Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 05:27 AM EDT

PDB ID	:	1Q81
Title	:	Crystal Structure of minihelix with 3' puromycin bound to A-site of the 50S ribosomal subunit.
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	2.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

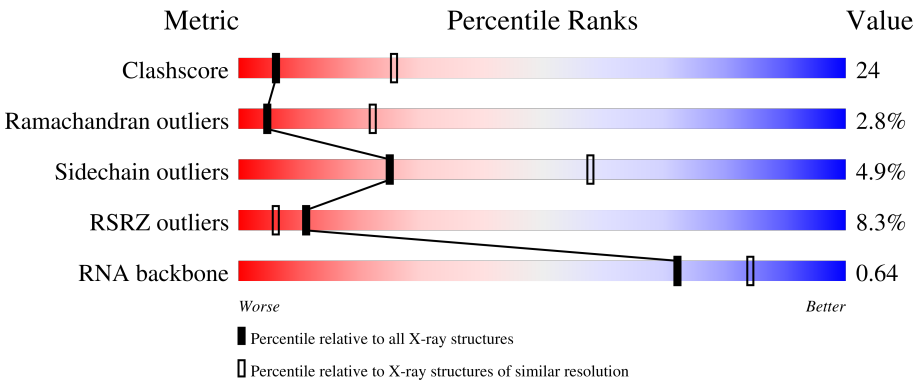
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	2922	2% 48% 39% 7% 6%
2	B	122	5% 39% 48% 11% •
3	5	2	100% 100%
4	C	239	10% 52% 41% 6% •
5	D	337	% 45% 50% 6%

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Mol	Chain	Length	Quality of chain
6	E	246	%, 50%, 46%
7	F	176	40%, 23%, 48%, 8%, 20%
8	G	177	14%, 46%, 50%
9	H	119	18%, 49%, 47%
10	I	348	5%, 92%
11	J	167	8%, 30%, 54%, 8%, 7%
12	K	145	2%, 47%, 44%, 7%
13	L	132	2%, 48%, 50%
14	M	164	18%, 43%, 42%, 12%
15	N	194	3%, 37%, 56%, 7%
16	O	186	18%, 34%, 57%, 9%
17	P	115	2%, 50%, 47%
18	Q	148	8%, 59%, 36%
19	R	95	%, 62%, 35%
20	S	154	%, 58%, 36%
21	T	84	2%, 64%, 31%
22	U	119	8%, 46%, 50%
23	V	66	23%, 35%, 44%, 20%
24	W	70	26%, 43%, 44%, 6%, 7%
25	X	154	44%, 49%, 6%
26	Y	91	10%, 40%, 44%, 7%, 10%
27	Z	240	3%, 33%, 23%, 41%
28	1	73	55%, 15%, 77%, 8%
29	2	56	62%, 38%
30	3	48	6%, 60%, 33%

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Mol	Chain	Length	Quality of chain
31	4	92	100% 27% 70%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	4	8078	-	-	-	X
32	MG	4	8114	-	-	-	X
32	MG	A	8024	-	-	-	X
32	MG	A	8070	-	-	-	X
32	MG	A	8097	-	-	-	X
34	NA	A	8355	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	B	8351	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	4	8504	-	-	-	X
35	CL	A	8515	-	-	-	X
37	CD	4	8404	-	-	-	X
37	CD	P	8405	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 98596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a RNA chain called minihelix-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	2	40	18	6	14	2	0	0	0

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
32	A	108	108	108	0	0
			Total	Mg		
32	B	1	1	1	0	0
			Total	Mg		
32	C	1	1	1	0	0
			Total	Mg		
32	D	1	1	1	0	0
			Total	Mg		
32	L	1	1	1	0	0
			Total	Mg		
32	U	1	1	1	0	0
			Total	Mg		
32	Z	1	1	1	0	0
			Total	Mg		
32	1	1	1	1	0	0
			Total	Mg		
32	4	2	2	2	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
34	A	73	73	73	0	0
			Total	Na		
34	B	2	2	2	0	0
			Total	Na		
34	C	1	1	1	0	0
			Total	Na		
34	E	1	1	1	0	0
			Total	Na		
34	J	1	1	1	0	0
			Total	Na		
34	K	1	1	1	0	0
			Total	Na		
34	M	1	1	1	0	0
			Total	Na		
34	N	1	1	1	0	0

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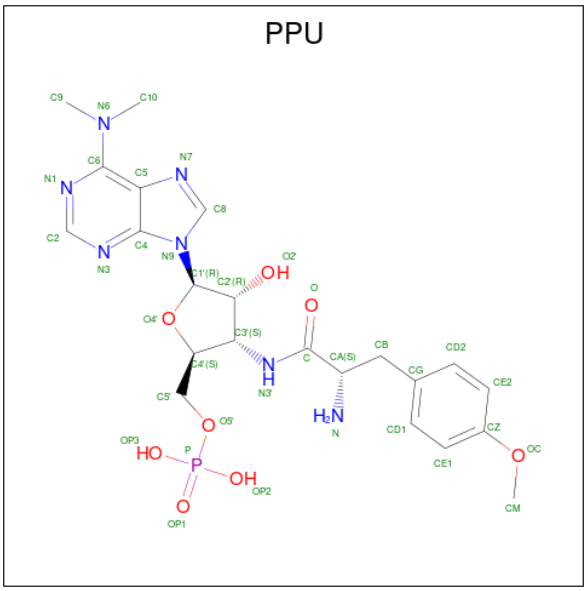
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0

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

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

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
36	5	1	37	22	7	7	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
37	P	1	1	1	0	0
37	V	1	1	1	0	0
37	1	1	1	1	0	0
37	2	1	1	1	0	0
37	4	1	1	1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
38	A	5871	5871	5871	0	0
38	B	147	147	147	0	0
38	C	135	135	135	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	155	Total O 155 155	0	0
38	E	171	Total O 171 171	0	0
38	F	51	Total O 51 51	0	0
38	G	44	Total O 44 44	0	0
38	H	26	Total O 26 26	0	0
38	I	20	Total O 20 20	0	0
38	J	77	Total O 77 77	0	0
38	K	55	Total O 55 55	0	0
38	L	63	Total O 63 63	0	0
38	M	90	Total O 90 90	0	0
38	N	125	Total O 125 125	0	0
38	O	64	Total O 64 64	0	0
38	P	44	Total O 44 44	0	0
38	Q	68	Total O 68 68	0	0
38	R	54	Total O 54 54	0	0
38	S	83	Total O 83 83	0	0
38	T	31	Total O 31 31	0	0
38	U	39	Total O 39 39	0	0
38	V	26	Total O 26 26	0	0
38	W	15	Total O 15 15	0	0
38	X	70	Total O 70 70	0	0

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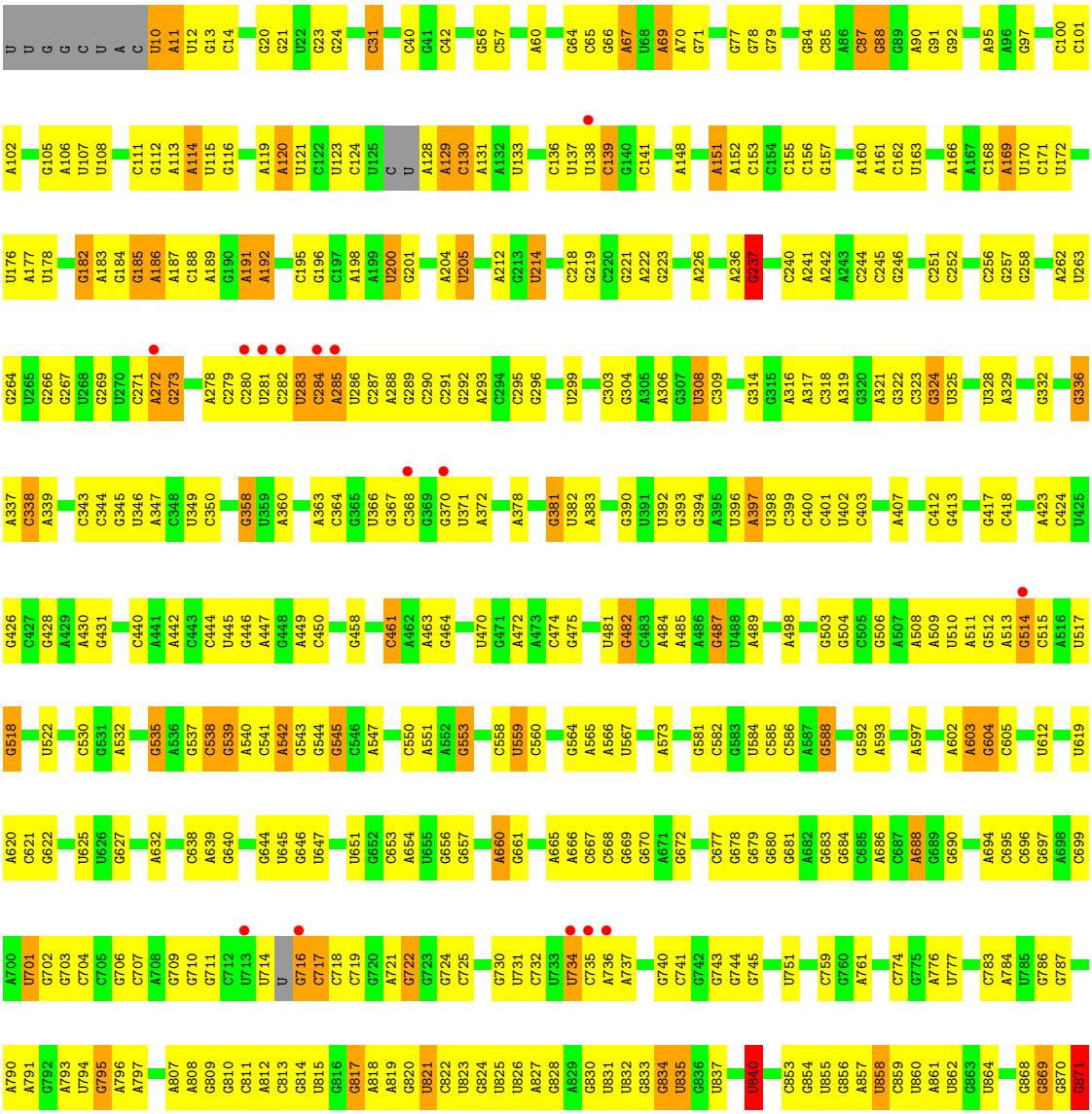
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Y	30	Total O 30 30	0	0
38	Z	102	Total O 102 102	0	0
38	1	38	Total O 38 38	0	0
38	2	56	Total O 56 56	0	0
38	3	47	Total O 47 47	0	0
38	4	72	Total O 72 72	0	0

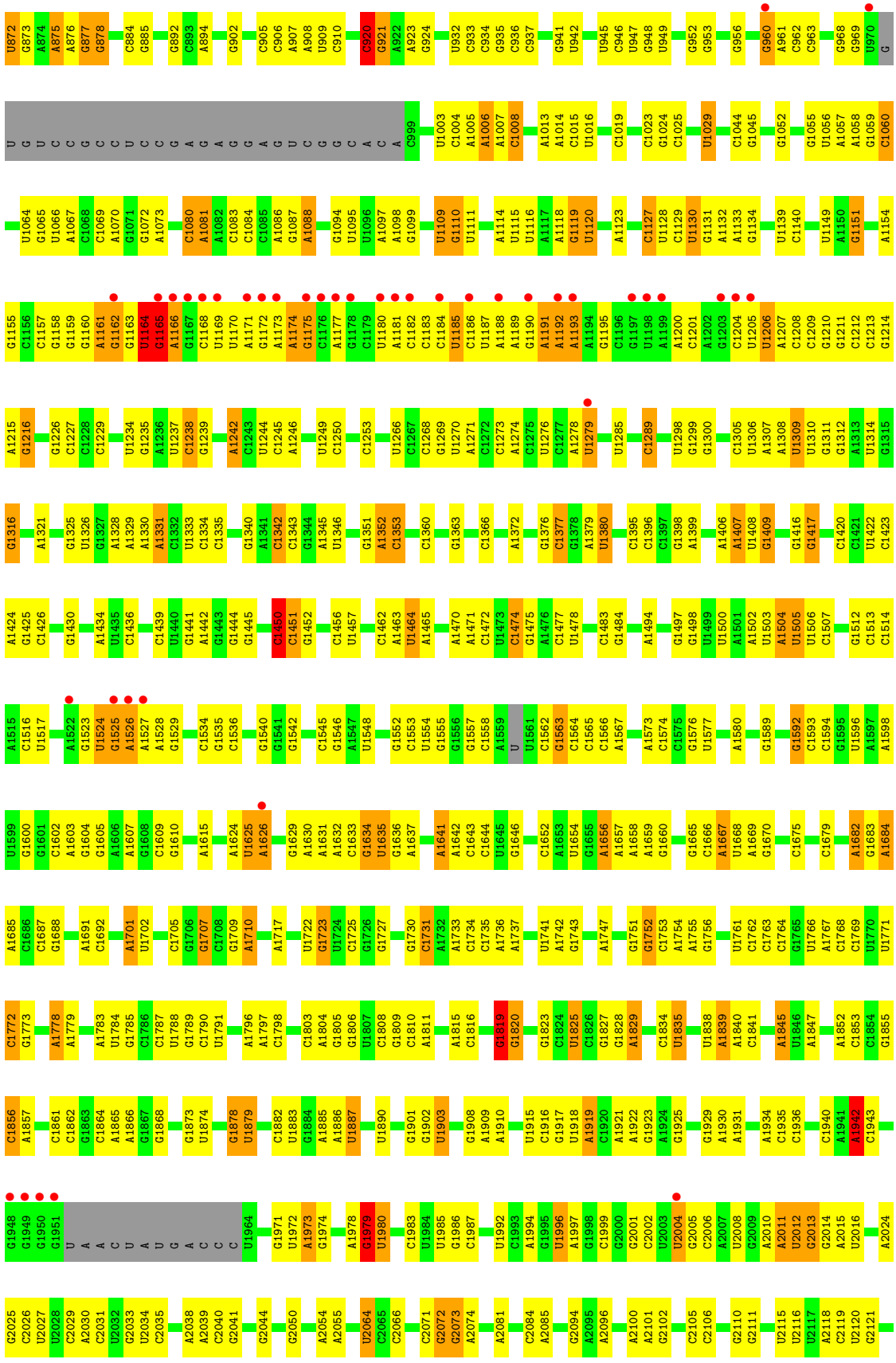
3 Residue-property plots (i)

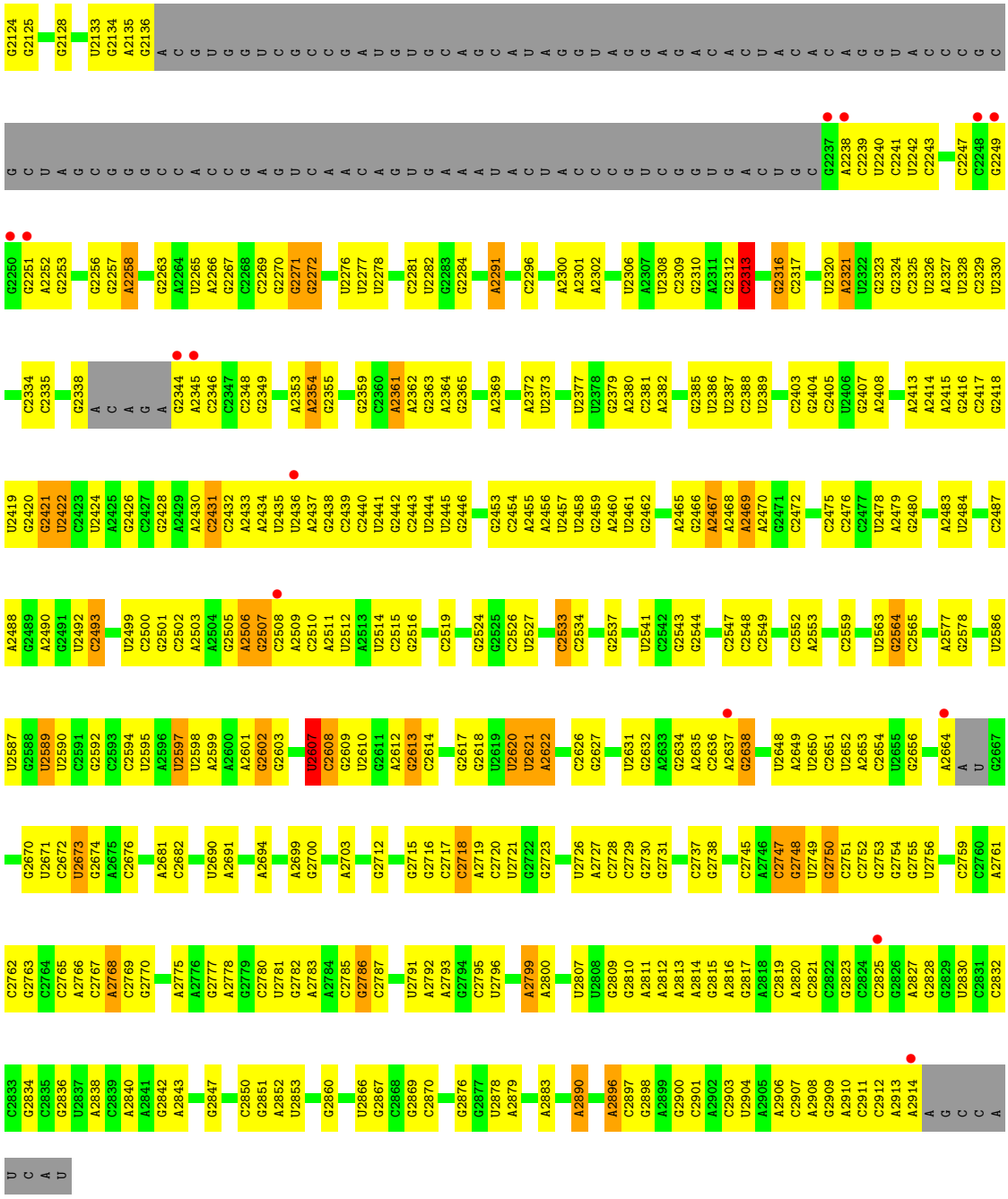
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S ribosomal rna

