	1:A:1052:G:O4'	2.21	0.41
1:A:1187:U:H3'	37:A:6434:HOH:O	2.20	0.41
1:A:1377:C:H5'	1:A:1377:C:C6	2.51	0.41
1:A:1444:G:O2'	1:A:1502:A:N1	2.44	0.41
1:A:2004:U:H2'	1:A:2005:G:OP1	2.20	0.41
1:A:2450:C:O5'	1:A:2450:C:H6	2.03	0.41
1:A:2735:U:H2'	1:A:2736:U:C6	2.55	0.41
2:B:3040:C:N4	6:F:51:ARG:HB2	2.35	0.41
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.36	0.41
4:D:87:TYR:OH	4:D:163:GLU:OE2	2.36	0.41
5:E:165:ASP:O	5:E:168:ARG:HB3	2.21	0.41
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.03	0.41
13:M:72:ASN:HB2	37:M:8587:HOH:O	2.20	0.41
14:N:20:ILE:O	14:N:24:MET:HG2	2.21	0.41
15:O:74:PRO:HG2	15:O:159:TYR:CZ	2.56	0.41
24:X:13:MET:HE2	24:X:18:GLN:N	2.35	0.41
24:X:14:HIS:HB2	24:X:17:ILE:HG13	2.02	0.41
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.65	0.41
27:1:38:LYS:HD3	37:1:8425:HOH:O	2.20	0.41
1:A:60:A:C2	1:A:61:G:C8	3.09	0.41
1:A:128:A:C8	1:A:128:A:C3'	3.03	0.41
1:A:171:C:OP2	14:N:84:LYS:HG3	2.21	0.41
1:A:308:U:H5'	21:U:97:ARG:NH2	2.36	0.41
1:A:432:G:N2	1:A:433:C:C2	2.89	0.41
1:A:696:C:O2'	1:A:697:G:H5'	2.20	0.41
1:A:834:G:H3'	1:A:835:U:H4'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:G:C6	1:A:942:U:C4	3.08	0.41
1:A:1021:G:O2'	1:A:1022:A:H5'	2.21	0.41
1:A:1064:U:H2'	1:A:1065:G:C8	2.56	0.41
1:A:1127:C:C2'	1:A:1128:U:H5'	2.50	0.41
1:A:1188:A:C5	1:A:1189:A:C2	3.09	0.41
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.41
1:A:1565:C:O4'	1:A:2738:G:H1'	2.21	0.41
1:A:1624:A:H5'	1:A:1626:A:O4'	2.21	0.41
1:A:1773:G:C8	27:1:16:PRO:CA	3.04	0.41
1:A:1821:A:O2'	1:A:1822:A:H5'	2.21	0.41
1:A:1839:A:H5'	1:A:2643:G:H4'	2.03	0.41
1:A:1840:A:H4'	1:A:1841:C:O5'	2.21	0.41
1:A:2039:A:H2'	1:A:2040:C:C6	2.56	0.41
1:A:2121:G:P	37:A:3085:HOH:O	2.67	0.41
1:A:2255:A:C6	1:A:2256:G:C5	3.08	0.41
1:A:2437:A:H2'	1:A:2438:G:C8	2.56	0.41
1:A:2577:A:H4'	1:A:2578:G:C8	2.55	0.41
1:A:2691:A:H8	1:A:2691:A:OP1	2.04	0.41
1:A:2900:G:H2'	1:A:2901:C:O4'	2.21	0.41
37:A:6119:HOH:O	2:B:3083:G:H4'	2.21	0.41
3:C:81:GLN:H	3:C:92:ASN:CG	2.29	0.41
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.86	0.41
4:D:224:LYS:HD3	4:D:224:LYS:HA	1.76	0.41
6:F:102:GLY:O	6:F:134:LEU:HD12	2.21	0.41
7:G:91:PHE:HA	7:G:92:PRO:HD3	1.90	0.41
7:G:137:ASP:OD1	7:G:137:ASP:C	2.63	0.41
9:I:64:ASN:N	9:I:64:ASN:ND2	2.67	0.41
10:J:45:GLN:CB	10:J:163:PRO:HD2	2.25	0.41
11:K:45:VAL:CG2	11:K:46:ILE:N	2.83	0.41
12:L:103:ASP:O	12:L:104:PRO:C	2.62	0.41
12:L:130:MET:SD	22:V:25:ASP:O	2.79	0.41
12:L:130:MET:SD	22:V:26:GLY:HA3	2.60	0.41
14:N:61:ILE:HA	37:N:8622:HOH:O	2.20	0.41
14:N:68:ARG:N	37:N:8544:HOH:O	2.51	0.41
14:N:69:LYS:HG2	14:N:127:LYS:HG3	2.01	0.41
14:N:115:LEU:O	14:N:116:ASN:CB	2.68	0.41
15:O:47:LEU:HD23	15:O:47:LEU:HA	1.79	0.41
15:O:143:ARG:HH12	15:O:173:ASP:CG	2.27	0.41
15:O:164:ASP:OD1	15:O:164:ASP:C	2.64	0.41
15:O:186:LEU:HD23	15:O:186:LEU:HA	1.88	0.41
19:S:89:LEU:HD23	19:S:89:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:80:ARG:HG2	37:T:4527:HOH:O	2.20	0.41
22:V:34:SER:O	22:V:38:ASN:ND2	2.54	0.41
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.46	0.41
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.52	0.41
25:Y:41:PHE:O	25:Y:42:SER:C	2.64	0.41
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.61	0.41
1:A:34:C:C4	1:A:35:U:C4	3.09	0.41
1:A:113:A:H3'	1:A:114:A:C5'	2.51	0.41
1:A:157:G:H4'	14:N:95:LYS:CE	2.48	0.41
1:A:542:A:C5'	1:A:542:A:C8	2.99	0.41
1:A:629:A:N7	37:A:9435:HOH:O	2.37	0.41
1:A:646:G:H2'	1:A:647:U:H6	1.84	0.41
1:A:716:G:C2'	1:A:717:C:O5'	2.69	0.41
1:A:816:G:C6	1:A:817:G:C6	3.09	0.41
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.50	0.41
1:A:1339:G:C5	1:A:1340:G:C6	3.09	0.41
1:A:1666:C:H2'	1:A:1667:A:H8	1.86	0.41
1:A:1886:A:H4'	37:1:8405:HOH:O	2.21	0.41
1:A:1946:C:H2'	1:A:1971:G:C8	2.56	0.41
1:A:1976:G:O2'	1:A:1977:U:H5'	2.21	0.41
1:A:2105:C:O2	1:A:2485:A:C6	2.74	0.41
1:A:2251:G:H2'	1:A:2252:A:H8	1.86	0.41
1:A:2323:G:H5'	37:A:6557:HOH:O	2.20	0.41
1:A:2791:U:H4'	1:A:2792:A:OP1	2.21	0.41
37:A:3579:HOH:O	4:D:48:MET:HB2	2.21	0.41
4:D:51:VAL:HG21	4:D:327:VAL:HG13	2.03	0.41
4:D:312:ARG:HG2	4:D:313:PRO:O	2.20	0.41
11:K:46:ILE:CG1	11:K:53:ILE:HD13	2.51	0.41
12:L:14:LYS:HD2	12:L:45:PRO:HG3	2.03	0.41
20:T:80:ARG:C	37:T:4895:HOH:O	2.64	0.41
21:U:63:ILE:O	21:U:63:ILE:HG22	2.20	0.41
21:U:69:LYS:O	21:U:71:VAL:HG23	2.21	0.41
30:4:84:ARG:HB3	37:4:8550:HOH:O	2.21	0.41
1:A:100:C:H4'	21:U:16:LEU:HB2	2.03	0.40
1:A:299:U:C5'	37:A:6872:HOH:O	2.63	0.40
1:A:401:C:H2'	1:A:402:U:C6	2.56	0.40
1:A:675:U:O2'	5:E:42:ARG:NH1	2.53	0.40
1:A:869:G:OP1	14:N:79:LYS:HE2	2.21	0.40
1:A:876:A:N7	1:A:878:G:H1'	2.36	0.40
1:A:1436:C:O2'	1:A:1437:A:H5'	2.21	0.40
1:A:1531:U:O2	1:A:1661:A:C2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1751:G:C3'	1:A:1752:G:H5''	2.51	0.40
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.40
1:A:2407:G:O2'	1:A:2408:A:H5'	2.21	0.40
1:A:2569:A:H8	1:A:2569:A:O5'	2.04	0.40
1:A:2667:G:H1'	1:A:2914:A:N3	2.35	0.40
1:A:2783:A:O2'	1:A:2784:A:H5'	2.20	0.40
3:C:33:GLU:CD	3:C:33:GLU:H	2.24	0.40
4:D:109:LEU:HG	4:D:113:LEU:HD12	2.03	0.40
6:F:84:LEU:C	6:F:86:THR:N	2.79	0.40