Chain A: 2% 48% 39% 7% 6%

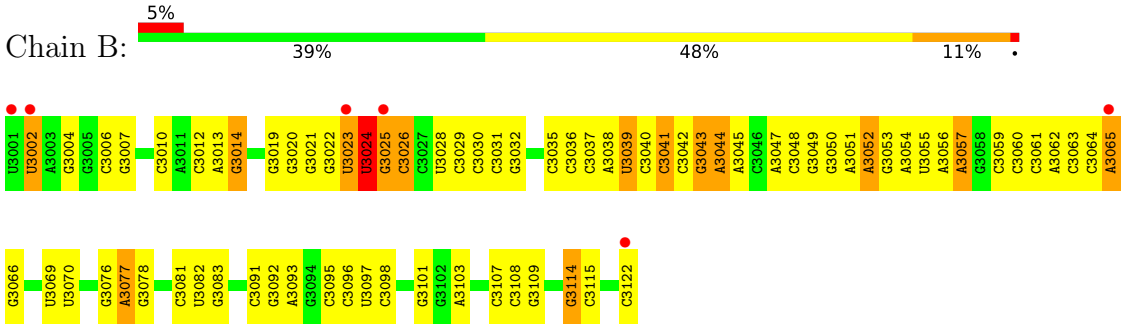






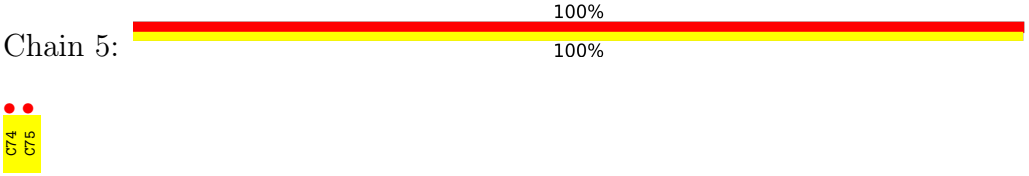
• Molecule 2: 5S ribosomal RNA

Chain B:



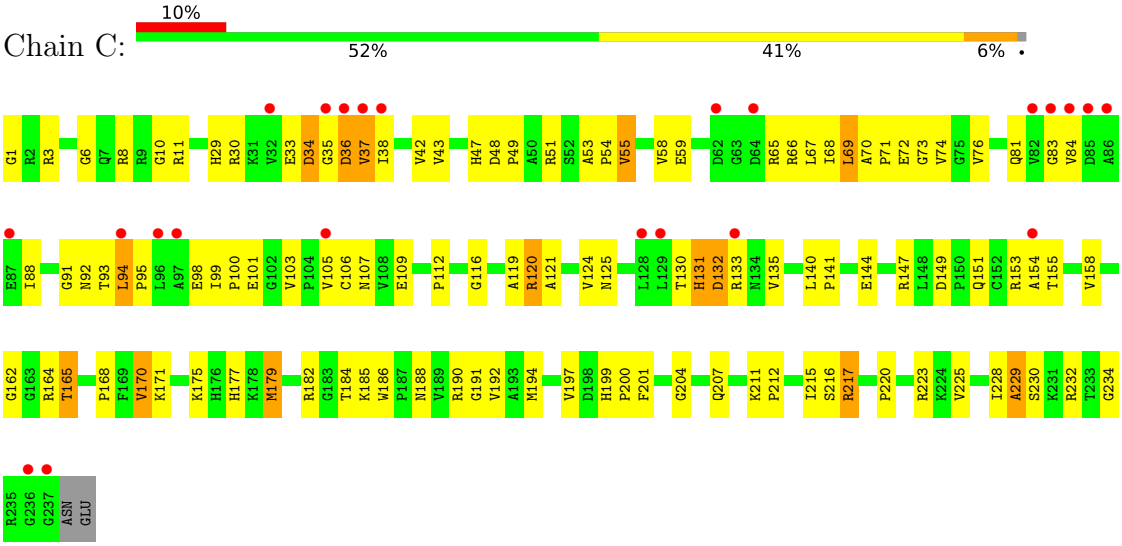
• Molecule 3: minihelix-puromycin

Chain 5:



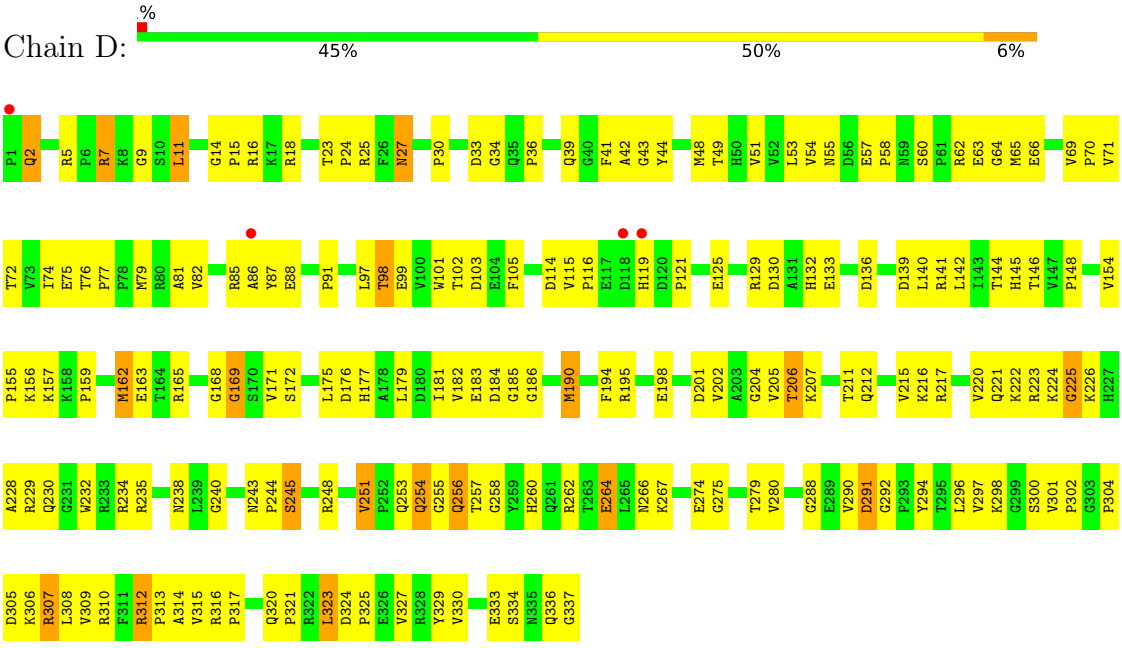
• Molecule 4: 50S ribosomal protein L2P

Chain C:



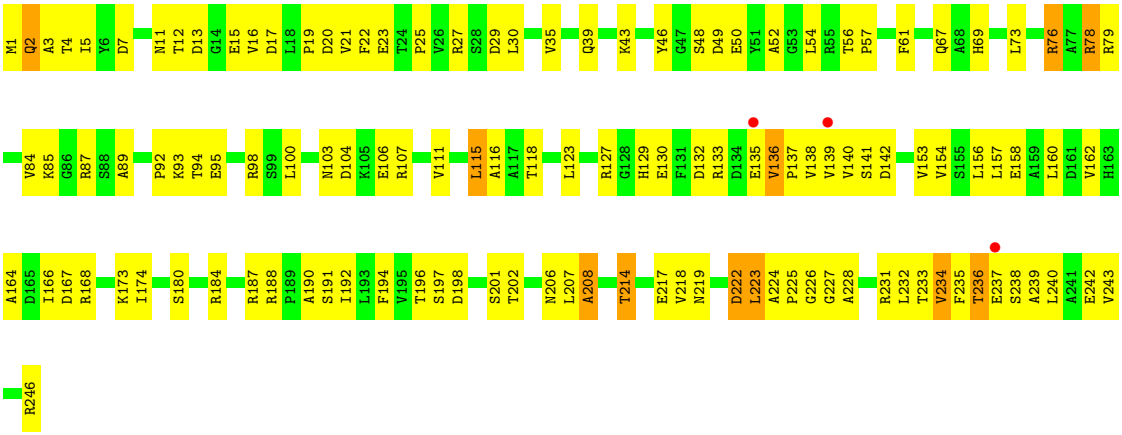
• Molecule 5: 50S ribosomal protein L3P

Chain D:



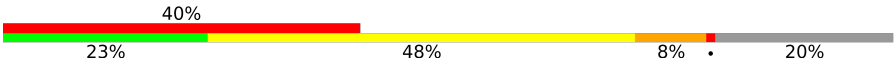
• Molecule 6: 50S ribosomal protein L4E

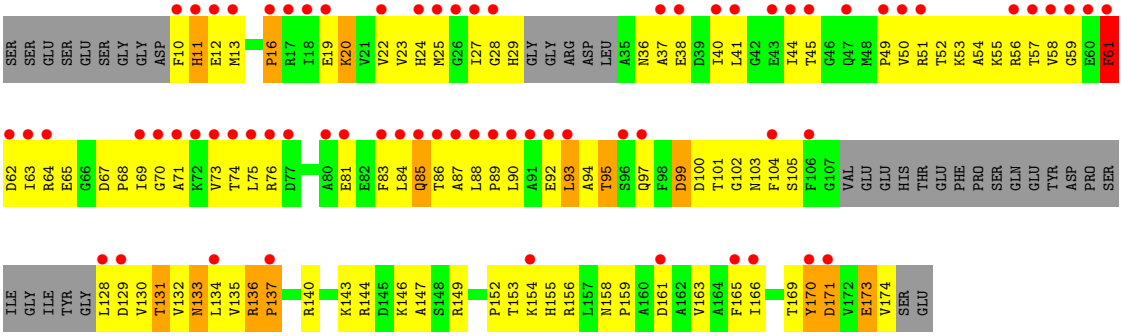
Chain E:



• Molecule 7: 50S ribosomal protein L5P

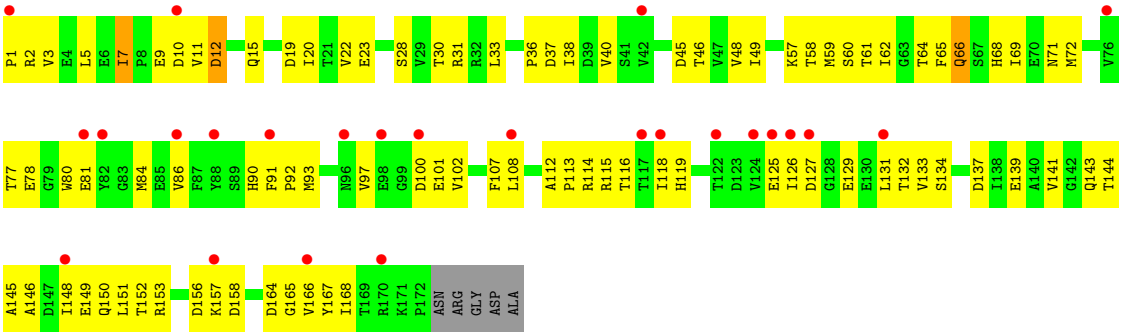
Chain F:





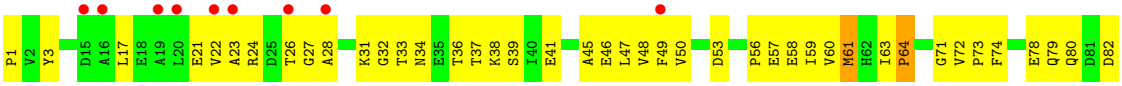
• Molecule 8: 50S ribosomal protein L6P

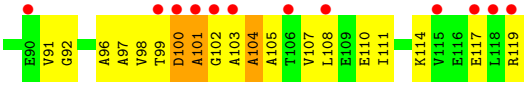
Chain G:



• Molecule 9: 50S ribosomal protein L7Ae

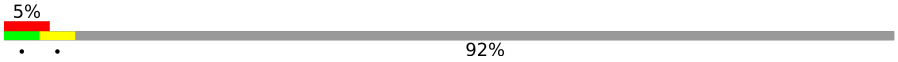
Chain H:

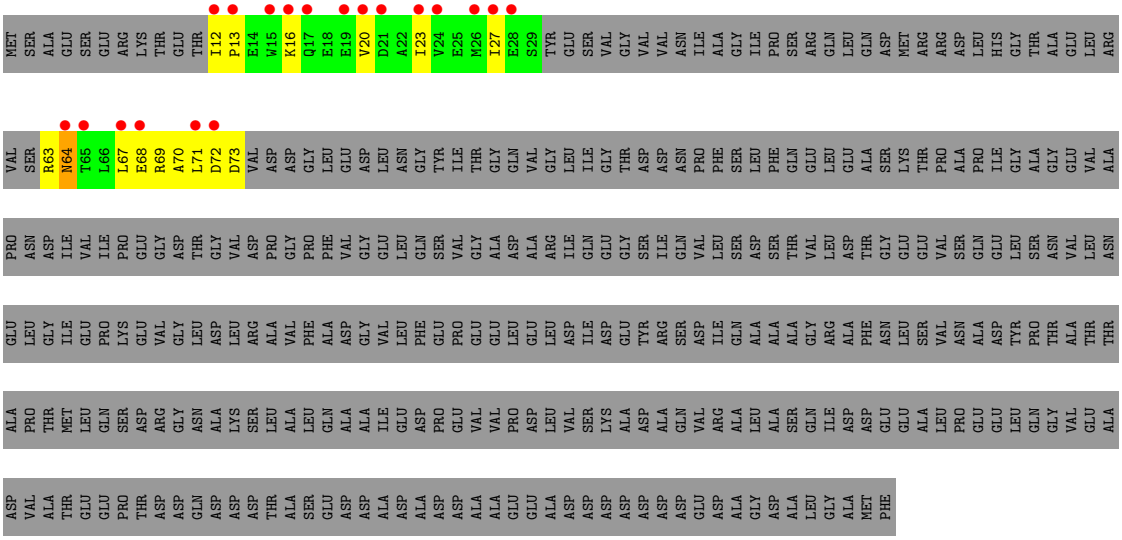




• Molecule 10: Acidic ribosomal protein P0 homolog

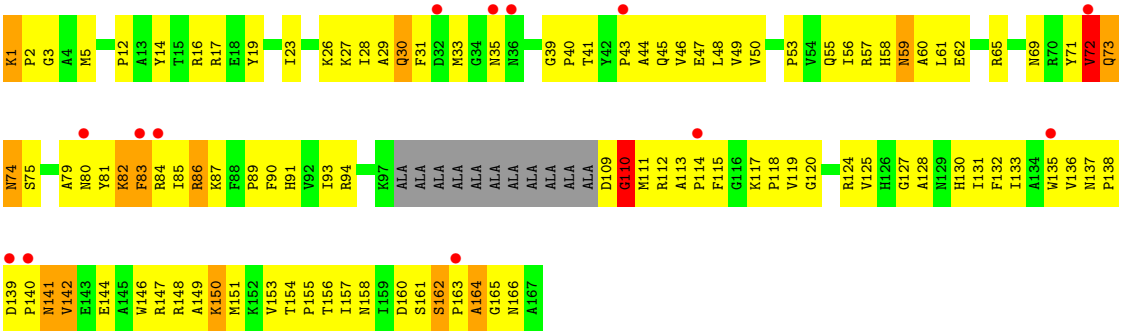
Chain I:





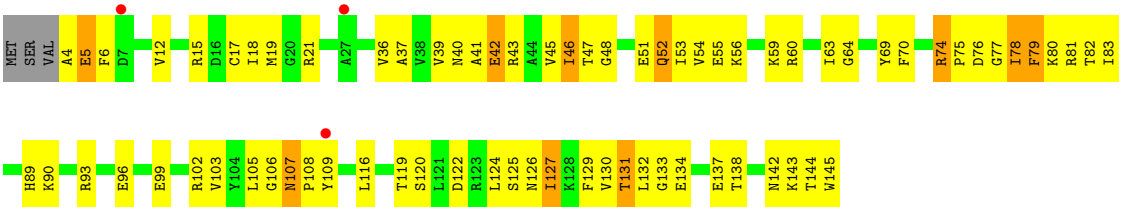
• Molecule 11: L10 Ribosomal Protein

Chain J:



• Molecule 12: 50S ribosomal protein L13P

Chain K:



• Molecule 13: 50S ribosomal protein L14P

Chain L: 2% 48% 50%

M1 E2 A3 L4 D7 V8 T9 Q10 K14 I18 T19 C20 A21 D22 N23 T24 G25 A26 R27 E28 L29 K30 V31 I32 S33 V34 Y37 S38 G39 T40 K41 N42 P45 K46 A47 G48 L49 I53 T54 V55 S56 V57 T58 P62 E63 M64 R65 R66 Q67 V72 V73 V74

R75 I80 R81 R82 F83 D84 G85 T86 R87 V88 K89 F90 N93 V98 D99 E100 N101 E102 G106 P112 I113 A114 R115 E116 V117 A118 Q119 R120 F121 G122 S123 V124 A125 S126 A127 V132

- Molecule 14: 50S ribosomal protein L15P

Chain M: 18% 43% 42% 12%

T1 K4 K5 R6 Q7 S10 R11 T12 H13 G16 S17 H18 R21 R22 H26 R30 G34 R35 H38 E39 F40 H43 E44 P45 L46 G50 R53 P54 V57 Q58 E59 E60 A61 A62 D65 V66 R67 E68 E71 N72 V73 T74 L75 L76 A77 A78

D79 D80 V81 A82 E83 VAL GLU ASP GLY GLY F89 R90 V91 D92 V93 R94 V97 E98 E99 A103 D104 Y105 V106 A111 V114 R115 H116 E117 L118 T119 L120 I121 A122 D123 D124 F125 G128 A129 R130 E131 K132 V133 E134 G135 A136 G137 G138 S139 V140 E141 L142 T143 D144 L145 G146

E147 E148 R149 Q150 ALA GLU ALA GLU GLU THR GLU ASP ALA ASP ALA ASP GLU GLU

- Molecule 15: L15 Ribosomal Protein

Chain N: 3% 37% 56% 7%

A1 R2 S3 A4 Y5 S6 R9 W12 K13 R14 E17 G18 Q19 I20 A21 E22 L23 H26 R27 M28 Q29 E30 W31 R32 N33 E34 P35 A36 V37 V38 R39 P43 T44 R45 L46 D47 R48 A49 R50 S51 L52 K57 G58 G59 I60 I61 V62 V63 R64 V65 A66 I67 R68 K69

R74 T75 R76 F77 N78 K79 G80 R81 R82 S83 K84 R85 M86 M87 V88 N89 R90 I91 T92 R93 K94 K95 R99 E102 E103 R104 A105 N106 R107 K108 F109 R113 V114 L115 N116 V120 G121 E122 K127 E130 I134 D137 H138 P139 A140 I141 K142 Q146 L147 S148

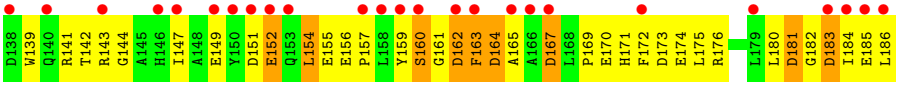
W149 I150 S151 R152 T153 R154 H155 R156 L157 R158 T159 F160 R161 G162 L163 T164 S165 A166 G167 R168 R169 C170 R171 G172 L173 R174 G175 K178 G179 K182 V183 R184 P185 S186 L187 R188 V189 K193 A194

- Molecule 16: 50S ribosomal protein L18P

Chain O: 18% 34% 57% 9%

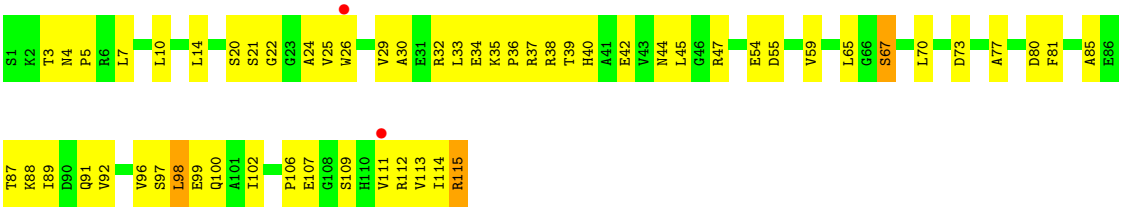
A1 T2 G3 P4 R5 Y6 K7 V8 P9 M10 R11 R12 R13 R14 E15 A16 R17 T18 D19 Y20 H21 Q22 R23 L24 R25 L26 L27 K28 S29 P32 R33 L34 V35 A36 R37 H42 V43 R44 A45 Q46 L47 V48 T49 L50 D55 D56 T57 L58 A61 H62 S63 S64 D65 L66 A67 E68

Y69 G70 W71 E72 A73 P74 T75 G76 N77 M78 P79 S80 A81 Y82 L83 L86 L87 A88 G89 L90 R91 A92 Q93 E94 A95 G96 V97 E98 E99 A100 I104 N107 S108 P109 S113 K114 V115 F116 A117 I118 Q119 E120 I123 D124 A125 G126 L127 D128 I129 N132 V135 L136 A137



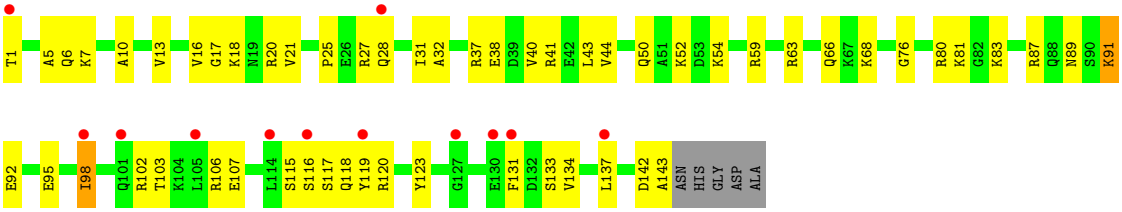
• Molecule 17: 50S ribosomal protein L18e

Chain P:



• Molecule 18: 50S ribosomal protein L19E

Chain Q:

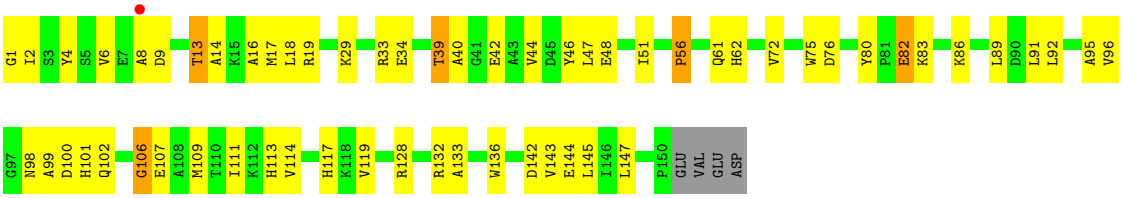


• Molecule 19: 50S ribosomal protein L21e

Chain R:

• Molecule 20: 50S ribosomal protein L22P

Chain S:

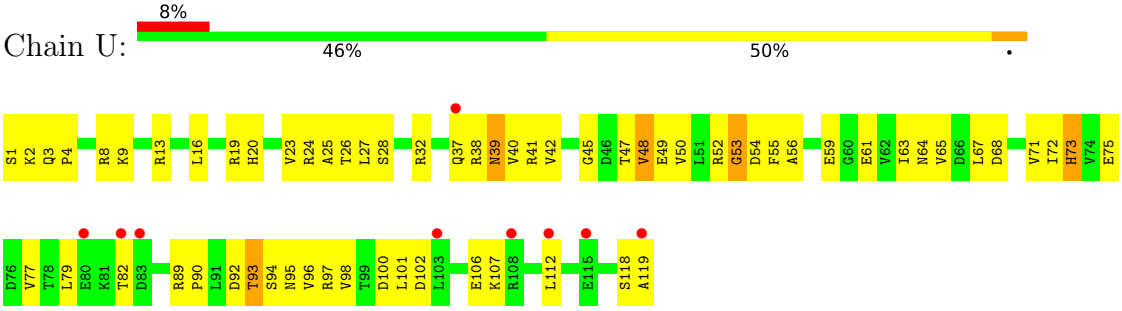


• Molecule 21: 50S ribosomal protein L23P

Chain T:

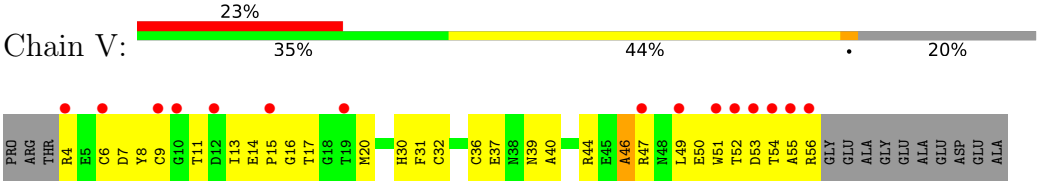
- Molecule 22: 50S ribosomal protein L24P

Chain U:



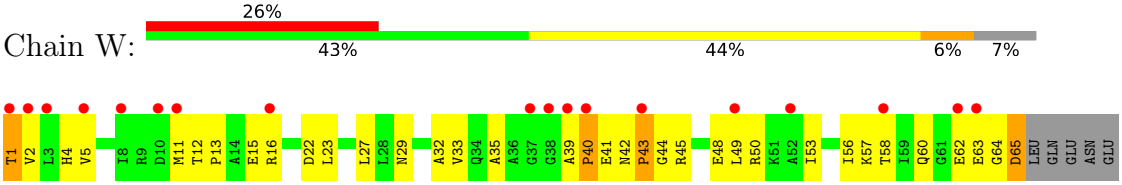
- Molecule 23: 50S ribosomal protein L24E

Chain V:



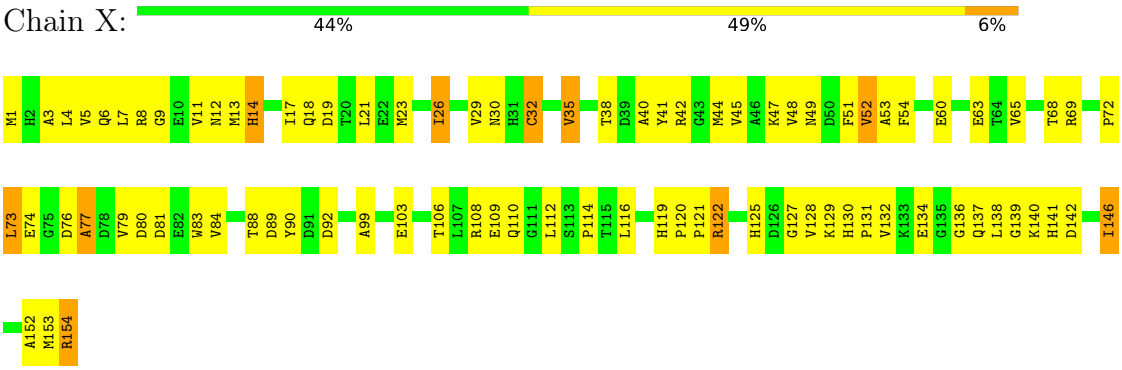
- Molecule 24: 50S ribosomal protein L29P

Chain W:



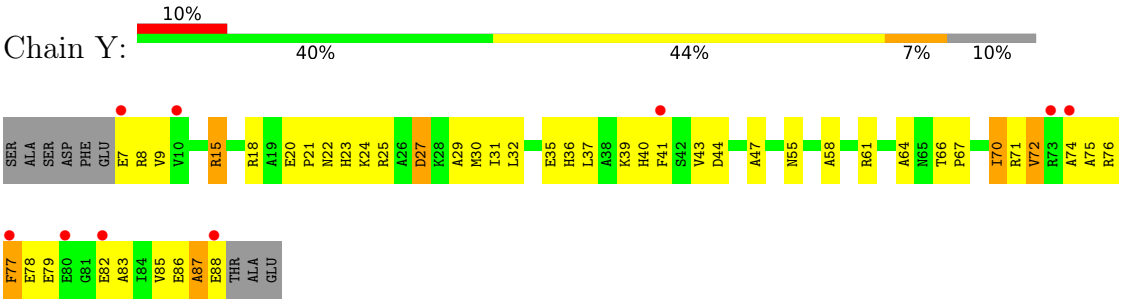
- Molecule 25: 50S ribosomal protein L30P

Chain X:



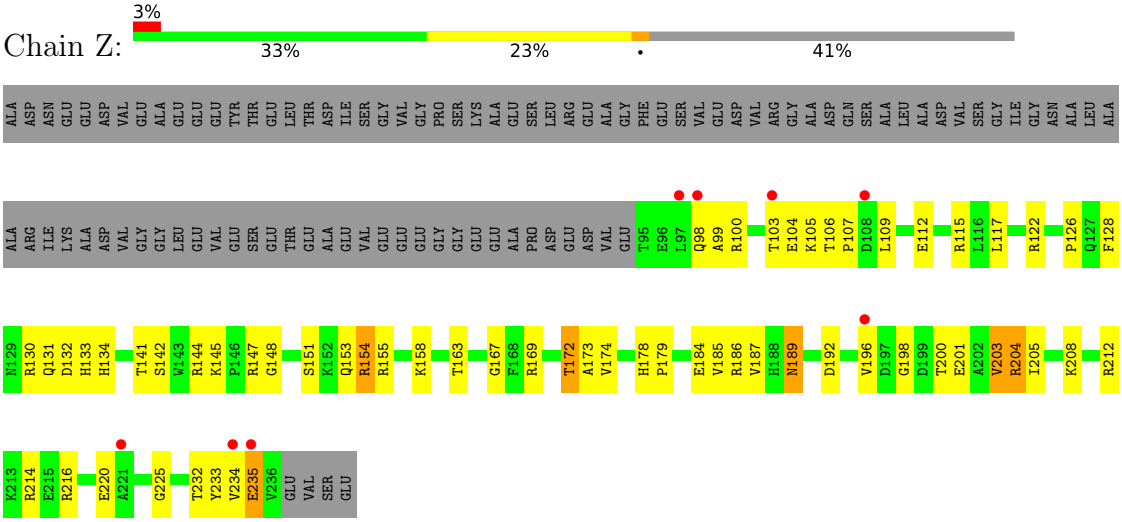
- Molecule 26: 50S ribosomal protein L31e

Chain Y:



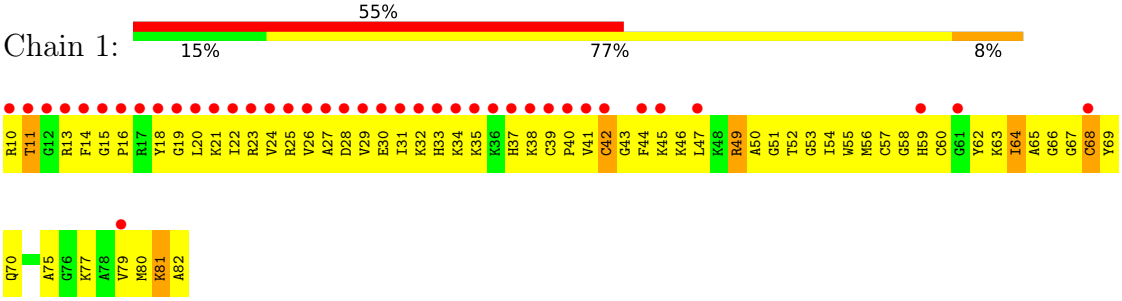
• Molecule 27: 50S ribosomal protein L32E

Chain Z:



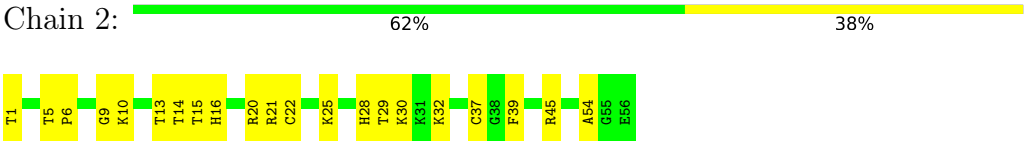
• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:



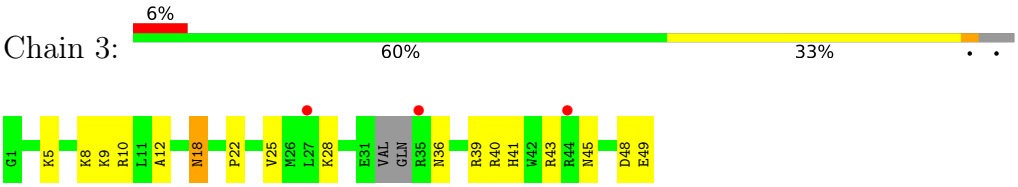
• Molecule 29: 50S ribosomal protein L37e

Chain 2:



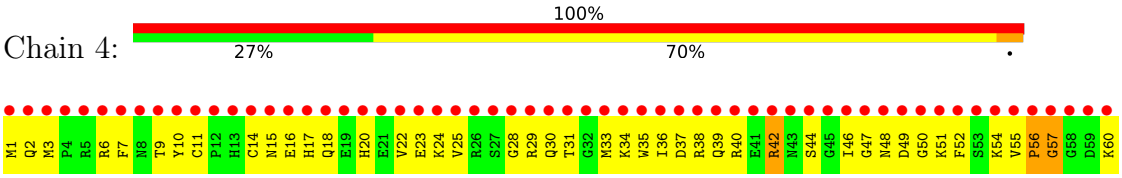
• Molecule 30: 50S ribosomal protein L39e

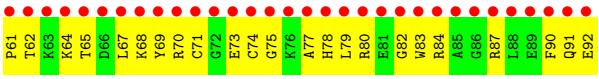
Chain 3:



• Molecule 31: 50S ribosomal protein L44E

Chain 4:




P61
T62
K63
K64
T65
D66
L67
K68
Y69
R70
C71
G72
E73
C74
G75
K76
A77
H78
L79
R80
E81
G82
W83
R84
A85
G86
R87
L88
E89
F90
Q91
E92

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 53.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.95) 90.6 (53.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.80 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.259 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	98596	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.53	6/66076 (0.0%)	0.72	18/103052 (0.0%)
2	B	0.49	0/2905	0.78	3/4528 (0.1%)
3	5	1.19	0/43	0.77	0/64
4	C	0.40	0/1787	0.71	0/2409
5	D	0.39	0/2689	0.69	0/3652
6	E	0.44	0/1883	0.68	0/2551
7	F	0.37	0/1111	0.62	0/1498
8	G	0.38	0/1382	0.62	0/1880
9	H	0.46	1/896 (0.1%)	0.73	3/1219 (0.2%)
10	I	0.42	0/241	0.62	0/324
11	J	0.44	0/1246	0.76	3/1686 (0.2%)
12	K	0.41	0/1135	0.67	0/1530
13	L	0.40	0/1003	0.73	0/1351
14	M	0.41	0/1126	0.72	0/1504
15	N	0.45	0/1633	0.74	2/2180 (0.1%)
16	O	0.36	0/1473	0.69	0/1999
17	P	0.41	0/873	0.71	0/1181
18	Q	0.41	0/1143	0.62	0/1521
19	R	0.42	0/748	0.74	1/1005 (0.1%)
20	S	0.42	0/1172	0.65	0/1578
21	T	0.39	0/648	0.63	0/875
22	U	0.36	0/957	0.66	0/1289
23	V	0.46	0/417	0.65	0/562
24	W	0.33	0/502	0.63	0/675
25	X	0.37	0/1218	0.67	0/1655
26	Y	0.40	0/664	0.66	0/895
27	Z	0.41	0/1146	0.67	0/1536
28	1	0.57	0/575	0.72	0/763
29	2	0.48	0/437	0.69	0/578
30	3	0.35	0/398	0.60	0/527
31	4	0.84	0/771	0.70	0/1024
All	All	0.50	7/98298 (0.0%)	0.71	30/147091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	58
2	B	1	0
All	All	1	58

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2617	G	C3'-O3'	12.86	1.60	1.42
1	A	2617	G	C4'-O4'	-6.15	1.37	1.45
9	H	3	TYR	CG-CD1	6.05	1.47	1.39
1	A	2618	G	P-OP2	-5.70	1.39	1.49
1	A	2617	G	N9-C8	5.65	1.41	1.37
1	A	2617	G	C2'-C1'	-5.40	1.47	1.53
1	A	2617	G	C4'-C3'	-5.38	1.47	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1165	G	O5'-P-OP2	10.73	123.58	110.70
1	A	1563	G	C2'-C3'-O3'	9.26	129.87	109.50
2	B	3024	U	C2'-C3'-O3'	9.18	129.70	109.50
9	H	3	TYR	CB-CG-CD2	9.11	126.47	121.00
1	A	1164	U	OP1-P-O3'	-8.57	86.34	105.20
1	A	1942	A	C5'-C4'-C3'	7.36	127.77	116.00
1	A	1164	U	OP2-P-O3'	-7.20	89.35	105.20
9	H	3	TYR	CG-CD2-CE2	6.82	126.76	121.30
1	A	871	G	C5'-C4'-O4'	-6.41	101.41	109.10
1	A	1504	A	N9-C1'-C2'	6.34	122.25	114.00
1	A	2617	G	C3'-C2'-C1'	-6.14	96.59	101.50
9	H	3	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	A	1979	G	C2'-C3'-O3'	6.10	123.46	113.70
1	A	381	G	N9-C1'-C2'	5.82	121.57	114.00
1	A	535	G	N9-C1'-C2'	5.82	121.56	114.00
11	J	74	ASN	N-CA-C	-5.75	95.48	111.00
1	A	2291	A	N9-C1'-C2'	5.74	121.47	114.00
1	A	1504	A	C1'-O4'-C4'	-5.64	105.39	109.90
15	N	127	LYS	N-CA-C	-5.56	95.99	111.00
19	R	68	GLY	N-CA-C	-5.42	99.55	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3024	U	C4'-C3'-O3'	5.34	123.69	113.00
2	B	3039	U	N1-C1'-C2'	5.32	120.91	114.00
1	A	2313	C	C5'-C4'-O4'	5.31	115.47	109.10
11	J	141	ASN	N-CA-C	-5.30	96.70	111.00
1	A	2431	C	C5'-C4'-C3'	-5.22	107.64	116.00
1	A	2607	U	N1-C1'-C2'	5.11	120.64	114.00
1	A	237	G	O4'-C4'-C3'	-5.10	98.90	104.00
11	J	110	GLY	N-CA-C	-5.07	100.42	113.10
1	A	1450	C	N1-C1'-C2'	-5.01	106.48	112.00
15	N	139	PRO	N-CA-C	-5.01	99.08	112.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3024	U	C3'

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1055	G	Sidechain
1	A	1191	A	Sidechain
1	A	1309	U	Sidechain
1	A	1316	G	Sidechain
1	A	1351	G	Sidechain
1	A	1376	G	Sidechain
1	A	1380	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1464	U	Sidechain
1	A	148	A	Sidechain
1	A	1635	U	Sidechain
1	A	1641	A	Sidechain
1	A	1707	G	Sidechain
1	A	176	U	Sidechain
1	A	1772	C	Sidechain
1	A	1819	G	Sidechain
1	A	182	G	Sidechain
1	A	1825	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1845	A	Sidechain
1	A	1861	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1878	G	Sidechain
1	A	1887	U	Sidechain
1	A	1903	U	Sidechain
1	A	1996	U	Sidechain
1	A	205	U	Sidechain
1	A	214	U	Sidechain
1	A	2308	U	Sidechain
1	A	2313	C	Sidechain
1	A	2316	G	Sidechain
1	A	2421	G	Sidechain
1	A	2493	C	Sidechain
1	A	2506	A	Sidechain
1	A	2552	C	Sidechain
1	A	2564	G	Sidechain
1	A	2597	U	Sidechain
1	A	2599	A	Sidechain
1	A	2607	U	Sidechain
1	A	2622	A	Sidechain
1	A	264	G	Sidechain
1	A	2673	U	Sidechain
1	A	2753	G	Sidechain
1	A	2793	A	Sidechain
1	A	2799	A	Sidechain
1	A	324	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain
1	A	535	G	Sidechain
1	A	619	U	Sidechain
1	A	651	U	Sidechain
1	A	722	G	Sidechain
1	A	734	U	Sidechain
1	A	795	G	Sidechain
1	A	817	G	Sidechain
1	A	840	U	Sidechain
1	A	920	C	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29805	1413	0
2	B	2600	0	1326	101	0
3	5	40	0	22	7	0
4	C	1754	0	1763	136	0
5	D	2624	0	2533	221	0
6	E	1858	0	1816	138	0
7	F	1094	0	1085	149	0
8	G	1357	0	1266	101	0
9	H	885	0	854	76	0
10	I	240	0	231	24	0
11	J	1215	0	1215	172	0
12	K	1119	0	1098	86	0
13	L	993	0	1027	73	0
14	M	1114	0	1072	76	0
15	N	1605	0	1676	178	0
16	O	1444	0	1401	159	0
17	P	864	0	873	74	0
18	Q	1133	0	1127	64	0
19	R	734	0	728	36	0
20	S	1149	0	1122	76	0
21	T	641	0	605	23	0
22	U	949	0	923	76	0
23	V	410	0	367	46	0
24	W	499	0	511	37	0
25	X	1195	0	1137	111	0
26	Y	654	0	653	53	0
27	Z	1130	0	1133	77	0
28	1	563	0	600	89	0
29	2	430	0	426	24	0
30	3	393	0	406	17	0
31	4	755	0	732	108	0
32	1	1	0	0	0	0
32	4	2	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0
32	C	1	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	2	0	0	0	0
34	A	73	0	0	0	0
34	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	1	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	1	0
35	A	11	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	38	0	0	14	0
38	2	56	0	0	9	0
38	3	47	0	0	2	0
38	4	72	0	0	13	0
38	A	5871	0	0	307	0
38	B	147	0	0	14	0
38	C	135	0	0	24	0
38	D	155	0	0	28	0
38	E	171	0	0	31	0
38	F	51	0	0	25	0
38	G	44	0	0	14	0
38	H	26	0	0	12	0
38	I	20	0	0	6	0
38	J	77	0	0	27	0
38	K	55	0	0	5	0
38	L	63	0	0	14	0
38	M	90	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	125	0	0	27	0
38	O	64	0	0	26	0
38	P	44	0	0	13	0
38	Q	68	0	0	10	0
38	R	54	0	0	5	0
38	S	83	0	0	9	0
38	T	31	0	0	4	0
38	U	39	0	0	8	0
38	V	26	0	0	7	0
38	W	15	0	0	5	0
38	X	70	0	0	14	0
38	Y	30	0	0	5	0
38	Z	102	0	0	19	0
All	All	98596	0	59561	3672	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 24.