7:G:84:MET:HB2	7:G:131:LEU:HB2	2.03	0.40
7:G:143:GLN:NE2	37:G:2113:HOH:O	2.53	0.40
12:L:118:ALA:C	12:L:120:ARG:N	2.79	0.40
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.51	0.40
14:N:39:ARG:CZ	37:N:8622:HOH:O	2.68	0.40
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.51	0.40
15:O:71:TRP:N	37:O:8539:HOH:O	2.54	0.40
16:P:96:VAL:HG13	16:P:100:GLN:HB2	2.03	0.40
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.56	0.40
19:S:106:GLY:HA2	19:S:109:MET:CE	2.49	0.40
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.21	0.40
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.55	0.40
1:A:1352:A:N1	5:E:48:SER:HB3	2.36	0.40
1:A:1828:G:C2'	1:A:1829:A:H5'	2.51	0.40
1:A:2101:A:H5'	5:E:63:SER:HB3	2.04	0.40
1:A:2422:U:OP1	37:A:6479:HOH:O	2.21	0.40
2:B:3036:C:C5	2:B:3037:C:C5	3.09	0.40
4:D:32:ASP:HA	37:D:8577:HOH:O	2.21	0.40
5:E:136:VAL:HG22	5:E:137:PRO:HA	2.02	0.40
7:G:84:MET:HE2	7:G:133:VAL:HG23	2.02	0.40
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.21	0.40
12:L:22:ASP:CG	12:L:24:THR:HG23	2.45	0.40
14:N:77:PHE:CD2	14:N:86:MET:HA	2.56	0.40
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.84	0.40
19:S:104:PHE:HB3	19:S:109:MET:HE2	2.02	0.40
20:T:57:THR:CG2	20:T:58:MET:N	2.85	0.40
30:4:60:LYS:HG3	30:4:61:PRO:HD2	2.03	0.40
1:A:90:A:H2'	1:A:91:G:O4'	2.22	0.40
1:A:664:U:O4	1:A:681:G:H5''	2.20	0.40
1:A:1076:G:C2	1:A:1084:C:C2	3.09	0.40
1:A:2266:A:C5'	37:A:5407:HOH:O	2.68	0.40
1:A:2547:C:H2'	1:A:2548:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2681:A:H4'	1:A:2682:C:H5'	2.03	0.40
2:B:3076:G:H2'	2:B:3077:A:OP1	2.21	0.40
2:B:3092:G:H22	10:J:52:LYS:NZ	2.19	0.40
2:B:3113:C:H5''	37:B:2295:HOH:O	2.21	0.40
3:C:164:ARG:HA	27:1:69:TYR:CE1	2.57	0.40
4:D:255:GLY:O	4:D:257:THR:HG23	2.21	0.40
7:G:81:GLU:HA	7:G:133:VAL:O	2.20	0.40
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.84	0.40
10:J:72:VAL:O	10:J:72:VAL:HG13	2.20	0.40
37:L:1387:HOH:O	22:V:20:MET:HE3	2.21	0.40
14:N:46:LEU:HD22	14:N:50:ARG:HG3	2.02	0.40
15:O:35:VAL:HG12	15:O:37:ARG:HG2	2.02	0.40
15:O:82:TYR:OH	15:O:176:ARG:NH1	2.54	0.40
18:R:9:GLY:HA2	37:R:6663:HOH:O	2.20	0.40
24:X:97:ALA:O	24:X:98:PHE:C	2.62	0.40
24:X:122:ARG:HG2	24:X:122:ARG:NH1	2.27	0.40
29:3:41:HIS:O	29:3:45:ASN:HB2	2.20	0.40
1:A:67:A:H5''	1:A:69:A:C8	2.57	0.40
1:A:920:C:N4	1:A:2467:A:C8	2.89	0.40
1:A:1123:A:N6	1:A:1238:C:H5'	2.36	0.40
1:A:1267:C:OP2	37:A:3759:HOH:O	2.22	0.40
1:A:1522:A:H2'	1:A:1523:G:H5'	2.02	0.40
1:A:1621:G:O2'	1:A:1622:G:H5'	2.22	0.40
1:A:1983:C:O5'	1:A:1983:C:H6	2.05	0.40
1:A:2379:G:N7	1:A:2408:A:N1	2.70	0.40
1:A:2912:C:H2'	1:A:2913:A:O4'	2.22	0.40
2:B:3003:A:H61	2:B:3022:G:H1'	1.86	0.40
4:D:145:HIS:CD2	4:D:146:THR:O	2.64	0.40
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.83	0.40
8:H:6:PHE:CD1	8:H:6:PHE:C	3.00	0.40
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.46	0.40
15:O:44:ARG:HG3	15:O:45:ALA:N	2.36	0.40
16:P:41:ALA:HA	37:P:5104:HOH:O	2.21	0.40
22:V:14:GLU:HA	22:V:15:PRO:HD2	1.94	0.40
24:X:90:TYR:N	37:X:6679:HOH:O	2.54	0.40
26:Z:197:ASP:OD1	26:Z:199:ASP:HB2	2.21	0.40
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.36	0.40
1:A:688:A:H62	13:M:111:ALA:HB2	1.85	0.40
1:A:736:A:H2'	1:A:737:A:O4'	2.21	0.40
1:A:1025:C:H5'	24:X:23:MET:O	2.21	0.40
1:A:1652:C:O2	3:C:164:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2379:G:H4'	1:A:2380:A:C5'	2.51	0.40
1:A:2731:G:H2'	1:A:2732:U:O4'	2.21	0.40
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.36	0.40
2:B:3078:G:N2	2:B:3102:G:H2'	2.36	0.40
4:D:190:MET:HE3	4:D:190:MET:HA	2.04	0.40
5:E:4:THR:HB	5:E:135:GLU:OE1	2.21	0.40
6:F:27:ILE:HD11	6:F:37:ALA:HB3	2.03	0.40
6:F:86:THR:CG2	37:F:7477:HOH:O	2.69	0.40
14:N:61:ILE:CG2	14:N:62:VAL:N	2.84	0.40
15:O:74:PRO:CD	15:O:159:TYR:CE2	3.04	0.40
16:P:60:VAL:C	16:P:62:GLY:H	2.25	0.40
19:S:145:LEU:HD12	19:S:146:ILE:N	2.35	0.40
27:1:39:CYS:HA	27:1:47:LEU:CG	2.51	0.40
27:1:57:CYS:O	27:1:61:GLY:N	2.52	0.40
28:2:22:CYS:HB2	37:2:8423:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	207 (88%)	25 (11%)	3 (1%)	9	38
4	D	335/337 (99%)	303 (90%)	24 (7%)	8 (2%)	4	24
5	E	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	0	3
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	4	23
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	14 (9%)	6 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	3	20
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	35
13	M	141/164 (86%)	118 (84%)	21 (15%)	2 (1%)	9	36
14	N	192/194 (99%)	170 (88%)	20 (10%)	2 (1%)	12	45
15	O	184/186 (99%)	163 (89%)	15 (8%)	6 (3%)	3	17
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	18	53
18	R	93/95 (98%)	84 (90%)	8 (9%)	1 (1%)	11	43
19	S	148/154 (96%)	138 (93%)	9 (6%)	1 (1%)	18	53
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	18
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	53
25	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	4	23
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	62 (87%)	8 (11%)	1 (1%)	9	36
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3295 (91%)	279 (8%)	59 (2%)	7	34