All (3672) 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)
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.56	1.19
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.28	1.14
6:E:236:THR:HG22	6:E:239:ALA:H	1.10	1.10
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.99	1.10
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.30	1.09
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.30	1.08
2:B:3006:C:H5"	16:O:37:ARG:HH12	0.91	1.05
2:B:3056:A:H2'	2:B:3057:A:H5"	1.35	1.05
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.39	1.04
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.34	1.04
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.40	1.03
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.40	1.03
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.73	1.02
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.42	1.02
1:A:1679:C:H5'	38:A:8832:HOH:O	1.59	1.02
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.22	1.02
2:B:3006:C:C5'	16:O:37:ARG:HH12	1.72	1.02
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.38	1.01
1:A:541:C:H2'	1:A:542:A:H5"	1.41	1.00
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.45	0.99
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.45	0.99
1:A:1165:G:OP1	1:A:1165:G:H3'	1.62	0.98
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.45	0.98
5:D:248:ARG:O	5:D:251:VAL:HG12	1.62	0.98
1:A:962:C:H1'	16:O:5:ARG:NH1	1.79	0.98
1:A:1160:G:H5'	1:A:1161:A:H5'	1.45	0.98
5:D:238:ASN:HD22	5:D:240:GLY:H	1.12	0.97
11:J:27:LYS:H	11:J:58:HIS:HD2	1.08	0.97
13:L:10:GLN:NE2	13:L:10:GLN:H	1.61	0.97
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.43	0.96
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.48	0.96
1:A:156:C:H5"	15:N:171:ARG:HD3	1.48	0.96
1:A:1751:G:H2'	1:A:1752:G:H5"	1.48	0.95
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.48	0.95
28:1:39:CYS:SG	28:1:47:LEU:HD21	2.07	0.94
1:A:856:G:H2'	38:A:4907:HOH:O	1.66	0.94
1:A:2717:C:H2'	1:A:2718:C:H5"	1.49	0.94
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.29	0.94
18:Q:115:SER:H	18:Q:118:GLN:HE21	1.14	0.94
1:A:960:G:H4'	38:A:6895:HOH:O	1.68	0.94
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.68	0.94
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.33	0.93
5:D:140:LEU:HA	38:D:8587:HOH:O	1.66	0.93
8:G:97:VAL:HG12	38:G:4191:HOH:O	1.66	0.93
1:A:2716:G:H5"	5:D:206:THR:HG21	1.47	0.93
27:Z:220:GLU:HG2	38:Z:8551:HOH:O	1.67	0.93
6:E:61:PHE:HB3	38:E:8444:HOH:O	1.66	0.93
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.83	0.93
1:A:1242:A:H5'	12:K:82:THR:HG23	1.50	0.93
2:B:3076:G:H3'	2:B:3077:A:H5"	1.52	0.92
14:M:68:GLU:HA	38:M:8419:HOH:O	1.68	0.92
2:B:3056:A:C2'	2:B:3057:A:H5"	1.98	0.92
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.69	0.92
1:A:1134:G:H4'	11:J:151:MET:HE1	1.51	0.92
7:F:25:MET:HE2	7:F:41:LEU:HG	1.52	0.91
17:P:32:ARG:HB2	38:P:4656:HOH:O	1.71	0.91
1:A:871:G:H5'	1:A:871:G:C8	2.06	0.91
7:F:105:SER:HB2	7:F:131:THR:HG23	1.53	0.91
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.53	0.90
1:A:1625:U:H4'	38:A:4147:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:41:HIS:H	30:3:45:ASN:HD22	1.16	0.90
1:A:1119:G:H2'	12:K:52:GLN:NE2	1.87	0.90
2:B:3023:U:H3'	38:B:8484:HOH:O	1.72	0.90
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.02	0.90
23:V:30:HIS:HB3	38:V:6215:HOH:O	1.72	0.89
1:A:21:G:H5'	20:S:2:ILE:HA	1.53	0.89
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.53	0.89
1:A:1667:A:H5'	1:A:1667:A:H8	1.34	0.89
5:D:321:PRO:HA	38:D:8666:HOH:O	1.72	0.89
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.54	0.89
11:J:162:SER:HB2	11:J:163:PRO:CD	2.00	0.89
1:A:711:G:H1'	38:A:6564:HOH:O	1.72	0.89
1:A:1702:U:H5"	38:A:6683:HOH:O	1.72	0.89
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.54	0.89
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.52	0.89
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.54	0.89
1:A:1166:A:H1'	1:A:1192:A:C2	2.08	0.88
11:J:5:MET:HG3	38:J:8354:HOH:O	1.71	0.88
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.36	0.88
1:A:289:G:H22	1:A:363:A:H2	1.20	0.88
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.55	0.88
1:A:2812:A:H2	1:A:2814:A:H62	1.20	0.88
12:K:19:MET:HE2	12:K:79:PHE:HA	1.55	0.88
15:N:87:MET:CB	31:4:46:ILE:HD13	2.04	0.88
38:B:8478:HOH:O	16:O:23:ARG:HD3	1.74	0.88
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.20	0.88
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.87	0.87
1:A:541:C:C2'	1:A:542:A:H5"	2.04	0.87
5:D:86:ALA:HA	38:D:8587:HOH:O	1.75	0.87
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.56	0.87
1:A:346:U:H4'	38:A:6311:HOH:O	1.74	0.87
15:N:64:ARG:HD2	38:N:8580:HOH:O	1.73	0.87
1:A:214:U:H5'	38:A:5630:HOH:O	1.75	0.87
1:A:2506:A:HO2'	1:A:2507:G:H8	0.89	0.86
9:H:107:VAL:HG23	38:H:6617:HOH:O	1.76	0.86
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.56	0.86
1:A:542:A:H5'	1:A:542:A:H8	1.40	0.86
26:Y:25:ARG:HD2	38:Y:3861:HOH:O	1.74	0.86
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.40	0.86
16:O:144:GLY:O	16:O:147:ILE:HG22	1.76	0.86
12:K:52:GLN:HG3	12:K:53:ILE:N	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:14:GLU:OE1	23:V:15:PRO:HD2	1.76	0.86
1:A:1191:A:H3'	1:A:1192:A:H5"	1.57	0.85
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.56	0.85
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.58	0.85
1:A:2459:G:OP1	31:4:64:LYS:N	2.08	0.85
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.58	0.85
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.58	0.85
14:M:148:GLU:HA	38:M:8448:HOH:O	1.75	0.85
28:1:59:HIS:HA	38:1:8441:HOH:O	1.77	0.85
38:A:3220:HOH:O	15:N:157:LEU:HD11	1.76	0.85
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.58	0.85
1:A:1164:U:C4'	1:A:1165:G:OP1	2.21	0.84
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.42	0.84
11:J:165:GLY:HA3	38:J:8384:HOH:O	1.77	0.84
38:A:4706:HOH:O	13:L:39:GLY:HA2	1.77	0.84
2:B:3023:U:H4'	2:B:3024:U:OP2	1.77	0.84
6:E:180:SER:HB2	38:E:8445:HOH:O	1.77	0.84
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.59	0.84
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.43	0.84
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.59	0.84
13:L:10:GLN:H	13:L:10:GLN:HE21	1.25	0.84
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.58	0.84
1:A:506:G:H22	1:A:509:A:H5'	1.43	0.84
6:E:242:GLU:HG3	38:E:8382:HOH:O	1.77	0.84
25:X:122:ARG:NH2	25:X:154:ARG:HD2	1.93	0.84
31:4:60:LYS:HD2	31:4:61:PRO:HD2	1.60	0.84
1:A:1702:U:H5'	38:A:9923:HOH:O	1.77	0.84
23:V:9:CYS:HA	23:V:52:THR:HG23	1.58	0.83
1:A:1634:G:H3'	38:A:3391:HOH:O	1.76	0.83
1:A:2435:U:OP1	31:4:28:GLY:HA3	1.79	0.83
4:C:35:GLY:O	4:C:36:ASP:HB3	1.78	0.83
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.61	0.83
1:A:1120:U:H6	1:A:1120:U:H5"	1.44	0.83
1:A:2586:U:H3	1:A:2592:G:H22	1.22	0.83
1:A:2256:G:H2'	1:A:2257:G:H5'	1.61	0.83
1:A:1835:U:H5	1:A:1840:A:N7	1.76	0.83
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.79	0.83
1:A:1164:U:H4'	1:A:1165:G:OP1	1.79	0.83
1:A:2004:U:H4'	38:A:4789:HOH:O	1.79	0.83
15:N:164:THR:HG22	15:N:167:GLY:H	1.41	0.83
38:A:5274:HOH:O	15:N:170:CYS:SG	2.37	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.61	0.83
1:A:962:C:H1'	16:O:5:ARG:HH12	1.42	0.82
5:D:179:LEU:O	5:D:183:GLU:HG2	1.79	0.82
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.60	0.82
5:D:258:GLY:H	5:D:260:HIS:CE1	1.97	0.82
6:E:76:ARG:HD2	38:E:8432:HOH:O	1.78	0.82
11:J:2:PRO:HB2	38:J:8354:HOH:O	1.78	0.82
6:E:237:GLU:HB2	38:E:8429:HOH:O	1.80	0.82
24:W:56:ILE:O	24:W:60:GLN:HG3	1.78	0.82
1:A:1773:G:C8	28:1:16:PRO:HA	2.15	0.82
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.61	0.82
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.50	0.82
38:A:3049:HOH:O	15:N:152:ARG:HG3	1.78	0.82
6:E:236:THR:HA	38:E:8450:HOH:O	1.78	0.82
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.09	0.82
1:A:1164:U:H3	1:A:1192:A:H2	1.27	0.82
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.60	0.82
11:J:139:ASP:N	11:J:140:PRO:HD3	1.95	0.82
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.62	0.81
31:4:22:VAL:HG11	31:4:67:LEU:HD13	1.63	0.81
1:A:877:G:H5'	1:A:878:G:OP1	1.81	0.81
5:D:162:MET:CE	5:D:308:LEU:HD21	2.10	0.81
20:S:9:ASP:O	20:S:13:THR:HB	1.80	0.81
14:M:148:GLU:HB2	38:M:8467:HOH:O	1.81	0.81
1:A:545:G:H5'	1:A:545:G:H8	1.46	0.81
11:J:162:SER:CB	11:J:163:PRO:HD3	2.09	0.81
1:A:2256:G:C2'	1:A:2257:G:H5'	2.11	0.81
15:N:104:ARG:O	15:N:108:LYS:HG2	1.81	0.81
1:A:1116:U:HO2'	1:A:1118:A:H2	0.83	0.81
11:J:59:ASN:H	11:J:59:ASN:HD22	1.27	0.81
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.63	0.81
26:Y:15:ARG:HB3	26:Y:15:ARG:HH11	1.45	0.81
38:A:7028:HOH:O	31:4:60:LYS:HG3	1.80	0.81
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.62	0.81
15:N:87:MET:CG	31:4:46:ILE:HG21	2.10	0.80
1:A:1474:C:H6	1:A:1474:C:H5'	1.46	0.80
18:Q:103:THR:HA	18:Q:106:ARG:NH1	1.95	0.80
22:U:19:ARG:HD3	22:U:67:LEU:O	1.81	0.80
11:J:142:VAL:HG13	38:J:8369:HOH:O	1.81	0.80
15:N:52:LEU:HD11	38:N:8610:HOH:O	1.81	0.80
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2830:U:H3'	38:A:4713:HOH:O	1.80	0.80
9:H:91:VAL:HG12	9:H:92:GLY:N	1.96	0.80
7:F:27:ILE:HG22	7:F:28:GLY:H	1.45	0.80
4:C:6:GLY:HA3	38:C:8578:HOH:O	1.81	0.79
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.27	0.79
12:K:76:ASP:HA	38:K:5907:HOH:O	1.81	0.79
7:F:154:LYS:H	7:F:154:LYS:HD2	1.47	0.79
11:J:137:ASN:O	11:J:139:ASP:N	2.15	0.79
15:N:94:LYS:HE3	38:N:8578:HOH:O	1.80	0.79
1:A:513:A:N3	38:A:3157:HOH:O	2.16	0.79
1:A:560:C:H42	1:A:597:A:H61	1.31	0.79
1:A:1923:G:H4'	31:4:31:THR:O	1.83	0.79
2:B:3042:C:H2'	38:B:8506:HOH:O	1.80	0.79
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.62	0.79
25:X:88:THR:HB	38:X:6679:HOH:O	1.81	0.79
3:5:74:C:C2'	3:5:75:C:H5'	2.12	0.79
14:M:133:VAL:HA	38:M:8449:HOH:O	1.81	0.79
5:D:238:ASN:ND2	5:D:240:GLY:H	1.79	0.79
6:E:236:THR:HG22	6:E:239:ALA:N	1.95	0.79
1:A:1878:G:H1'	38:A:5611:HOH:O	1.81	0.78
5:D:119:HIS:O	5:D:121:PRO:HD3	1.83	0.78
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.66	0.78
1:A:870:G:H2'	1:A:871:G:H5"	1.64	0.78
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.66	0.78
14:M:35:ARG:O	14:M:40:PHE:HA	1.83	0.78
5:D:125:GLU:O	5:D:129:ARG:HG3	1.82	0.78
6:E:1:MET:HG2	6:E:2:GLN:H	1.47	0.78
1:A:2717:C:C2'	1:A:2718:C:H5"	2.14	0.78
1:A:871:G:C5'	1:A:871:G:H8	1.95	0.78
38:A:4346:HOH:O	15:N:14:ARG:HG2	1.84	0.78
38:A:6242:HOH:O	16:O:4:PRO:HD2	1.83	0.78
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.66	0.78
5:D:141:ARG:HD2	5:D:163:GLU:OE2	1.83	0.78
31:4:31:THR:HB	31:4:33:MET:CE	2.14	0.78
1:A:1886:A:N3	38:A:4306:HOH:O	2.17	0.78
13:L:22:ASP:HB2	38:L:5264:HOH:O	1.83	0.78
23:V:14:GLU:O	23:V:17:THR:HB	1.84	0.78
1:A:1185:U:H2'	1:A:1186:C:C6	2.19	0.78
2:B:3025:G:H3'	2:B:3026:C:C5'	2.14	0.78
2:B:3029:C:H2'	2:B:3030:C:H5'	1.66	0.78
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.66	0.78
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.65	0.78
1:A:2432:C:O2'	1:A:2433:A:H5'	1.83	0.77
1:A:1474:C:H5'	1:A:1474:C:C6	2.20	0.77
1:A:1936:C:H3'	38:A:6641:HOH:O	1.83	0.77
2:B:3025:G:H3'	2:B:3026:C:H5'	1.64	0.77
1:A:1372:A:H3'	38:A:6654:HOH:O	1.84	0.77
4:C:121:ALA:O	4:C:124:VAL:HG22	1.83	0.77
5:D:41:PHE:CD2	5:D:190:MET:HE3	2.18	0.77
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.64	0.77
1:A:1507:C:H4'	38:A:3100:HOH:O	1.84	0.77
15:N:99:ARG:HD2	15:N:167:GLY:HA2	1.66	0.77
4:C:192:VAL:HB	38:C:8607:HOH:O	1.85	0.77
1:A:871:G:H5'	1:A:871:G:H8	1.46	0.77
21:T:6:LYS:HB2	21:T:27:ALA:O	1.85	0.77
27:Z:109:LEU:HD23	38:Z:8573:HOH:O	1.84	0.77
1:A:1328:A:OP1	27:Z:169:ARG:HD2	1.85	0.77
2:B:3107:C:H5	38:B:8439:HOH:O	1.68	0.77
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.66	0.77
8:G:37:ASP:OD1	12:K:125:SER:HB3	1.85	0.77
24:W:16:ARG:NH2	24:W:63:GLU:HG3	2.00	0.77
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.64	0.77
11:J:59:ASN:HD22	11:J:59:ASN:N	1.82	0.77
1:A:871:G:C8	1:A:871:G:C5'	2.69	0.76
9:H:46:GLU:O	9:H:73:PRO:HD2	1.85	0.76
15:N:60:ILE:C	15:N:61:ILE:HD12	2.06	0.76
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.66	0.76
1:A:1450:C:H4'	1:A:1451:C:OP2	1.84	0.76
9:H:99:THR:HA	38:H:3461:HOH:O	1.84	0.76
29:2:25:LYS:HG2	29:2:25:LYS:O	1.84	0.76
15:N:172:GLY:O	15:N:183:VAL:HG11	1.86	0.76
1:A:1377:C:H6	1:A:1377:C:H5'	1.51	0.76
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.66	0.76
6:E:111:VAL:HB	38:E:8321:HOH:O	1.85	0.76
7:F:19:GLU:O	7:F:20:LYS:HG2	1.85	0.76
1:A:1187:U:H2'	38:A:6366:HOH:O	1.84	0.76
8:G:166:VAL:HG12	38:G:3134:HOH:O	1.86	0.76
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.48	0.76
1:A:157:G:H4'	15:N:95:LYS:HE3	1.67	0.76
1:A:559:U:H6	1:A:559:U:H5'	1.51	0.76
1:A:1213:C:O2'	1:A:1214:G:H5'	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:A:H4'	1:A:1702:U:H5"	1.68	0.76
1:A:2291:A:C8	1:A:2309:C:H5'	2.21	0.76
15:N:80:GLY:O	15:N:81:ARG:HD3	1.86	0.76
5:D:62:ARG:HA	5:D:65:MET:HE3	1.67	0.75
15:N:164:THR:CG2	15:N:167:GLY:H	2.00	0.75
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.01	0.75
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.66	0.75
1:A:1160:G:H5'	1:A:1161:A:C5'	2.16	0.75
1:A:2533:C:H6	1:A:2533:C:H5'	1.52	0.75
15:N:164:THR:HG22	15:N:167:GLY:N	2.01	0.75
1:A:236:A:H4'	1:A:237:G:H5'	1.69	0.75
1:A:2433:A:O4'	38:A:5776:HOH:O	2.03	0.75
1:A:92:G:H5'	38:W:7247:HOH:O	1.85	0.75
1:A:1116:U:H3	1:A:1246:A:H62	1.35	0.75
1:A:2578:G:H5'	1:A:2578:G:H8	1.51	0.75
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.50	0.75
31:4:51:LYS:HA	31:4:54:LYS:HE3	1.67	0.75
1:A:2768:A:H2'	1:A:2769:C:O4'	1.87	0.75
24:W:1:THR:HG23	24:W:2:VAL:H	1.49	0.75
5:D:275:GLY:O	5:D:291:ASP:HA	1.86	0.75
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.83	0.75
8:G:7:ILE:HG22	8:G:45:ASP:O	1.86	0.74
1:A:272:A:H5'	1:A:273:G:OP2	1.87	0.74
1:A:338:C:H4'	6:E:174:ILE:HD11	1.68	0.74
1:A:2420:G:O2'	1:A:2421:G:H5'	1.87	0.74
1:A:2506:A:O2'	1:A:2507:G:H8	1.68	0.74
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.51	0.74
1:A:1735:C:O2'	1:A:1736:A:H5'	1.86	0.74
1:A:2526:C:O2'	1:A:2527:U:H5'	1.86	0.74
14:M:67:ARG:O	14:M:71:GLU:HG3	1.88	0.74
2:B:3014:G:H5'	2:B:3014:G:H8	1.51	0.74
9:H:91:VAL:HG12	9:H:92:GLY:H	1.48	0.74
15:N:139:PRO:O	15:N:140:ALA:HB3	1.88	0.74
1:A:1080:C:H4'	1:A:1081:A:OP1	1.87	0.74
15:N:30:GLU:O	15:N:34:GLU:HG3	1.87	0.74
1:A:506:G:H22	1:A:509:A:C5'	2.01	0.74
1:A:1160:G:N3	38:A:5114:HOH:O	2.20	0.74
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.68	0.74
19:R:23:THR:HA	38:R:4792:HOH:O	1.88	0.74
1:A:544:G:H2'	1:A:545:G:H5"	1.70	0.74
1:A:282:C:O2'	1:A:283:U:H5'	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.86	0.74
30:3:41:HIS:H	30:3:45:ASN:ND2	1.85	0.74
31:4:22:VAL:CG1	31:4:67:LEU:HD13	2.18	0.74
1:A:553:G:P	27:Z:204:ARG:HH22	2.11	0.73
7:F:20:LYS:HA	7:F:75:LEU:O	1.88	0.73
1:A:2896:A:H5"	38:A:5590:HOH:O	1.87	0.73
5:D:238:ASN:HD22	5:D:240:GLY:N	1.84	0.73
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.18	0.73
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.86	0.73
1:A:2426:G:H1'	38:A:5583:HOH:O	1.87	0.73
16:O:113:SER:HB2	38:O:8556:HOH:O	1.89	0.73
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.54	0.73
28:1:39:CYS:SG	28:1:57:CYS:HB2	2.29	0.73
28:1:46:LYS:O	28:1:57:CYS:HA	1.88	0.73
1:A:2786:G:H2'	38:A:6652:HOH:O	1.88	0.73
6:E:39:GLN:O	6:E:43:LYS:HD3	1.87	0.73
1:A:1864:C:OP1	15:N:75:THR:HG23	1.89	0.73
1:A:1909:A:N1	1:A:2128:G:H1'	2.03	0.73
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.70	0.73
5:D:211:THR:HA	5:D:255:GLY:O	1.88	0.73
14:M:79:ASP:HB3	38:M:8434:HOH:O	1.87	0.73
4:C:135:VAL:HG21	4:C:147:ARG:NH1	2.03	0.73
6:E:132:ASP:HB3	38:E:8365:HOH:O	1.89	0.73
19:R:46:SER:O	19:R:48:PRO:HD3	1.88	0.73
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.18	0.73
1:A:1119:G:N2	1:A:1246:A:C2	2.57	0.73
2:B:3049:G:H5"	38:B:8469:HOH:O	1.89	0.73
13:L:81:ARG:HB2	13:L:87:ARG:NH1	2.04	0.73
14:M:26:HIS:HB2	38:M:8381:HOH:O	1.88	0.73
30:3:39:ARG:HG2	38:3:3143:HOH:O	1.87	0.73
1:A:20:G:H21	20:S:117:HIS:HD2	1.37	0.73
3:5:74:C:H2'	3:5:75:C:H5'	1.68	0.73
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.69	0.73
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.71	0.73
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.89	0.73
12:K:93:ARG:HB3	12:K:93:ARG:HH11	1.53	0.73
28:1:42:CYS:SG	28:1:43:GLY:N	2.62	0.73
7:F:25:MET:CE	7:F:41:LEU:HG	2.18	0.72
11:J:75:SER:O	11:J:79:ALA:HB2	1.89	0.72
28:1:22:ILE:O	28:1:26:VAL:HG23	1.88	0.72
1:A:1165:G:H4'	1:A:1174:A:O2'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.70	0.72
11:J:132:PHE:O	11:J:133:ILE:HD13	1.89	0.72
15:N:87:MET:CB	31:4:46:ILE:HG21	2.19	0.72
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.54	0.72
1:A:1751:G:C2'	1:A:1752:G:H5"	2.18	0.72
1:A:2320:U:H4'	1:A:2321:A:O4'	1.90	0.72
1:A:2780:C:H2'	1:A:2781:U:H6	1.54	0.72
38:A:6343:HOH:O	15:N:178:LYS:HB2	1.88	0.72
15:N:61:ILE:HG13	38:N:8619:HOH:O	1.89	0.72
1:A:1120:U:H5"	1:A:1120:U:C6	2.25	0.72
7:F:19:GLU:HG3	38:F:6165:HOH:O	1.87	0.72
1:A:584:U:H3'	38:A:5586:HOH:O	1.88	0.72
1:A:2432:C:H4'	31:4:36:ILE:HG12	1.72	0.72
11:J:26:LYS:HG2	11:J:28:ILE:H	1.53	0.72
12:K:39:VAL:HG13	12:K:106:GLY:O	1.90	0.72
19:R:93:ARG:HH11	19:R:93:ARG:HG3	1.54	0.72
1:A:288:A:H61	1:A:364:C:H42	1.36	0.72
24:W:39:ALA:N	24:W:40:PRO:HD2	2.05	0.72
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.15	0.72
1:A:195:C:H2'	1:A:196:G:H5'	1.70	0.72
1:A:1160:G:C5'	1:A:1161:A:H5'	2.18	0.72
22:U:37:GLN:HB3	38:U:6711:HOH:O	1.90	0.72
20:S:99:ALA:HB1	20:S:109:MET:CE	2.19	0.72
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.72	0.72
1:A:21:G:C5'	20:S:2:ILE:HA	2.18	0.72
2:B:3023:U:H3'	2:B:3024:U:H5"	1.72	0.72
11:J:41:THR:HA	38:J:8382:HOH:O	1.89	0.72
12:K:74:ARG:HD3	38:K:5061:HOH:O	1.88	0.72
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.72	0.72
17:P:87:THR:O	17:P:91:GLN:HG3	1.90	0.72
27:Z:235:GLU:H	27:Z:235:GLU:CD	1.93	0.72
1:A:1667:A:H5'	1:A:1667:A:C8	2.23	0.72
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.72	0.72
1:A:1666:C:O2'	1:A:1667:A:H5"	1.90	0.71
1:A:1887:U:OP1	28:1:21:LYS:HG3	1.90	0.71
22:U:48:VAL:HG23	22:U:98:VAL:HA	1.72	0.71
1:A:444:C:H1'	38:A:3535:HOH:O	1.88	0.71
1:A:2382:A:H1'	31:4:10:TYR:CE2	2.25	0.71
1:A:2780:C:H2'	1:A:2781:U:C6	2.25	0.71
6:E:154:VAL:O	6:E:158:GLU:HG3	1.90	0.71
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.20	0.71
1:A:2851:G:O2'	1:A:2852:A:H5'	1.91	0.71
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.71	0.71
15:N:87:MET:HG2	31:4:46:ILE:CG2	2.19	0.71
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.71	0.71
1:A:1116:U:O2'	1:A:1118:A:H2	1.66	0.71
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.54	0.71
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.71
12:K:131:THR:HG22	12:K:134:GLU:H	1.52	0.71
1:A:1118:A:H8	1:A:1118:A:H3'	1.56	0.71
12:K:52:GLN:HG3	12:K:53:ILE:H	1.51	0.71
1:A:681:G:H5'	1:A:681:G:N3	2.06	0.71
31:4:31:THR:HB	31:4:33:MET:HE2	1.70	0.71
1:A:2256:G:H2'	1:A:2257:G:C5'	2.21	0.71
38:B:8469:HOH:O	16:O:147:ILE:HD12	1.90	0.71
6:E:235:PHE:CE2	6:E:243:VAL:HG21	2.25	0.71
27:Z:212:ARG:HD2	38:Z:8606:HOH:O	1.89	0.71
1:A:2727:A:H2'	1:A:2728:C:H5'	1.72	0.71
7:F:53:LYS:HA	7:F:67:ASP:O	1.90	0.71
25:X:81:ASP:OD1	25:X:92:ASP:HB2	1.90	0.71
5:D:175:LEU:HD23	5:D:175:LEU:C	2.12	0.70
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.26	0.70
15:N:139:PRO:O	15:N:140:ALA:CB	2.39	0.70
11:J:140:PRO:HB3	38:J:8369:HOH:O	1.89	0.70
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.56	0.70
31:4:65:THR:HG23	31:4:67:LEU:HG	1.73	0.70
8:G:7:ILE:HD11	8:G:11:VAL:C	2.11	0.70
15:N:84:LYS:HE2	38:N:8572:HOH:O	1.90	0.70
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.22	0.70
1:A:272:A:H3'	38:A:7000:HOH:O	1.90	0.70
1:A:1123:A:C6	1:A:1238:C:H5'	2.26	0.70
38:A:9065:HOH:O	5:D:267:LYS:HD3	1.90	0.70
1:A:2637:A:H5'	38:A:8783:HOH:O	1.91	0.70
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.72	0.70
1:A:2815:G:N7	12:K:80:LYS:NZ	2.39	0.70
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.74	0.70
15:N:39:ARG:HA	15:N:63:VAL:HG22	1.74	0.70
7:F:95:THR:O	7:F:97:GLN:N	2.21	0.70
16:O:7:LYS:HE3	19:R:21:ARG:O	1.91	0.70
1:A:1773:G:H8	28:1:16:PRO:HA	1.56	0.70
23:V:6:CYS:HA	23:V:13:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:110:GLN:HE21	25:X:110:GLN:HA	1.56	0.70
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.72	0.69
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.21	0.69
29:2:1:THR:HB	38:2:6858:HOH:O	1.92	0.69
1:A:1127:C:H2'	1:A:1128:U:H5'	1.74	0.69
1:A:2502:C:H4'	11:J:151:MET:HG2	1.74	0.69
12:K:74:ARG:HH11	12:K:74:ARG:CB	2.04	0.69
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.28	0.69
1:A:119:A:H2'	1:A:120:A:H5"	1.74	0.69
1:A:2414:A:H2'	1:A:2415:A:C8	2.26	0.69
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.55	0.69
15:N:134:ILE:HG23	15:N:141:ILE:HD13	1.75	0.69
1:A:694:A:H2'	1:A:695:C:H5'	1.74	0.69
11:J:27:LYS:H	11:J:58:HIS:CD2	2.01	0.69
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.75	0.69
13:L:106:GLY:HA3	38:L:5264:HOH:O	1.91	0.69
38:A:9470:HOH:O	6:E:174:ILE:HD12	1.93	0.69
2:B:3092:G:H2'	2:B:3093:A:C8	2.27	0.69
4:C:105:VAL:HG12	4:C:106:CYS:N	2.08	0.69
12:K:74:ARG:O	12:K:78:ILE:HG12	1.92	0.69
15:N:153:THR:O	15:N:156:ARG:HG3	1.93	0.69
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.92	0.69
1:A:2054:A:N3	20:S:128:ARG:NH2	2.41	0.69
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.58	0.69
8:G:137:ASP:O	8:G:141:VAL:HG23	1.93	0.69
1:A:284:C:H4'	1:A:285:A:O5'	1.90	0.69
1:A:541:C:H2'	1:A:542:A:C5'	2.20	0.69
1:A:2346:C:O2'	7:F:52:THR:HG21	1.92	0.69
6:E:93:LYS:O	6:E:98:ARG:NH2	2.26	0.69
10:I:64:ASN:HD22	10:I:64:ASN:N	1.91	0.69
16:O:151:ASP:HB3	38:O:8528:HOH:O	1.93	0.69
20:S:39:THR:HG22	20:S:42:GLU:H	1.56	0.69
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.27	0.69
1:A:1603:A:H5'	1:A:1605:G:O4'	1.92	0.69
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.69
38:A:8962:HOH:O	20:S:83:LYS:HD3	1.90	0.69
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.58	0.69
1:A:1118:A:H3'	1:A:1118:A:C8	2.27	0.68
8:G:7:ILE:HD11	8:G:11:VAL:O	1.93	0.68
12:K:103:VAL:HG12	38:K:5907:HOH:O	1.91	0.68
28:1:42:CYS:SG	28:1:44:PHE:N	2.65	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.68
1:A:2638:G:H1'	38:A:7228:HOH:O	1.93	0.68
1:A:2795:C:O2'	1:A:2796:U:H5'	1.92	0.68
13:L:115:ARG:HG3	13:L:116:GLU:N	2.08	0.68
1:A:289:G:N2	1:A:363:A:H2	1.90	0.68
38:A:4434:HOH:O	2:B:3103:A:H4'	1.93	0.68
5:D:16:ARG:HB3	5:D:217:ARG:NH2	2.09	0.68
27:Z:185:VAL:HA	38:Z:8565:HOH:O	1.91	0.68
28:1:28:ASP:O	28:1:31:ILE:HG22	1.93	0.68
2:B:3020:G:O2'	2:B:3021:G:H5'	1.93	0.68
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.92	0.68
7:F:23:VAL:HG23	7:F:23:VAL:O	1.93	0.68
15:N:14:ARG:HB3	15:N:17:GLU:HG3	1.75	0.68
25:X:129:LYS:HG2	38:X:1990:HOH:O	1.93	0.68
38:A:8899:HOH:O	15:N:94:LYS:HE2	1.94	0.68
4:C:223:ARG:HG3	38:C:8617:HOH:O	1.94	0.68
12:K:45:VAL:HG23	12:K:130:VAL:O	1.92	0.68
23:V:9:CYS:CA	23:V:52:THR:HG23	2.24	0.68
27:Z:185:VAL:HG12	38:Z:8572:HOH:O	1.92	0.68
1:A:603:A:H5"	1:A:604:G:OP1	1.92	0.68
38:A:3178:HOH:O	15:N:79:LYS:HD3	1.93	0.68
2:B:3023:U:H6	2:B:3023:U:H5"	1.58	0.68
8:G:11:VAL:HG12	8:G:12:ASP:N	2.08	0.68
17:P:25:VAL:O	17:P:29:VAL:HG23	1.94	0.68
1:A:1819:G:H2'	1:A:1820:G:H4'	1.76	0.68
38:A:4999:HOH:O	5:D:298:LYS:HD3	1.92	0.68
7:F:62:ASP:HA	38:F:4233:HOH:O	1.93	0.68
16:O:5:ARG:HG3	19:R:18:PRO:CB	2.24	0.68
1:A:1333:U:H2'	1:A:1334:C:C6	2.29	0.68
1:A:1919:A:H4'	38:A:4333:HOH:O	1.94	0.68
1:A:2890:A:H1'	23:V:56:ARG:NH2	2.08	0.68
38:A:8896:HOH:O	28:1:34:LYS:HD3	1.93	0.68
5:D:41:PHE:HA	5:D:79:MET:HE2	1.76	0.68
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.07	0.68
18:Q:18:LYS:O	18:Q:21:VAL:HG22	1.92	0.68
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.23	0.68
8:G:149:GLU:OE1	8:G:168:ILE:HG12	1.94	0.68
1:A:2382:A:H1'	31:4:10:TYR:CD2	2.29	0.68
1:A:1187:U:O2'	1:A:1189:A:H2	1.77	0.67
1:A:2421:G:H3'	1:A:2422:U:C5'	2.24	0.67
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:39:ALA:O	24:W:41:GLU:N	2.27	0.67
1:A:1886:A:H4'	38:1:8405:HOH:O	1.93	0.67
1:A:2508:C:H2'	38:A:6224:HOH:O	1.93	0.67
29:2:25:LYS:HE2	38:2:7213:HOH:O	1.93	0.67
1:A:1857:A:N6	1:A:2247:C:H1'	2.09	0.67
4:C:94:LEU:N	4:C:94:LEU:HD23	2.09	0.67
5:D:333:GLU:HB2	38:V:3564:HOH:O	1.93	0.67
6:E:139:VAL:HG13	38:E:8448:HOH:O	1.95	0.67
20:S:40:ALA:O	20:S:44:VAL:HG23	1.95	0.67
7:F:97:GLN:HG2	7:F:97:GLN:O	1.94	0.67
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.76	0.67
13:L:22:ASP:OD1	13:L:24:THR:HG23	1.95	0.67
26:Y:15:ARG:HB3	26:Y:15:ARG:NH1	2.09	0.67
1:A:2265:U:H2'	1:A:2266:A:C8	2.30	0.67
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.23	0.67
4:C:8:ARG:HG2	38:C:8559:HOH:O	1.94	0.67
4:C:179:MET:HG2	4:C:186:TRP:CB	2.25	0.67
5:D:175:LEU:HD23	5:D:175:LEU:O	1.95	0.67
1:A:2278:U:H2'	38:A:7073:HOH:O	1.95	0.67
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.42	0.67
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.30	0.67
28:1:20:LEU:O	28:1:24:VAL:HG23	1.94	0.67
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.30	0.67
1:A:2506:A:H1'	38:A:3244:HOH:O	1.94	0.67
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.43	0.67
6:E:214:THR:HG21	38:E:8402:HOH:O	1.95	0.67
6:E:236:THR:CG2	6:E:239:ALA:H	2.00	0.67
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.24	0.67
1:A:1163:G:N2	38:A:5536:HOH:O	2.24	0.66
5:D:11:LEU:HA	38:D:8622:HOH:O	1.94	0.66
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.60	0.66
1:A:21:G:H4'	20:S:2:ILE:HG22	1.75	0.66