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
11	K	7	ASP
11	K	143	LYS
13	M	80	ASP

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Mol	Chain	Res	Type
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
24	X	77	ALA
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	20	LYS
6	F	171	ASP
10	J	72	VAL
10	J	138	PRO
10	J	164	ALA
11	K	5	GLU
15	O	162	ASP
17	Q	116	SER
23	W	43	PRO
30	4	57	GLY
3	C	132	ASP
4	D	184	ASP
6	F	16	PRO
6	F	36	ASN
6	F	82	GLU
8	H	64	PRO
12	L	119	GLN
13	M	35	ARG
14	N	140	ALA
15	O	167	ASP
15	O	181	ASP
25	Y	77	PHE
27	1	81	LYS
30	4	56	PRO
6	F	61	PHE
6	F	147	ALA
8	H	61	MET
10	J	40	PRO
12	L	126	SER
4	D	185	GLY
4	D	2	GLN
4	D	107	SER
4	D	306	LYS

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Mol	Chain	Res	Type
14	N	165	SER
23	W	40	PRO
11	K	78	ILE
18	R	54	PRO
10	J	140	PRO
19	S	81	PRO
25	Y	70	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	168 (94%)	11 (6%)	17	49
4	D	282/282 (100%)	263 (93%)	19 (7%)	15	46
5	E	193/193 (100%)	178 (92%)	15 (8%)	11	39
6	F	117/147 (80%)	108 (92%)	9 (8%)	12	40
7	G	152/155 (98%)	147 (97%)	5 (3%)	33	67
8	H	92/92 (100%)	91 (99%)	1 (1%)	65	83
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	109 (89%)	13 (11%)	6	26
11	K	118/121 (98%)	110 (93%)	8 (7%)	14	45
12	L	106/106 (100%)	103 (97%)	3 (3%)	38	70
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	71
14	N	166/166 (100%)	158 (95%)	8 (5%)	23	57
15	O	149/149 (100%)	141 (95%)	8 (5%)	20	53
16	P	93/93 (100%)	90 (97%)	3 (3%)	34	67
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	71
18	R	79/79 (100%)	74 (94%)	5 (6%)	16	48
19	S	117/121 (97%)	114 (97%)	3 (3%)	40	72
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	105/105 (100%)	101 (96%)	4 (4%)	29	63
22	V	44/52 (85%)	43 (98%)	1 (2%)	44	74
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
24	X	130/130 (100%)	120 (92%)	10 (8%)	12	40
25	Y	66/73 (90%)	62 (94%)	4 (6%)	17	49
26	Z	120/195 (62%)	112 (93%)	8 (7%)	15	46
27	1	56/56 (100%)	53 (95%)	3 (5%)	20	53
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
30	4	79/79 (100%)	74 (94%)	5 (6%)	16	48
All	All	3027/3441 (88%)	2872 (95%)	155 (5%)	21	55

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	131	HIS
3	C	153	ARG
3	C	175	LYS
3	C	179	MET
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	84	LEU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	175	LEU
4	D	195	ARG

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Mol	Chain	Res	Type
4	D	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	67	GLN
5	E	81	PRO
5	E	91	PRO
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
5	E	243	VAL
6	F	24	HIS
6	F	50	VAL
6	F	92	GLU
6	F	95	THR
6	F	99	ASP
6	F	131	THR
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	7	ILE
7	G	36	PRO
7	G	54	ASP
7	G	86	VAL
7	G	102	VAL
8	H	46	GLU
10	J	1	LYS
10	J	18	GLU
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL

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Mol	Chain	Res	Type
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	93	ILE
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	74	ARG
11	K	76	ASP
11	K	93	ARG
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	35	ARG
13	M	117	GLU
13	M	140	VAL
14	N	38	VAL
14	N	46	LEU
14	N	81	ARG
14	N	84	LYS
14	N	87	MET
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	12	ARG
15	O	26	LEU
15	O	43	VAL
15	O	47	LEU
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
16	P	98	LEU
16	P	111	VAL
17	Q	52	LYS

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Mol	Chain	Res	Type
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	54	PRO
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
20	T	10	VAL
21	U	39	ASN
21	U	47	THR
21	U	48	VAL
21	U	96	VAL
22	V	28	THR
23	W	43	PRO
24	X	4	LEU
24	X	26	ILE
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	120	PRO
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	72	VAL
25	Y	85	VAL
26	Z	103	THR
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	32	LYS
27	1	64	ILE

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Mol	Chain	Res	Type
29	3	18	ASN
30	4	14	CYS
30	4	38	ARG
30	4	42	ARG
30	4	56	PRO
30	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	55	ASN
4	D	145	HIS
4	D	221	GLN
4	D	238	ASN
4	D	260	HIS
4	D	318	ASN
5	E	2	GLN
5	E	39	GLN
5	E	67	GLN
5	E	129	HIS
5	E	163	HIS
6	F	103	ASN
7	G	106	ASN
7	G	119	HIS
7	G	143	GLN
8	H	80	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	74	ASN
10	J	80	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN

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Mol	Chain	Res	Type
10	J	166	ASN
11	K	29	GLN
11	K	52	GLN
11	K	107	ASN
12	L	10	GLN
13	M	18	HIS
13	M	41	HIS
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	98	GLN
14	N	176	GLN
15	O	22	GLN
15	O	107	ASN
15	O	140	GLN
15	O	153	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
18	R	67	GLN
19	S	22	GLN
19	S	61	GLN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	122	GLN
19	S	123	GLN
19	S	140	GLN
20	T	51	GLN
20	T	53	ASN
21	U	39	ASN
21	U	73	HIS
22	V	39	ASN
23	W	4	HIS
23	W	60	GLN
24	X	6	GLN
24	X	27	HIS

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Mol	Chain	Res	Type
24	X	28	HIS
24	X	31	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	119	GLN
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	37	HIS
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	17	GLN
29	3	18	ASN
29	3	41	HIS
29	3	45	ASN
30	4	20	HIS
30	4	30	GLN
30	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	258 (9%)	35 (1%)
2	B	121/122 (99%)	15 (12%)	6 (4%)
All	All	2868/3044 (94%)	273 (9%)	41 (1%)

All (273) 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

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Mol	Chain	Res	Type
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
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	318	C
1	A	336	G
1	A	337	A
1	A	338	C
1	A	339	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

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Mol	Chain	Res	Type
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	645	U
1	A	660	A
1	A	688	A
1	A	701	U
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	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
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

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Mol	Chain	Res	Type
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	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	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	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	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C

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Mol	Chain	Res	Type
1	A	1378	G
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
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	1668	U
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1857	A
1	A	1879	U
1	A	1904	A

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Mol	Chain	Res	Type
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2008	U
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	2101	A
1	A	2102	G
1	A	2103	A
1	A	2104	C
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2291	A
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G

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Mol	Chain	Res	Type
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2526	C
1	A	2527	U
1	A	2533	C
1	A	2537	G
1	A	2540	G
1	A	2541	U
1	A	2553	A
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	2638	G
1	A	2649	A
1	A	2650	U
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	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A

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Mol	Chain	Res	Type
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3004	G
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (41) 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	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G

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Mol	Chain	Res	Type
1	A	1667	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2102	G
1	A	2103	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3002	U
2	B	3003	A
2	B	3023	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 233 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CAI	A	4000	1	61,62,62	2.84	19 (31%)	75,90,90	1.90	21 (28%)

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
31	CAI	A	4000	1	-	9/66/110/110	0/3/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	4000	CAI	C2-C3	-10.37	1.29	1.52
31	A	4000	CAI	C20-C21	8.22	1.71	1.50
31	A	4000	CAI	C6-C5	-6.34	1.40	1.52
31	A	4000	CAI	O21-C21	5.63	1.52	1.20
31	A	4000	CAI	O3-C3	5.44	1.55	1.46
31	A	4000	CAI	C2A-C3A	5.43	1.62	1.53
31	A	4000	CAI	C4A-C5A	4.64	1.60	1.52
31	A	4000	CAI	O4B-C4B	4.09	1.52	1.45
31	A	4000	CAI	C2-C1	-3.92	1.43	1.50
31	A	4000	CAI	C5-C4	3.65	1.58	1.52
31	A	4000	CAI	C6A-C5A	-3.32	1.43	1.51
31	A	4000	CAI	C8-C9	-3.20	1.46	1.51
31	A	4000	CAI	O3B-C3B	2.95	1.49	1.44
31	A	4000	CAI	C4A-C3A	-2.80	1.47	1.53
31	A	4000	CAI	O3-C17	2.68	1.41	1.35
31	A	4000	CAI	C12-C11	2.54	1.58	1.50
31	A	4000	CAI	O1A-C1A	2.35	1.48	1.41
31	A	4000	CAI	O5B-C1B	2.33	1.48	1.42
31	A	4000	CAI	O12-C13	2.09	1.49	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4000	CAI	O21-C21-C20	-7.74	102.86	125.38
31	A	4000	CAI	C5-C4-C3	4.50	121.25	113.16
31	A	4000	CAI	C19-O4-C4	-3.65	105.09	114.47
31	A	4000	CAI	O3-C17-O17	-3.44	116.34	122.99
31	A	4000	CAI	C4A-C3A-N3A	-3.37	103.71	111.68
31	A	4000	CAI	O4B-C1C-O1C	3.01	130.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4000	CAI	O1B-C4A-C5A	2.85	114.03	106.77
31	A	4000	CAI	O5A-C5A-C6A	-2.85	100.42	106.74
31	A	4000	CAI	O4B-C1C-C2C	-2.83	106.36	111.43
31	A	4000	CAI	C22-C8-C7	-2.73	106.12	111.52
31	A	4000	CAI	C12-C11-C10	-2.72	119.64	125.10
31	A	4000	CAI	C1B-O1B-C4A	-2.71	109.33	114.72
31	A	4000	CAI	O3B-C3B-C2B	2.67	113.98	108.05
31	A	4000	CAI	O3-C3-C2	2.56	113.42	107.01
31	A	4000	CAI	C15-O15-C1	-2.49	114.19	117.78
31	A	4000	CAI	C3-C2-C1	2.47	119.30	112.90
31	A	4000	CAI	O1B-C4A-C3A	-2.17	103.56	109.02
31	A	4000	CAI	C3-O3-C17	2.12	120.84	117.47
31	A	4000	CAI	C1A-O5A-C5A	-2.07	110.10	113.63
31	A	4000	CAI	O1B-C1B-C2B	-2.01	105.64	108.99
31	A	4000	CAI	O15-C1-O1	-2.00	119.03	123.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	4000	CAI	C2-C3-C4-C5
31	A	4000	CAI	C2B-C1B-O1B-C4A
31	A	4000	CAI	O5B-C1B-O1B-C4A
31	A	4000	CAI	C2-C3-C4-O4
31	A	4000	CAI	O3-C3-C4-C5
31	A	4000	CAI	O3-C3-C4-O4
31	A	4000	CAI	O5A-C1A-O1A-C5
31	A	4000	CAI	C2A-C1A-O1A-C5
31	A	4000	CAI	C1C-C2C-C3C-C4C