1:A:317:A:H5"	22:U:52:ARG:HD2	1.77	0.66
1:A:821:U:H2'	1:A:822:C:H6	1.60	0.66
1:A:1161:A:H8	1:A:1161:A:O5'	1.78	0.66
4:C:33:GLU:O	4:C:34:ASP:HB2	1.93	0.66
13:L:10:GLN:HE21	13:L:10:GLN:N	1.92	0.66
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.60	0.66
20:S:44:VAL:O	20:S:48:GLU:HG3	1.95	0.66
1:A:157:G:H4'	15:N:95:LYS:CE	2.26	0.66
1:A:639:A:H2'	1:A:640:G:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:2:ARG:HH21	8:G:48:VAL:HG21	1.59	0.66
10:I:12:ILE:N	10:I:13:PRO:HD3	2.09	0.66
10:I:63:ARG:N	38:I:2569:HOH:O	2.28	0.66
15:N:45:ARG:HB3	15:N:48:ARG:HB2	1.76	0.66
24:W:44:GLY:O	24:W:48:GLU:HG2	1.95	0.66
1:A:1589:G:N2	1:A:1605:G:H1'	2.09	0.66
1:A:2415:A:C2	16:O:25:ARG:HB3	2.29	0.66
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.78	0.66
5:D:75:GLU:C	5:D:77:PRO:HD3	2.14	0.66
6:E:246:ARG:HB3	6:E:246:ARG:NH1	2.10	0.66
9:H:104:ALA:HA	38:H:6617:HOH:O	1.96	0.66
23:V:52:THR:HG22	23:V:54:THR:H	1.61	0.66
31:4:64:LYS:HE3	31:4:84:ARG:NH1	2.10	0.66
11:J:140:PRO:O	38:J:8355:HOH:O	2.13	0.66
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.77	0.66
1:A:450:C:OP1	6:E:184:ARG:NH2	2.25	0.66
1:A:2421:G:H3'	1:A:2422:U:H5"	1.76	0.66
5:D:51:VAL:HG23	5:D:330:VAL:HG22	1.78	0.66
5:D:144:THR:HG22	5:D:145:HIS:N	2.11	0.66
6:E:198:ASP:O	38:E:8471:HOH:O	2.14	0.66
11:J:49:VAL:O	11:J:157:ILE:HG23	1.96	0.66
25:X:88:THR:HG23	25:X:110:GLN:NE2	2.11	0.66
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.30	0.66
38:A:8729:HOH:O	4:C:11:ARG:HD3	1.94	0.66
8:G:132:THR:HB	38:G:2227:HOH:O	1.96	0.66
12:K:99:GLU:HA	38:K:7377:HOH:O	1.94	0.66
14:M:1:THR:HA	38:M:8395:HOH:O	1.96	0.66
26:Y:41:PHE:O	26:Y:43:VAL:HG23	1.95	0.66
1:A:2911:C:H3'	38:A:5034:HOH:O	1.95	0.66
8:G:84:MET:HE3	8:G:148:ILE:HG21	1.78	0.66
22:U:106:GLU:HG3	38:U:4913:HOH:O	1.95	0.66
1:A:2252:A:C5	1:A:2253:G:H1'	2.31	0.66
9:H:38:LYS:NZ	15:N:3:SER:HA	2.10	0.66
15:N:120:VAL:HG11	15:N:130:GLU:OE2	1.97	0.66
22:U:38:ARG:NH1	38:U:6217:HOH:O	2.29	0.66
27:Z:103:THR:HG22	27:Z:104:GLU:OE2	1.95	0.66
31:4:60:LYS:CD	31:4:61:PRO:HD2	2.25	0.66
4:C:105:VAL:HG13	4:C:155:THR:O	1.96	0.65
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.26	0.65
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.26	0.65
15:N:38:VAL:O	15:N:63:VAL:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:89:GLY:O	16:O:92:ALA:HB3	1.96	0.65
1:A:1675:C:H5"	30:3:5:LYS:HD2	1.77	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.96	0.65
9:H:28:ALA:HB3	9:H:99:THR:O	1.95	0.65
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.77	0.65
28:1:21:LYS:O	28:1:25:ARG:HG3	1.96	0.65
31:4:39:GLN:HA	31:4:42:ARG:NH2	2.12	0.65
1:A:162:C:H2'	1:A:163:U:H5'	1.78	0.65
1:A:2382:A:H5'	38:4:8535:HOH:O	1.95	0.65
5:D:62:ARG:HA	5:D:65:MET:CE	2.26	0.65
1:A:710:G:O2'	1:A:711:G:H5'	1.95	0.65
1:A:2717:C:OP1	5:D:207:LYS:HG3	1.96	0.65
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.78	0.65
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.76	0.65
15:N:74:ARG:CD	15:N:91:ILE:HD12	2.26	0.65
1:A:282:C:H1'	1:A:368:C:N4	2.11	0.65
1:A:522:U:O2'	1:A:1366:C:H5'	1.96	0.65
7:F:49:PRO:HG3	38:F:5828:HOH:O	1.96	0.65
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.77	0.65
11:J:50:VAL:HA	11:J:157:ILE:HG12	1.78	0.65
15:N:138:HIS:ND1	15:N:139:PRO:O	2.26	0.65
23:V:6:CYS:SG	23:V:31:PHE:HA	2.37	0.65
25:X:106:THR:OG1	25:X:109:GLU:HG3	1.97	0.65
1:A:56:G:H5"	24:W:50:ARG:NH1	2.11	0.65
1:A:407:A:H5'	38:A:5513:HOH:O	1.96	0.65
14:M:114:VAL:HG11	38:M:8449:HOH:O	1.96	0.65
15:N:186:SER:O	15:N:189:VAL:HG12	1.95	0.65
16:O:80:SER:HB2	38:O:8534:HOH:O	1.96	0.65
24:W:4:HIS:HB3	38:W:6622:HOH:O	1.95	0.65
1:A:1416:G:H1'	38:A:8527:HOH:O	1.95	0.65
1:A:1909:A:H2'	1:A:1910:A:C8	2.31	0.65
4:C:55:VAL:HG13	4:C:67:LEU:HD22	1.77	0.65
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.79	0.65
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.94	0.65
1:A:2243:C:H5"	38:A:3248:HOH:O	1.97	0.65
1:A:2346:C:O3'	7:F:52:THR:HG23	1.97	0.65
2:B:3029:C:C2'	2:B:3030:C:H5'	2.27	0.65
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.27	0.65
31:4:44:SER:HA	31:4:49:ASP:OD1	1.97	0.65
1:A:514:G:H8	1:A:514:G:O5'	1.80	0.65
1:A:645:U:OP2	14:M:4:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.62	0.65
7:F:140:ARG:N	38:F:3723:HOH:O	2.27	0.64
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.12	0.64
16:O:170:GLU:O	16:O:174:GLU:HG3	1.97	0.64
1:A:2359:G:H3'	38:A:5173:HOH:O	1.97	0.64
14:M:143:THR:HG21	38:M:8413:HOH:O	1.97	0.64
20:S:39:THR:HG23	20:S:107:GLU:O	1.97	0.64
1:A:316:A:H5'	22:U:54:ASP:OD2	1.96	0.64
1:A:1191:A:C3'	1:A:1192:A:H5"	2.28	0.64
38:A:6888:HOH:O	22:U:9:LYS:HB2	1.96	0.64
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.78	0.64
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.09	0.64
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.80	0.64
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.28	0.64
1:A:2597:U:H2'	1:A:2598:U:H5'	1.79	0.64
17:P:42:GLU:HB2	38:P:2176:HOH:O	1.97	0.64
18:Q:143:ALA:HA	38:Q:5521:HOH:O	1.97	0.64
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.80	0.64
27:Z:186:ARG:HG2	27:Z:186:ARG:HH11	1.62	0.64
31:4:3:MET:O	31:4:90:PHE:HA	1.96	0.64
1:A:1829:A:H5"	38:A:9585:HOH:O	1.97	0.64
1:A:2549:C:H1'	5:D:248:ARG:NH2	2.13	0.64
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.80	0.64
17:P:26:TRP:HB2	38:P:3062:HOH:O	1.98	0.64
25:X:72:PRO:O	38:X:7874:HOH:O	2.15	0.64
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.79	0.64
1:A:2608:C:H3'	38:A:7277:HOH:O	1.98	0.64
16:O:154:LEU:O	16:O:155:GLU:HB3	1.96	0.64
1:A:138:U:H5"	1:A:139:C:OP2	1.97	0.64
1:A:1162:G:H2'	38:A:6057:HOH:O	1.97	0.64
1:A:1929:G:H1'	38:A:4641:HOH:O	1.98	0.64
1:A:2310:G:OP2	11:J:114:PRO:HD2	1.98	0.64
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.27	0.64
31:4:7:PHE:HE2	31:4:22:VAL:CG2	2.11	0.64
1:A:339:A:H2'	38:A:3705:HOH:O	1.98	0.64
1:A:2281:C:C2'	1:A:2282:U:H5'	2.27	0.64
2:B:3064:C:C2'	2:B:3065:A:H5'	2.28	0.64
7:F:27:ILE:HG22	7:F:28:GLY:N	2.13	0.64
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.79	0.64
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.38	0.64
31:4:57:GLY:HA2	38:4:8528:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2265:U:H2'	1:A:2266:A:H8	1.61	0.63
1:A:2415:A:H2'	1:A:2416:G:H5'	1.78	0.63
1:A:2524:G:H21	1:A:2526:C:N4	1.95	0.63
2:B:3024:U:O2'	2:B:3025:G:H4'	1.97	0.63
4:C:179:MET:HG2	4:C:186:TRP:HB2	1.79	0.63
15:N:69:LYS:HG2	15:N:127:LYS:HG3	1.80	0.63
25:X:65:VAL:HA	25:X:68:THR:HG22	1.80	0.63
1:A:281:U:H2'	1:A:282:C:O4'	1.98	0.63
1:A:1942:A:O2'	1:A:1943:C:H5'	1.98	0.63
4:C:43:VAL:HG21	4:C:59:GLU:HG3	1.78	0.63
5:D:51:VAL:HG13	5:D:53:LEU:HD13	1.79	0.63
8:G:20:ILE:HD11	8:G:40:VAL:CG1	2.28	0.63
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.63
16:O:164:ASP:CG	16:O:167:ASP:HA	2.19	0.63
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.78	0.63
28:1:10:ARG:HA	38:1:8414:HOH:O	1.98	0.63
38:A:9125:HOH:O	9:H:38:LYS:HD2	1.97	0.63
2:B:3023:U:H5"	2:B:3023:U:C6	2.33	0.63
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.79	0.63
10:I:16:LYS:O	10:I:20:VAL:HG23	1.97	0.63
28:1:46:LYS:HB3	38:1:8436:HOH:O	1.97	0.63
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.79	0.63
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.33	0.63
38:O:8540:HOH:O	19:R:19:ARG:HD3	1.97	0.63
17:P:21:SER:CB	17:P:106:PRO:O	2.47	0.63
1:A:656:G:OP2	17:P:37:ARG:HD2	1.98	0.63
1:A:1185:U:H5'	38:A:6934:HOH:O	1.99	0.63
1:A:1210:G:O2'	1:A:1211:G:H5'	1.98	0.63
1:A:2325:C:H1'	38:A:3637:HOH:O	1.97	0.63
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.28	0.63
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.81	0.63
8:G:133:VAL:HG12	8:G:141:VAL:HG13	1.80	0.63
9:H:110:GLU:O	9:H:114:LYS:HG3	1.99	0.63
30:3:41:HIS:N	30:3:45:ASN:HD22	1.92	0.63
1:A:1641:A:H2'	1:A:1642:A:H5'	1.81	0.63
2:B:3047:A:H4'	38:O:8549:HOH:O	1.98	0.63
1:A:95:A:H5"	1:A:97:G:O4'	1.98	0.63
1:A:1701:A:H5'	38:A:5769:HOH:O	1.97	0.63
38:A:6922:HOH:O	5:D:211:THR:HG21	1.97	0.63
7:F:136:ARG:HD2	7:F:155:HIS:O	1.98	0.63
8:G:11:VAL:HG11	8:G:22:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:74:ARG:HD3	15:N:91:ILE:HD12	1.81	0.63
1:A:182:G:H4'	15:N:157:LEU:HD13	1.81	0.63
1:A:195:C:H5"	38:N:8599:HOH:O	1.97	0.63
7:F:81:GLU:O	7:F:85:GLN:HG3	1.98	0.63
12:K:133:GLY:O	12:K:137:GLU:HG3	1.99	0.63
1:A:218:C:P	31:4:39:GLN:HE21	2.20	0.63
1:A:2501:G:N7	38:A:9280:HOH:O	2.31	0.63
25:X:110:GLN:HA	25:X:110:GLN:NE2	2.13	0.63
25:X:154:ARG:C	38:X:4276:HOH:O	2.37	0.63
4:C:101:GLU:OE2	4:C:131:HIS:HB2	1.99	0.62
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.81	0.62
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.13	0.62
16:O:82:TYR:C	16:O:82:TYR:CD2	2.73	0.62
31:4:73:GLU:HB3	38:4:8561:HOH:O	1.98	0.62
1:A:1741:U:H5'	1:A:1742:A:OP1	1.99	0.62
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.80	0.62
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.28	0.62
17:P:4:ASN:HB2	38:P:6939:HOH:O	1.98	0.62
24:W:12:THR:HG22	24:W:15:GLU:CG	2.18	0.62
14:M:66:VAL:HG23	14:M:67:ARG:N	2.14	0.62
24:W:39:ALA:C	24:W:41:GLU:H	2.01	0.62
1:A:12:U:H2'	1:A:13:G:H5'	1.81	0.62
1:A:2365:G:H4'	19:R:45:PRO:O	2.00	0.62
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.81	0.62
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.32	0.62
14:M:12:THR:HG21	14:M:16:GLY:O	1.99	0.62
22:U:38:ARG:HH11	22:U:38:ARG:HG3	1.63	0.62
1:A:2459:G:P	31:4:64:LYS:HB2	2.40	0.62
4:C:73:GLY:N	28:1:65:ALA:O	2.21	0.62
7:F:37:ALA:O	7:F:40:ILE:HG12	1.99	0.62
22:U:48:VAL:HG22	22:U:97:ARG:C	2.20	0.62
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.81	0.62
16:O:32:PRO:HD2	16:O:99:GLU:O	2.00	0.62
16:O:91:ARG:HG3	16:O:186:LEU:HD23	1.82	0.62
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.80	0.62
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.30	0.62
17:P:35:LYS:HD3	38:P:3360:HOH:O	1.99	0.62
21:T:51:GLN:HE21	21:T:53:ASN:ND2	1.97	0.62
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.35	0.62
1:A:2256:G:O2'	1:A:2257:G:H5'	1.98	0.62
1:A:2470:A:H5"	38:A:9742:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:224:LYS:NZ	38:D:8551:HOH:O	2.33	0.62
6:E:166:ILE:HG23	6:E:208:ALA:HB3	1.82	0.62
22:U:20:HIS:ND1	22:U:41:ARG:NE	2.38	0.62
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.12	0.62
1:A:855:U:H5"	38:A:3129:HOH:O	1.98	0.62
1:A:1165:G:OP1	1:A:1165:G:C3'	2.43	0.62
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.30	0.62
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.81	0.62
16:O:73:ALA:N	38:O:8563:HOH:O	2.32	0.62
25:X:88:THR:HG22	25:X:89:ASP:H	1.64	0.62
25:X:54:PHE:CZ	25:X:140:LYS:HB2	2.35	0.62
1:A:1316:G:H1'	1:A:1340:G:N2	2.15	0.61
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.29	0.61
14:M:143:THR:HG22	14:M:144:ASP:N	2.15	0.61
15:N:60:ILE:HG12	15:N:134:ILE:HD12	1.81	0.61
1:A:338:C:H4'	6:E:174:ILE:CD1	2.30	0.61
1:A:669:G:O2'	1:A:670:G:H5'	2.00	0.61
1:A:2031:C:O3'	38:A:3995:HOH:O	2.16	0.61
1:A:2432:C:C1'	38:A:3570:HOH:O	2.47	0.61
7:F:50:VAL:O	7:F:71:ALA:HA	2.00	0.61
9:H:46:GLU:N	38:H:3461:HOH:O	2.33	0.61
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.15	0.61
1:A:1901:G:O2'	1:A:1902:G:H5'	2.00	0.61
1:A:2635:A:O2'	1:A:2636:C:H5'	2.00	0.61
1:A:2712:G:H5'	38:A:4706:HOH:O	2.01	0.61
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.66	0.61
1:A:57:C:H5"	38:A:6229:HOH:O	1.99	0.61
1:A:316:A:N3	1:A:336:G:O2'	2.33	0.61
2:B:3014:G:H5'	2:B:3014:G:C8	2.34	0.61
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.31	0.61
1:A:960:G:H2'	1:A:960:G:N3	2.16	0.61
8:G:81:GLU:HB3	38:G:4761:HOH:O	2.00	0.61
1:A:1766:U:O2	1:A:1778:A:H5'	2.00	0.61
1:A:2106:C:H5'	1:A:2284:G:H21	1.64	0.61
38:A:7028:HOH:O	31:4:61:PRO:HG2	2.00	0.61
4:C:131:HIS:O	4:C:132:ASP:HB2	1.98	0.61
8:G:3:VAL:CG2	8:G:49:ILE:HB	2.29	0.61
12:K:48:GLY:HA3	12:K:53:ILE:HD11	1.81	0.61
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.14	0.61
1:A:544:G:C2'	1:A:545:G:H5"	2.30	0.61
1:A:1209:C:H2'	1:A:1210:G:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:A:H2'	1:A:1529:G:O4'	2.00	0.61
1:A:2748:G:H2'	38:A:7012:HOH:O	2.01	0.61
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.14	0.61
2:B:3054:A:O2'	2:B:3055:U:H5'	2.01	0.61
23:V:9:CYS:HA	23:V:52:THR:CG2	2.28	0.61
25:X:131:PRO:HB2	38:X:5904:HOH:O	1.98	0.61
31:4:7:PHE:HE2	31:4:22:VAL:HG21	1.64	0.61
17:P:73:ASP:HA	17:P:92:VAL:O	2.01	0.61
27:Z:155:ARG:NH1	38:Z:8560:HOH:O	2.34	0.61
15:N:154:ARG:HG3	38:N:8607:HOH:O	2.01	0.61
1:A:2900:G:H2'	1:A:2901:C:O4'	2.01	0.61
38:A:6692:HOH:O	15:N:13:LYS:HE2	2.00	0.61
2:B:3039:U:H1'	2:B:3044:A:H61	1.66	0.61
16:O:37:ARG:NE	38:O:8532:HOH:O	2.34	0.61
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.82	0.61
1:A:2338:G:H1'	7:F:105:SER:OG	2.01	0.60
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.34	0.60