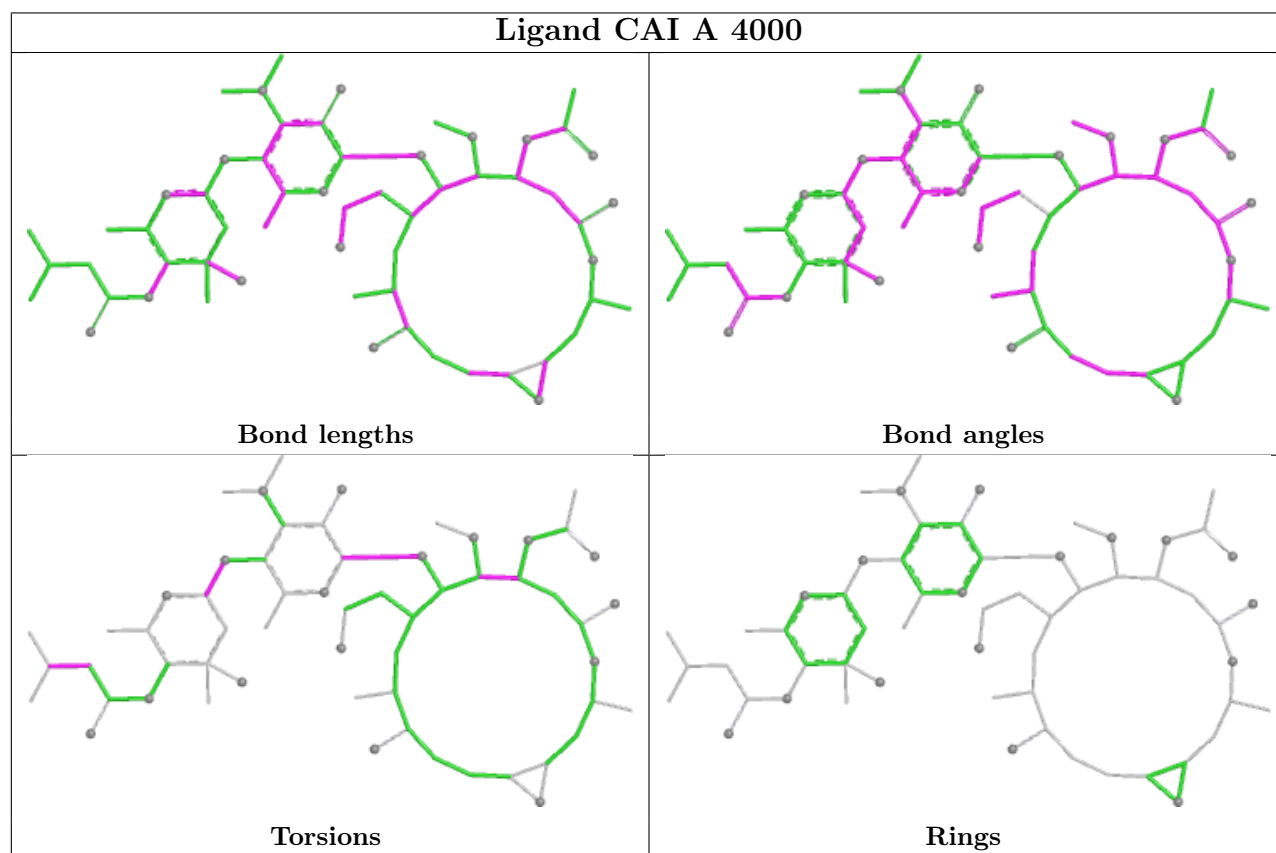
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	4000	CAI	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	-0.18	45 (1%) 70 47	25, 51, 97, 142	0
2	B	122/122 (100%)	0.30	5 (4%) 41 23	33, 69, 99, 152	0
3	C	237/239 (99%)	0.15	2 (0%) 82 64	30, 64, 95, 112	0
4	D	337/337 (100%)	-0.02	1 (0%) 90 79	24, 57, 84, 96	0
5	E	246/246 (100%)	-0.10	1 (0%) 88 76	23, 50, 74, 84	0
6	F	140/176 (79%)	0.93	8 (5%) 29 15	63, 104, 122, 128	0
7	G	172/177 (97%)	0.21	4 (2%) 61 38	41, 68, 90, 94	0
8	H	119/119 (100%)	0.55	1 (0%) 82 64	63, 81, 102, 108	0
9	I	29/348 (8%)	1.14	4 (13%) 6 4	77, 93, 100, 104	0
10	J	156/167 (93%)	0.17	2 (1%) 75 53	36, 57, 84, 93	0
11	K	142/145 (97%)	-0.12	0 100 100	30, 50, 75, 84	0
12	L	132/132 (100%)	-0.00	0 100 100	34, 56, 79, 85	0
13	M	145/164 (88%)	0.27	4 (2%) 55 32	30, 75, 106, 114	0
14	N	194/194 (100%)	0.37	18 (9%) 14 7	36, 56, 95, 105	0
15	O	186/186 (100%)	0.61	13 (6%) 22 12	45, 74, 112, 124	0
16	P	115/115 (100%)	0.12	0 100 100	40, 57, 75, 79	0
17	Q	143/148 (96%)	0.06	2 (1%) 73 51	40, 61, 77, 84	0
18	R	95/95 (100%)	-0.11	1 (1%) 78 57	36, 50, 65, 79	0
19	S	150/154 (97%)	-0.34	0 100 100	31, 45, 67, 75	0
20	T	81/84 (96%)	0.06	0 100 100	48, 66, 86, 89	0
21	U	119/119 (100%)	0.19	2 (1%) 69 45	44, 62, 88, 100	0
22	V	53/66 (80%)	1.42	8 (15%) 5 3	84, 96, 103, 112	0
23	W	65/70 (92%)	0.40	3 (4%) 37 20	56, 81, 110, 116	0
24	X	154/154 (100%)	-0.21	0 100 100	32, 46, 65, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.11	3 (3%) 45 25	41, 59, 84, 100	0
26	Z	142/240 (59%)	-0.18	0 100 100	27, 46, 69, 87	0
27	1	73/73 (100%)	1.79	25 (34%) 1 1	82, 97, 105, 106	0
28	2	56/56 (100%)	-0.50	0 100 100	28, 38, 45, 49	0
29	3	46/48 (95%)	0.23	0 100 100	38, 68, 89, 104	0
30	4	92/92 (100%)	2.43	58 (63%) 0 0	94, 109, 114, 119	0
All	All	6577/7279 (90%)	0.07	210 (3%) 50 29	23, 57, 104, 152	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	80	GLY	6.8
23	W	1	THR	6.7
14	N	89	ASN	6.4
1	A	1173	A	6.2
30	4	12	PRO	6.1
14	N	70	GLY	5.8
30	4	60	LYS	5.3
1	A	2433	A	5.0
27	1	26	VAL	4.8
27	1	12	GLY	4.8
27	1	22	ILE	4.6
17	Q	116	SER	4.6
30	4	1	MET	4.6
1	A	1925	G	4.5
1	A	1176	C	4.5
14	N	81	ARG	4.5
30	4	84	ARG	4.5
14	N	83	SER	4.4
27	1	18	TYR	4.4
1	A	2432	C	4.4
30	4	33	MET	4.4
1	A	1175	G	4.3
30	4	48	ASN	4.3
6	F	10	PHE	4.2
14	N	82	ARG	4.1
14	N	71	SER	4.1
30	4	83	TRP	4.1
1	A	1160	G	4.1
27	1	40	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
27	1	16	PRO	4.0
30	4	43	ASN	4.0
30	4	88	LEU	4.0
1	A	1190	G	4.0
30	4	79	LEU	3.9
30	4	51	LYS	3.8
30	4	31	THR	3.8
1	A	2345	A	3.7
5	E	135	GLU	3.7
27	1	20	LEU	3.7
15	O	148	ALA	3.6
2	B	3001	U	3.6
30	4	39	GLN	3.6
30	4	61	PRO	3.6
2	B	3022	G	3.5
1	A	735	C	3.5
27	1	44	PHE	3.5
30	4	76	LYS	3.5
30	4	77	ALA	3.5
30	4	85	ALA	3.5
1	A	1168	C	3.5
27	1	31	ILE	3.5
30	4	7	PHE	3.4
27	1	15	GLY	3.4
30	4	36	ILE	3.4
1	A	736	A	3.4
6	F	63	ILE	3.4
30	4	52	PHE	3.3
14	N	72	SER	3.2
27	1	41	VAL	3.2
27	1	35	LYS	3.2
6	F	69	ILE	3.2
14	N	88	VAL	3.2
27	1	13	ARG	3.1
1	A	1171	A	3.1
4	D	1	PRO	3.1
30	4	10	TYR	3.1
1	A	1184	C	3.1
7	G	45	ASP	3.1
30	4	64	LYS	3.1
22	V	13	ILE	3.1
30	4	13	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
30	4	78	HIS	3.0
1	A	1167	G	3.0
30	4	56	PRO	3.0
15	O	168	LEU	3.0
27	1	17	ARG	3.0
1	A	1165	G	3.0
30	4	11	CYS	3.0
22	V	49	LEU	2.9
30	4	9	THR	2.9
30	4	47	GLY	2.9
30	4	68	LYS	2.9
9	I	26	MET	2.9
30	4	62	THR	2.9
1	A	2436	U	2.9
30	4	22	VAL	2.9
1	A	1169	U	2.8
27	1	34	LYS	2.8
1	A	1964	U	2.8
15	O	162	ASP	2.8
30	4	42	ARG	2.8
9	I	71	LEU	2.8
30	4	3	MET	2.8
27	1	24	VAL	2.8
30	4	63	LYS	2.8
1	A	734	U	2.8
30	4	17	HIS	2.8
30	4	69	TYR	2.8
14	N	90	ARG	2.8
15	O	169	PRO	2.8
30	4	4	PRO	2.8
30	4	35	TRP	2.7
30	4	34	LYS	2.7
6	F	21	VAL	2.7
1	A	10	U	2.7
1	A	138	U	2.7
30	4	46	ILE	2.7
30	4	32	GLY	2.7
30	4	53	SER	2.7
1	A	1177	A	2.7
27	1	14	PHE	2.7
30	4	54	LYS	2.7
2	B	3025	G	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	3024	U	2.7
1	A	1174	A	2.6
14	N	84	LYS	2.6
23	W	2	VAL	2.6
1	A	1162	G	2.6
1	A	1170	U	2.6
30	4	8	ASN	2.6
25	Y	88	GLU	2.6
3	C	85	ASP	2.6
15	O	186	LEU	2.6
2	B	3002	U	2.6
15	O	147	ILE	2.5
22	V	31	PHE	2.5
15	O	167	ASP	2.5
1	A	1924	A	2.5
18	R	95	GLU	2.5
6	F	58	VAL	2.5
14	N	77	PHE	2.5
1	A	2257	G	2.5
6	F	102	GLY	2.5
30	4	55	VAL	2.5
1	A	1193	A	2.5
6	F	131	THR	2.5
27	1	39	CYS	2.4
1	A	1199	A	2.4
14	N	68	ARG	2.4
22	V	55	ALA	2.4
30	4	90	PHE	2.4
14	N	73	ARG	2.4
22	V	39	ASN	2.4
1	A	737	A	2.4
1	A	1198	U	2.4
1	A	2378	U	2.4
13	M	148	GLU	2.4
14	N	74	ARG	2.4
13	M	82	ALA	2.4
1	A	1188	A	2.4
30	4	67	LEU	2.4
22	V	51	TRP	2.4
25	Y	85	VAL	2.4
17	Q	110	ASP	2.4
30	4	2	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
22	V	42	LEU	2.4
30	4	57	GLY	2.3
30	4	38	ARG	2.3
10	J	167	ALA	2.3
15	O	166	ALA	2.3
30	4	74	CYS	2.3
10	J	40	PRO	2.3
9	I	27	ILE	2.3
15	O	158	LEU	2.3
15	O	172	PHE	2.3
30	4	58	GLY	2.3
30	4	82	GLY	2.3
1	A	1181	A	2.3
30	4	71	CYS	2.3
9	I	63	ARG	2.3
1	A	1195	G	2.2
1	A	1192	A	2.2
21	U	1	SER	2.2
23	W	39	ALA	2.2
30	4	65	THR	2.2
27	1	64	ILE	2.2
15	O	154	LEU	2.2
27	1	42	CYS	2.2
27	1	21	LYS	2.2
8	H	103	ALA	2.2
15	O	1	ALA	2.2
25	Y	82	GLU	2.2
30	4	15	ASN	2.2
6	F	171	ASP	2.2
7	G	10	ASP	2.2
7	G	100	ASP	2.2
30	4	75	GLY	2.1
14	N	78	ASN	2.1
1	A	1206	U	2.1
30	4	49	ASP	2.1
7	G	11	VAL	2.1
1	A	1161	A	2.1
13	M	83	GLU	2.1
15	O	179	LEU	2.1
22	V	40	ALA	2.1
1	A	2511	A	2.1
27	1	32	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1205	U	2.1
1	A	1561	U	2.1
3	C	36	ASP	2.1
14	N	75	THR	2.1
14	N	86	MET	2.1
27	1	11	THR	2.1
1	A	1917	G	2.1
1	A	2249	G	2.1
21	U	119	ALA	2.1
27	1	33	HIS	2.0
27	1	29	VAL	2.0
1	A	1172	G	2.0
13	M	81	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CD	4	8404	1/1	0.48	0.30	202,202,202,202	0
32	MG	A	8092	1/1	0.61	0.26	115,115,115,115	0
32	MG	A	8050	1/1	0.62	0.13	85,85,85,85	0
34	CL	4	8504	1/1	0.64	0.14	98,98,98,98	0
33	NA	A	8384	1/1	0.67	0.25	109,109,109,109	0
33	NA	S	8337	1/1	0.68	0.12	40,40,40,40	0
33	NA	A	8329	1/1	0.69	0.24	64,64,64,64	0
32	MG	A	8093	1/1	0.70	0.11	37,37,37,37	0
33	NA	B	8383	1/1	0.72	0.63	103,103,103,103	0
32	MG	A	8116	1/1	0.74	0.15	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	T	8312	1/1	0.74	0.11	61,61,61,61	0
34	CL	A	8515	1/1	0.75	0.28	92,92,92,92	0
33	NA	A	8326	1/1	0.75	0.14	61,61,61,61	0
33	NA	A	8373	1/1	0.75	0.17	71,71,71,71	0
33	NA	A	8356	1/1	0.77	0.24	52,52,52,52	0
35	K	A	8602	1/1	0.78	0.18	69,69,69,69	0
32	MG	A	8104	1/1	0.78	0.14	54,54,54,54	0
36	CD	1	8403	1/1	0.79	0.15	180,180,180,180	0
34	CL	P	8508	1/1	0.79	0.14	91,91,91,91	0
32	MG	A	8024	1/1	0.80	0.11	81,81,81,81	0
33	NA	A	8371	1/1	0.81	0.30	56,56,56,56	0
33	NA	A	8341	1/1	0.81	0.08	44,44,44,44	0
36	CD	V	8401	1/1	0.82	0.23	202,202,202,202	0
33	NA	A	8357	1/1	0.83	0.10	60,60,60,60	0
34	CL	R	8511	1/1	0.84	0.15	84,84,84,84	0
33	NA	A	8363	1/1	0.84	0.29	56,56,56,56	0
32	MG	A	8049	1/1	0.84	0.11	81,81,81,81	0
32	MG	A	8067	1/1	0.84	0.15	57,57,57,57	0
32	MG	A	8070	1/1	0.84	0.17	62,62,62,62	0
33	NA	B	8351	1/1	0.84	0.10	44,44,44,44	0
33	NA	A	8364	1/1	0.85	0.18	53,53,53,53	0
34	CL	C	8509	1/1	0.85	0.15	82,82,82,82	0
33	NA	A	8327	1/1	0.85	0.13	27,27,27,27	0
33	NA	A	8302	1/1	0.86	0.12	27,27,27,27	0
34	CL	A	8522	1/1	0.87	0.26	83,83,83,83	0
33	NA	A	8372	1/1	0.87	0.27	71,71,71,71	0
32	MG	A	8041	1/1	0.87	0.07	68,68,68,68	0
33	NA	A	8382	1/1	0.88	0.19	59,59,59,59	0
32	MG	A	8113	1/1	0.88	0.09	45,45,45,45	0
33	NA	A	8366	1/1	0.88	0.08	45,45,45,45	0
33	NA	A	8367	1/1	0.88	0.11	50,50,50,50	0
33	NA	E	8304	1/1	0.88	0.10	43,43,43,43	0
33	NA	N	8365	1/1	0.88	0.16	50,50,50,50	0
33	NA	A	8306	1/1	0.88	0.25	65,65,65,65	0
33	NA	A	8320	1/1	0.88	0.12	35,35,35,35	0
33	NA	A	8331	1/1	0.88	0.12	46,46,46,46	0
32	MG	A	8101	1/1	0.89	0.14	59,59,59,59	0
34	CL	A	8505	1/1	0.89	0.17	95,95,95,95	0
33	NA	A	8303	1/1	0.89	0.14	43,43,43,43	0
32	MG	A	8053	1/1	0.89	0.06	45,45,45,45	0
32	MG	A	8119	1/1	0.89	0.08	19,19,19,19	0
33	NA	A	8301	1/1	0.89	0.10	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8102	1/1	0.90	0.50	109,109,109,109	0
34	CL	D	8519	1/1	0.90	0.14	71,71,71,71	0
34	CL	M	8510	1/1	0.90	0.18	108,108,108,108	0
33	NA	A	8355	1/1	0.90	0.19	54,54,54,54	0
33	NA	A	8328	1/1	0.90	0.07	47,47,47,47	0
33	NA	A	8324	1/1	0.90	0.39	61,61,61,61	0
33	NA	A	8374	1/1	0.90	0.27	75,75,75,75	0
32	MG	4	8078	1/1	0.90	0.15	74,74,74,74	0
33	NA	A	8332	1/1	0.90	0.13	57,57,57,57	0
33	NA	A	8340	1/1	0.90	0.07	42,42,42,42	0
32	MG	D	8055	1/1	0.91	0.06	77,77,77,77	0
34	CL	A	8523	1/1	0.91	0.15	56,56,56,56	0
33	NA	A	8319	1/1	0.91	0.12	49,49,49,49	0
32	MG	A	8082	1/1	0.91	0.08	63,63,63,63	0
33	NA	A	8336	1/1	0.91	0.07	49,49,49,49	0
33	NA	A	8339	1/1	0.91	0.10	33,33,33,33	0
33	NA	A	8369	1/1	0.91	0.21	60,60,60,60	0
32	MG	A	8114	1/1	0.91	0.12	97,97,97,97	0
32	MG	A	8046	1/1	0.91	0.07	48,48,48,48	0
32	MG	A	8066	1/1	0.91	0.13	66,66,66,66	0
34	CL	A	8512	1/1	0.91	0.09	39,39,39,39	0
33	NA	A	8305	1/1	0.91	0.07	20,20,20,20	0
32	MG	A	8089	1/1	0.92	0.12	64,64,64,64	0
33	NA	A	8378	1/1	0.92	0.16	37,37,37,37	0
33	NA	A	8362	1/1	0.92	0.13	56,56,56,56	0
31	CAI	A	4000	59/59	0.92	0.11	40,47,60,62	0
33	NA	A	8368	1/1	0.92	0.08	41,41,41,41	0
33	NA	A	8316	1/1	0.93	0.12	53,53,53,53	0
33	NA	A	8318	1/1	0.93	0.18	42,42,42,42	0
32	MG	A	8022	1/1	0.93	0.32	56,56,56,56	0
33	NA	A	8352	1/1	0.93	0.12	46,46,46,46	0
36	CD	P	8405	1/1	0.93	0.09	136,136,136,136	0
32	MG	C	8105	1/1	0.93	0.09	40,40,40,40	0
32	MG	A	8094	1/1	0.93	0.17	63,63,63,63	0
33	NA	A	8310	1/1	0.93	0.09	42,42,42,42	0
32	MG	A	8045	1/1	0.94	0.07	50,50,50,50	0
32	MG	A	8040	1/1	0.94	0.20	124,124,124,124	0
33	NA	A	8323	1/1	0.94	0.15	53,53,53,53	0
32	MG	A	8062	1/1	0.94	0.06	80,80,80,80	0
33	NA	A	8350	1/1	0.94	0.11	38,38,38,38	0
34	CL	A	8514	1/1	0.94	0.07	57,57,57,57	0
32	MG	A	8088	1/1	0.94	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	CL	A	8516	1/1	0.94	0.13	43,43,43,43	0
32	MG	A	8001	1/1	0.94	0.07	30,30,30,30	0
33	NA	A	8377	1/1	0.94	0.18	71,71,71,71	0
32	MG	A	8103	1/1	0.94	0.14	57,57,57,57	0
33	NA	A	8379	1/1	0.94	0.09	44,44,44,44	0
33	NA	A	8314	1/1	0.94	0.14	35,35,35,35	0
34	CL	N	8518	1/1	0.94	0.12	51,51,51,51	0
33	NA	A	8330	1/1	0.94	0.07	39,39,39,39	0
32	MG	U	8073	1/1	0.94	0.04	40,40,40,40	0
32	MG	A	8090	1/1	0.94	0.22	67,67,67,67	0
33	NA	C	8345	1/1	0.94	0.06	43,43,43,43	0
35	K	A	8603	1/1	0.94	0.09	67,67,67,67	0
33	NA	A	8334	1/1	0.94	0.08	30,30,30,30	0
33	NA	K	8346	1/1	0.94	0.06	27,27,27,27	0
33	NA	M	8380	1/1	0.94	0.07	52,52,52,52	0
33	NA	N	8347	1/1	0.94	0.06	25,25,25,25	0
32	MG	A	8117	1/1	0.95	0.04	17,17,17,17	0
33	NA	A	8325	1/1	0.95	0.10	60,60,60,60	0
32	MG	A	8086	1/1	0.95	0.05	44,44,44,44	0
33	NA	A	8308	1/1	0.95	0.09	53,53,53,53	0
34	CL	A	8513	1/1	0.95	0.10	60,60,60,60	0
33	NA	A	8375	1/1	0.95	0.13	54,54,54,54	0
33	NA	A	8353	1/1	0.95	0.05	32,32,32,32	0
32	MG	A	8087	1/1	0.95	0.06	41,41,41,41	0
32	MG	A	8076	1/1	0.95	0.06	76,76,76,76	0
33	NA	A	8381	1/1	0.95	0.05	42,42,42,42	0
33	NA	A	8315	1/1	0.95	0.06	40,40,40,40	0
33	NA	A	8359	1/1	0.95	0.11	64,64,64,64	0
33	NA	A	8385	1/1	0.95	0.13	34,34,34,34	0
33	NA	A	8360	1/1	0.95	0.16	36,36,36,36	0
34	CL	O	8507	1/1	0.95	0.08	58,58,58,58	0
32	MG	A	8079	1/1	0.95	0.05	56,56,56,56	0
32	MG	A	8081	1/1	0.95	0.06	44,44,44,44	0
34	CL	Z	8520	1/1	0.95	0.07	39,39,39,39	0
33	NA	A	8333	1/1	0.95	0.10	37,37,37,37	0
35	K	A	8601	1/1	0.95	0.23	62,62,62,62	0
33	NA	J	8309	1/1	0.95	0.07	21,21,21,21	0
33	NA	J	8322	1/1	0.95	0.11	59,59,59,59	0
32	MG	A	8091	1/1	0.95	0.07	53,53,53,53	0
32	MG	A	8075	1/1	0.95	0.09	33,33,33,33	0
33	NA	A	8338	1/1	0.95	0.09	79,79,79,79	0
32	MG	A	8085	1/1	0.95	0.06	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8043	1/1	0.96	0.06	52,52,52,52	0
32	MG	A	8012	1/1	0.96	0.08	25,25,25,25	0
32	MG	A	8118	1/1	0.96	0.14	22,22,22,22	0
33	NA	A	8321	1/1	0.96	0.12	50,50,50,50	0
34	CL	K	8501	1/1	0.96	0.05	50,50,50,50	0
32	MG	A	8071	1/1	0.96	0.05	66,66,66,66	0
32	MG	A	8106	1/1	0.96	0.06	59,59,59,59	0
33	NA	R	8348	1/1	0.96	0.03	23,23,23,23	0
32	MG	A	8112	1/1	0.96	0.06	52,52,52,52	0
33	NA	A	8313	1/1	0.96	0.06	75,75,75,75	0
34	CL	S	8506	1/1	0.96	0.10	48,48,48,48	0
33	NA	U	8343	1/1	0.96	0.03	18,18,18,18	0
34	CL	A	8503	1/1	0.96	0.09	63,63,63,63	0
32	MG	A	8099	1/1	0.96	0.07	51,51,51,51	0
33	NA	A	8344	1/1	0.96	0.04	24,24,24,24	0
32	MG	A	8072	1/1	0.96	0.07	83,83,83,83	0
32	MG	A	8115	1/1	0.96	0.05	47,47,47,47	0
33	NA	A	8317	1/1	0.96	0.05	27,27,27,27	0
33	NA	A	8354	1/1	0.96	0.08	44,44,44,44	0
34	CL	A	8517	1/1	0.96	0.04	52,52,52,52	0
33	NA	A	8307	1/1	0.97	0.05	34,34,34,34	0
32	MG	A	8098	1/1	0.97	0.17	23,23,23,23	0
33	NA	A	8370	1/1	0.97	0.15	39,39,39,39	0
32	MG	A	8051	1/1	0.97	0.05	57,57,57,57	0
33	NA	A	8311	1/1	0.97	0.05	34,34,34,34	0
32	MG	A	8100	1/1	0.97	0.08	65,65,65,65	0
32	MG	A	8027	1/1	0.97	0.07	69,69,69,69	0
32	MG	A	8060	1/1	0.97	0.06	62,62,62,62	0
33	NA	A	8361	1/1	0.97	0.09	63,63,63,63	0
32	MG	A	8047	1/1	0.97	0.07	41,41,41,41	0
32	MG	A	8064	1/1	0.97	0.17	23,23,23,23	0
33	NA	A	8349	1/1	0.97	0.06	56,56,56,56	0
32	MG	A	8096	1/1	0.97	0.06	48,48,48,48	0
32	MG	B	8095	1/1	0.97	0.05	67,67,67,67	0
34	CL	K	8521	1/1	0.97	0.05	43,43,43,43	0
32	MG	A	8083	1/1	0.98	0.07	44,44,44,44	0
32	MG	A	8084	1/1	0.98	0.09	40,40,40,40	0
34	CL	K	8502	1/1	0.98	0.03	48,48,48,48	0
32	MG	A	8033	1/1	0.98	0.06	19,19,19,19	0
32	MG	A	8039	1/1	0.98	0.09	76,76,76,76	0
32	MG	A	8068	1/1	0.98	0.04	52,52,52,52	0
32	MG	A	8052	1/1	0.98	0.05	43,43,43,43	0

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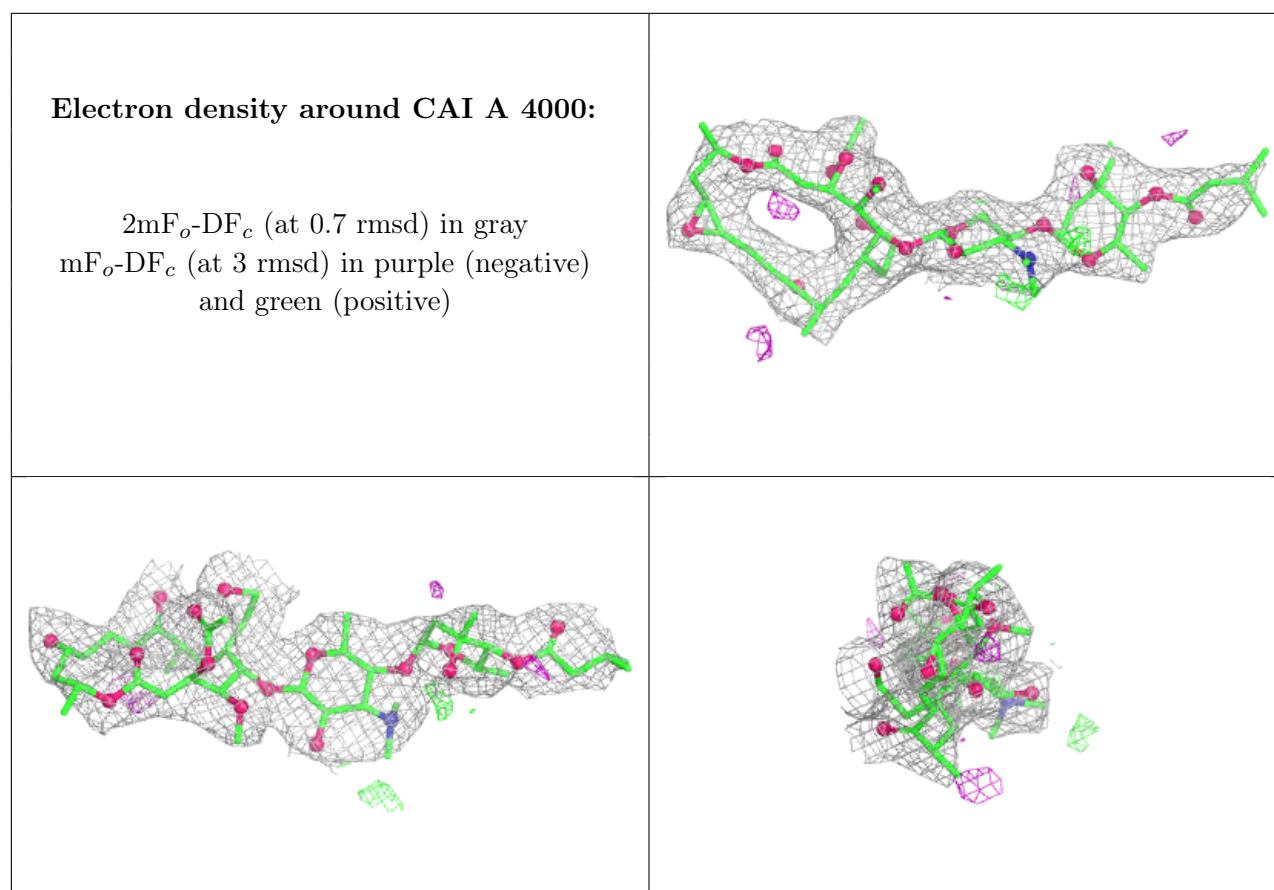
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	L	8069	1/1	0.98	0.05	78,78,78,78	0
32	MG	A	8006	1/1	0.98	0.03	61,61,61,61	0
33	NA	A	8335	1/1	0.98	0.09	61,61,61,61	0
32	MG	Z	8109	1/1	0.98	0.08	42,42,42,42	0
32	MG	A	8056	1/1	0.98	0.06	40,40,40,40	0
32	MG	A	8111	1/1	0.98	0.03	47,47,47,47	0
32	MG	A	8057	1/1	0.98	0.05	48,48,48,48	0
32	MG	A	8059	1/1	0.98	0.03	35,35,35,35	0
33	NA	A	8342	1/1	0.98	0.09	60,60,60,60	0
32	MG	A	8008	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8048	1/1	0.98	0.03	54,54,54,54	0
32	MG	A	8042	1/1	0.98	0.08	46,46,46,46	0
32	MG	C	8065	1/1	0.99	0.03	48,48,48,48	0
32	MG	A	8030	1/1	0.99	0.03	19,19,19,19	0
32	MG	A	8097	1/1	0.99	0.10	29,29,29,29	0
32	MG	A	8007	1/1	0.99	0.03	25,25,25,25	0
32	MG	A	8035	1/1	0.99	0.04	49,49,49,49	0
32	MG	A	8037	1/1	0.99	0.04	30,30,30,30	0
32	MG	A	8080	1/1	0.99	0.06	31,31,31,31	0
32	MG	A	8054	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8013	1/1	0.99	0.03	56,56,56,56	0
32	MG	A	8014	1/1	0.99	0.05	14,14,14,14	0
32	MG	A	8058	1/1	0.99	0.03	57,57,57,57	0
32	MG	A	8107	1/1	0.99	0.02	40,40,40,40	0
32	MG	A	8108	1/1	0.99	0.07	67,67,67,67	0
32	MG	A	8110	1/1	0.99	0.05	41,41,41,41	0
32	MG	A	8015	1/1	0.99	0.03	43,43,43,43	0
32	MG	A	8016	1/1	0.99	0.03	59,59,59,59	0
32	MG	A	8018	1/1	0.99	0.03	43,43,43,43	0
32	MG	A	8063	1/1	0.99	0.04	67,67,67,67	0
32	MG	A	8044	1/1	0.99	0.08	70,70,70,70	0
32	MG	A	8004	1/1	0.99	0.03	52,52,52,52	0
32	MG	A	8023	1/1	0.99	0.02	29,29,29,29	0
32	MG	A	8009	1/1	0.99	0.05	24,24,24,24	0
32	MG	A	8010	1/1	0.99	0.03	48,48,48,48	0
36	CD	2	8402	1/1	0.99	0.04	60,60,60,60	0
32	MG	A	8028	1/1	0.99	0.06	34,34,34,34	0
32	MG	A	8019	1/1	1.00	0.04	34,34,34,34	0
32	MG	A	8031	1/1	1.00	0.04	32,32,32,32	0
32	MG	A	8032	1/1	1.00	0.08	23,23,23,23	0
32	MG	A	8020	1/1	1.00	0.03	33,33,33,33	0
32	MG	A	8034	1/1	1.00	0.03	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8021	1/1	1.00	0.02	19,19,19,19	0
32	MG	A	8036	1/1	1.00	0.02	28,28,28,28	0
32	MG	A	8074	1/1	1.00	0.09	12,12,12,12	0
32	MG	A	8002	1/1	1.00	0.03	25,25,25,25	0
32	MG	A	8038	1/1	1.00	0.01	33,33,33,33	0
32	MG	A	8077	1/1	1.00	0.04	21,21,21,21	0
32	MG	A	8011	1/1	1.00	0.04	24,24,24,24	0
32	MG	A	8005	1/1	1.00	0.03	41,41,41,41	0
32	MG	A	8025	1/1	1.00	0.02	41,41,41,41	0
32	MG	A	8026	1/1	1.00	0.04	12,12,12,12	0
32	MG	A	8017	1/1	1.00	0.03	24,24,24,24	0
32	MG	A	8061	1/1	1.00	0.04	33,33,33,33	0
32	MG	A	8003	1/1	1.00	0.04	14,14,14,14	0
32	MG	A	8029	1/1	1.00	0.01	36,36,36,36	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.