5:D:7:ARG:HD3	5:D:9:GLY:O	2.01	0.60
6:E:76:ARG:HD3	38:E:8368:HOH:O	2.00	0.60
8:G:77:THR:OG1	8:G:78:GLU:N	2.34	0.60
8:G:100:ASP:HB2	38:G:2789:HOH:O	2.01	0.60
10:I:23:ILE:CD1	10:I:67:LEU:HD23	2.23	0.60
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.49	0.60
17:P:106:PRO:HG2	17:P:107:GLU:OE2	2.01	0.60
23:V:6:CYS:HB2	23:V:32:CYS:HB3	1.82	0.60
1:A:314:G:N2	1:A:316:A:H3'	2.16	0.60
1:A:1211:G:O2'	1:A:1212:C:H5'	2.00	0.60
1:A:2827:A:H2'	1:A:2828:G:O4'	2.00	0.60
4:C:191:GLY:HA2	4:C:194:MET:CE	2.31	0.60
1:A:88:G:H5'	1:A:88:G:H8	1.66	0.60
1:A:1669:A:H2	38:A:3200:HOH:O	1.84	0.60
2:B:3064:C:H2'	2:B:3065:A:H5'	1.81	0.60
4:C:179:MET:HG2	4:C:186:TRP:CG	2.36	0.60
17:P:39:THR:HB	38:P:3360:HOH:O	2.00	0.60
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.49	0.60
4:C:211:LYS:HB2	38:C:8632:HOH:O	2.02	0.60
7:F:95:THR:C	7:F:97:GLN:H	2.05	0.60
11:J:141:ASN:HA	38:J:8355:HOH:O	2.01	0.60
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.16	0.60
14:M:104:ASP:HB2	38:M:8452:HOH:O	2.00	0.60
1:A:2433:A:O3'	31:4:30:GLN:OE1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:10:PHE:CD1	7:F:11:HIS:N	2.69	0.60
7:F:45:THR:HG22	7:F:75:LEU:HD11	1.84	0.60
11:J:30:GLN:H	11:J:65:ARG:NH1	1.98	0.60
38:L:408:HOH:O	23:V:37:GLU:HB3	2.01	0.60
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.81	0.60
28:1:46:LYS:HE2	38:1:8436:HOH:O	2.00	0.60
5:D:24:PRO:HG3	5:D:204:GLY:HA2	1.82	0.60
5:D:36:PRO:HA	5:D:168:GLY:CA	2.32	0.60
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.37	0.60
6:E:219:ASN:O	6:E:222:ASP:OD1	2.20	0.60
9:H:58:GLU:HA	9:H:61:MET:HE2	1.83	0.60
10:I:71:LEU:C	10:I:73:ASP:H	2.05	0.60
11:J:14:TYR:H	11:J:91:HIS:CE1	2.20	0.60
13:L:55:VAL:HG12	13:L:56:SER:H	1.67	0.60
17:P:97:SER:OG	17:P:100:GLN:HG3	2.01	0.60
21:T:22:ASN:ND2	21:T:68:LEU:HB2	2.17	0.60
26:Y:30:MET:HE1	26:Y:55:ASN:HA	1.82	0.60
1:A:558:C:O2'	1:A:559:U:H5"	2.02	0.60
1:A:935:G:H4'	17:P:38:ARG:HH12	1.66	0.60
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.60
1:A:1804:A:H2'	1:A:1805:G:C8	2.36	0.60
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.32	0.60
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.83	0.60
25:X:122:ARG:HG2	25:X:152:ALA:O	2.02	0.60
27:Z:151:SER:HB3	27:Z:154:ARG:HB3	1.84	0.60
1:A:31:C:H4'	38:A:6888:HOH:O	2.02	0.60
1:A:1130:U:H2'	1:A:1131:G:O4'	2.01	0.60
1:A:1434:A:H2'	1:A:1436:C:C5	2.36	0.60
1:A:2832:C:H5'	38:A:6221:HOH:O	2.00	0.60
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.32	0.60
10:I:64:ASN:O	10:I:68:GLU:HG3	2.02	0.60
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.37	0.60
31:4:64:LYS:HE3	31:4:84:ARG:HH12	1.66	0.60
1:A:188:C:H5"	15:N:163:LEU:HD21	1.84	0.60
1:A:280:C:H2'	1:A:281:U:O4'	2.02	0.60
1:A:1353:C:P	38:A:4159:HOH:O	2.60	0.60
1:A:1535:G:H2'	1:A:1536:C:C6	2.37	0.60
2:B:3028:U:H2'	2:B:3029:C:C6	2.36	0.60
12:K:54:VAL:HG11	12:K:138:THR:HG21	1.84	0.60
1:A:558:C:H2'	1:A:559:U:C5'	2.32	0.60
1:A:665:A:H2'	1:A:666:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.35	0.60
1:A:2348:C:H5"	7:F:22:VAL:HG21	1.84	0.60
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.67	0.60
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.83	0.60
23:V:52:THR:HG22	23:V:54:THR:N	2.17	0.60
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.84	0.59
1:A:2381:C:O2'	31:4:10:TYR:HB3	2.02	0.59
9:H:91:VAL:CG1	9:H:92:GLY:H	2.15	0.59
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.83	0.59
22:U:38:ARG:NH1	22:U:38:ARG:HG3	2.16	0.59
25:X:13:MET:CE	25:X:17:ILE:HG22	2.32	0.59
25:X:122:ARG:NH1	25:X:152:ALA:O	2.35	0.59
1:A:1015:C:H2'	1:A:1016:U:C6	2.37	0.59
1:A:2475:C:O2	38:A:9234:HOH:O	2.15	0.59
5:D:48:MET:N	38:D:8564:HOH:O	2.32	0.59
6:E:127:ARG:HG2	6:E:127:ARG:HH11	1.68	0.59
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.32	0.59
14:M:149:ARG:O	14:M:150:GLN:HB2	2.02	0.59
16:O:164:ASP:OD2	16:O:167:ASP:HA	2.02	0.59
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.84	0.59
1:A:1805:G:O2'	1:A:1806:G:H5'	2.02	0.59
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.35	0.59
1:A:2502:C:C2'	1:A:2503:A:H5'	2.32	0.59
7:F:128:LEU:N	38:F:5495:HOH:O	2.35	0.59
8:G:127:ASP:HB3	38:G:6772:HOH:O	2.01	0.59
31:4:64:LYS:CE	31:4:84:ARG:HH12	2.16	0.59
1:A:182:G:H5'	38:A:4640:HOH:O	2.01	0.59
1:A:383:A:H4'	38:A:4810:HOH:O	2.01	0.59
1:A:399:C:H5'	15:N:179:GLY:O	2.02	0.59
1:A:2472:C:O2'	1:A:2634:G:H4'	2.02	0.59
1:A:2866:U:H4'	1:A:2867:G:H5'	1.83	0.59
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.84	0.59
11:J:27:LYS:N	11:J:58:HIS:HD2	1.91	0.59
17:P:30:ALA:O	17:P:34:GLU:HG3	2.02	0.59
25:X:84:VAL:HG12	38:X:6679:HOH:O	2.02	0.59
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.31	0.59
1:A:31:C:H2'	38:A:7160:HOH:O	2.02	0.59
1:A:1209:C:H4'	38:A:4763:HOH:O	2.00	0.59
9:H:28:ALA:CB	9:H:99:THR:HG23	2.31	0.59
11:J:71:TYR:C	11:J:73:GLN:H	2.06	0.59
11:J:136:VAL:HG23	38:J:8331:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:136:ALA:HB3	38:M:8449:HOH:O	2.02	0.59
23:V:6:CYS:HG	23:V:31:PHE:HA	1.68	0.59
1:A:709:G:O2'	17:P:25:VAL:HG12	2.03	0.59
1:A:1470:A:OP1	15:N:93:ARG:HD2	2.03	0.59
1:A:2434:A:OP1	31:4:30:GLN:HG2	2.02	0.59
6:E:115:LEU:HD13	6:E:223:LEU:CD2	2.19	0.59
6:E:127:ARG:HH21	6:E:225:PRO:HG2	1.65	0.59
12:K:19:MET:CE	12:K:132:LEU:HD11	2.32	0.59
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.84	0.59
25:X:65:VAL:HG12	25:X:116:LEU:HD13	1.85	0.59
1:A:119:A:H2'	1:A:120:A:C5'	2.33	0.59
1:A:328:U:O4'	6:E:202:THR:HG22	2.03	0.59
1:A:821:U:H2'	1:A:822:C:C6	2.37	0.59
1:A:1773:G:O2'	28:1:15:GLY:HA2	2.03	0.59
2:B:3107:C:C5	38:B:8439:HOH:O	2.49	0.59
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.84	0.59
16:O:154:LEU:HD11	16:O:157:PRO:HA	1.84	0.59
20:S:82:GLU:HG3	20:S:83:LYS:N	2.18	0.59
28:1:38:LYS:HG3	38:1:8426:HOH:O	2.02	0.59
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.42	0.59
31:4:35:TRP:HA	31:4:38:ARG:NH1	2.18	0.59
1:A:1771:U:O3'	28:1:23:ARG:NH2	2.35	0.59
9:H:38:LYS:HZ1	15:N:3:SER:HA	1.68	0.59
11:J:75:SER:C	11:J:79:ALA:HB2	2.23	0.59
12:K:15:ARG:NH1	12:K:43:ARG:NH1	2.50	0.59
15:N:184:ARG:HB2	15:N:184:ARG:NH1	2.18	0.59
23:V:52:THR:CG2	23:V:54:THR:HB	2.32	0.59
26:Y:85:VAL:HG12	26:Y:86:GLU:H	1.67	0.59
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.37	0.59
1:A:1652:C:O2	4:C:164:ARG:HD2	2.02	0.59
4:C:199:HIS:CD2	4:C:201:PHE:H	2.20	0.59
5:D:258:GLY:HA2	38:D:8563:HOH:O	2.03	0.59
1:A:2524:G:H21	1:A:2526:C:H41	1.50	0.59
1:A:2578:G:H5'	1:A:2578:G:C8	2.37	0.59
1:A:2620:U:O4	36:5:76:PPU:C	2.51	0.59
38:A:5781:HOH:O	7:F:99:ASP:HA	2.03	0.59
9:H:91:VAL:CG1	9:H:92:GLY:N	2.65	0.59
11:J:59:ASN:H	11:J:59:ASN:ND2	2.01	0.59
22:U:61:GLU:HG3	38:U:3851:HOH:O	2.02	0.59
29:2:10:LYS:HG3	38:2:2979:HOH:O	2.03	0.59
1:A:625:U:H5"	1:A:1044:C:N4	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:G:C5	1:A:686:A:C2	2.91	0.58
1:A:1119:G:H22	1:A:1246:A:H2	1.46	0.58
1:A:2445:U:H2'	1:A:2446:G:C8	2.38	0.58
1:A:2897:C:H2'	1:A:2898:G:H8	1.66	0.58
5:D:145:HIS:HD2	5:D:146:THR:O	1.85	0.58
7:F:128:LEU:HD23	7:F:128:LEU:C	2.24	0.58
7:F:140:ARG:O	7:F:144:ARG:HG2	2.02	0.58
8:G:166:VAL:HB	38:G:6341:HOH:O	2.03	0.58
13:L:28:GLU:OE2	13:L:58:THR:HG21	2.02	0.58
15:N:57:LYS:HE2	15:N:140:ALA:O	2.03	0.58
23:V:52:THR:HA	38:V:6796:HOH:O	2.02	0.58
1:A:329:A:OP2	6:E:206:ASN:HB2	2.03	0.58
1:A:1596:U:H2'	1:A:1598:A:OP2	2.02	0.58
1:A:2507:G:H2'	1:A:2510:C:H42	1.67	0.58
38:A:3966:HOH:O	31:4:51:LYS:HB2	2.02	0.58
1:A:245:C:H2'	38:A:5052:HOH:O	2.04	0.58
1:A:426:G:H5"	38:A:7097:HOH:O	2.02	0.58
1:A:2443:C:H3'	38:A:9967:HOH:O	2.03	0.58
6:E:236:THR:HG21	38:E:8374:HOH:O	2.03	0.58
7:F:146:LYS:NZ	16:O:107:ASN:HD21	2.02	0.58
13:L:55:VAL:HG12	13:L:56:SER:N	2.18	0.58
20:S:44:VAL:HG13	20:S:89:LEU:HD22	1.85	0.58
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.33	0.58
1:A:869:G:H1'	38:A:9812:HOH:O	2.01	0.58
1:A:2387:U:H2'	1:A:2388:C:C6	2.37	0.58
1:A:2912:C:OP2	38:A:5034:HOH:O	2.16	0.58
5:D:14:GLY:HA2	5:D:15:PRO:C	2.23	0.58
15:N:102:GLU:OE1	15:N:164:THR:HG21	2.04	0.58
19:R:93:ARG:HG3	19:R:93:ARG:NH1	2.18	0.58
1:A:120:A:H2'	1:A:120:A:N3	2.19	0.58
1:A:2469:A:OP2	38:A:6942:HOH:O	2.17	0.58
6:E:1:MET:HG2	6:E:2:GLN:N	2.18	0.58
8:G:12:ASP:HA	38:G:1750:HOH:O	2.03	0.58
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.18	0.58
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.19	0.58
15:N:48:ARG:NH1	38:N:8610:HOH:O	2.36	0.58
22:U:47:THR:HB	22:U:100:ASP:HB3	1.85	0.58
1:A:2094:G:H4'	5:D:245:SER:HB3	1.85	0.58
1:A:2727:A:C2'	1:A:2728:C:H5'	2.32	0.58
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.86	0.58
8:G:114:ARG:HA	38:G:3388:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:57:ARG:HH11	11:J:57:ARG:HG3	1.69	0.58
16:O:58:LEU:HD12	16:O:58:LEU:N	2.17	0.58
1:A:660:A:H4'	1:A:661:G:O5'	2.03	0.58
1:A:1763:C:O2'	1:A:1764:C:H5'	2.03	0.58
1:A:2419:U:H5"	1:A:2420:G:H5'	1.85	0.58
5:D:238:ASN:ND2	5:D:240:GLY:N	2.49	0.58
14:M:145:LEU:O	14:M:148:GLU:HG3	2.04	0.58
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.67	0.58
20:S:119:VAL:O	20:S:119:VAL:HG12	2.03	0.58
28:1:30:GLU:HA	28:1:33:HIS:CB	2.31	0.58
31:4:87:ARG:HD2	38:4:8526:HOH:O	2.04	0.58
1:A:2834:G:OP1	26:Y:39:LYS:HE2	2.04	0.58
11:J:117:LYS:O	11:J:119:VAL:HG13	2.03	0.58
12:K:142:ASN:O	12:K:144:THR:N	2.36	0.58
15:N:14:ARG:HB3	15:N:17:GLU:CG	2.34	0.58
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.04	0.58
17:P:59:VAL:HG23	17:P:111:VAL:HG23	1.85	0.58
22:U:2:LYS:HE2	38:U:7214:HOH:O	2.03	0.58
1:A:1497:G:H2'	1:A:1498:G:H8	1.69	0.58
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.86	0.58
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.33	0.58
7:F:166:ILE:HD12	38:F:6326:HOH:O	2.03	0.58
10:I:12:ILE:HB	38:I:4714:HOH:O	2.04	0.58
11:J:127:GLY:O	11:J:128:ALA:HB3	2.03	0.58
17:P:77:ALA:HB1	17:P:98:LEU:HD12	1.85	0.58
31:4:64:LYS:CE	31:4:84:ARG:NH1	2.67	0.58
1:A:251:C:H1'	15:N:58:GLN:HE22	1.67	0.58
1:A:263:U:O4'	9:H:59:ILE:HD13	2.03	0.58
1:A:1827:G:H2'	1:A:1828:G:C8	2.38	0.58
6:E:16:VAL:HG12	6:E:17:ASP:N	2.18	0.58
8:G:108:LEU:HD11	8:G:164:ASP:HB2	1.85	0.58
15:N:186:SER:OG	15:N:189:VAL:HG12	2.03	0.58
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.39	0.58
28:1:29:VAL:O	28:1:33:HIS:HB2	2.04	0.58
1:A:2382:A:OP1	31:4:80:ARG:HG2	2.03	0.57
2:B:3064:C:O2'	2:B:3065:A:H5'	2.03	0.57
4:C:72:GLU:HG3	28:1:66:GLY:HA2	1.86	0.57
5:D:253:GLN:HA	38:D:8629:HOH:O	2.04	0.57
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.33	0.57
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.86	0.57
27:Z:133:HIS:HD2	38:Z:8584:HOH:O	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:C:H2'	1:A:559:U:H5'	1.87	0.57
1:A:1189:A:H1'	1:A:1209:C:C1'	2.35	0.57
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.85	0.57
38:B:8391:HOH:O	16:O:7:LYS:HE2	2.02	0.57
5:D:55:ASN:HB3	5:D:63:GLU:CA	2.33	0.57
6:E:27:ARG:HD2	6:E:29:ASP:OD1	2.04	0.57
7:F:102:GLY:O	7:F:134:LEU:HD12	2.04	0.57
7:F:170:TYR:O	7:F:171:ASP:HB3	2.04	0.57
10:I:16:LYS:NZ	38:I:5575:HOH:O	2.20	0.57
14:M:73:VAL:HG23	14:M:74:THR:N	2.20	0.57
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.19	0.57
25:X:88:THR:HG22	25:X:89:ASP:N	2.19	0.57
1:A:1456:C:H2'	1:A:1457:U:C6	2.38	0.57
1:A:2898:G:H4'	5:D:288:GLY:HA2	1.84	0.57
6:E:7:ASP:OD1	6:E:11:ASN:O	2.23	0.57
8:G:101:GLU:HB2	8:G:116:THR:O	2.04	0.57
25:X:13:MET:HE1	25:X:18:GLN:HA	1.85	0.57
1:A:121:U:OP2	30:3:10:ARG:NH2	2.36	0.57
1:A:793:A:H5"	18:Q:83:LYS:HG2	1.86	0.57
1:A:1733:A:H4'	5:D:212:GLN:HA	1.85	0.57
1:A:2349:G:OP1	7:F:20:LYS:NZ	2.32	0.57
1:A:2526:C:C2'	1:A:2527:U:H5'	2.34	0.57
6:E:191:SER:OG	6:E:192:ILE:N	2.36	0.57
8:G:81:GLU:HG2	8:G:134:SER:CB	2.34	0.57
8:G:118:ILE:HG23	8:G:144:THR:HG21	1.85	0.57
29:2:45:ARG:NH2	38:2:2086:HOH:O	2.18	0.57
1:A:484:A:N1	1:A:506:G:H4'	2.18	0.57
1:A:542:A:H5'	1:A:542:A:C8	2.31	0.57
1:A:1624:A:H5'	1:A:1626:A:O4'	2.05	0.57
1:A:2672:C:P	5:D:25:ARG:NH1	2.77	0.57
1:A:2729:C:H2'	1:A:2730:G:H8	1.69	0.57
38:A:5395:HOH:O	15:N:189:VAL:HG23	2.03	0.57
5:D:162:MET:CE	5:D:310:ARG:HD3	2.34	0.57
7:F:10:PHE:CE1	7:F:11:HIS:HB3	2.39	0.57
15:N:52:LEU:HD21	38:N:8610:HOH:O	2.05	0.57
15:N:164:THR:HG23	15:N:165:SER:N	2.20	0.57
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	2.04	0.57
31:4:70:ARG:HD3	38:4:8541:HOH:O	2.05	0.57
1:A:2385:G:H2'	1:A:2386:U:C6	2.40	0.57
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.05	0.57
3:5:74:C:H2'	3:5:75:C:C5'	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:11:HIS:C	7:F:13:MET:H	2.08	0.57
17:P:25:VAL:HG23	17:P:26:TRP:N	2.19	0.57
26:Y:23:HIS:HA	26:Y:64:ALA:HB2	1.86	0.57
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.18	0.57
1:A:542:A:H2'	1:A:543:G:O4'	2.05	0.57
1:A:656:G:H5'	17:P:3:THR:HB	1.86	0.57
1:A:2769:C:H2'	1:A:2770:G:O4'	2.04	0.57
6:E:118:THR:HG22	6:E:137:PRO:HB3	1.86	0.57
11:J:163:PRO:HG2	38:J:8326:HOH:O	2.03	0.57
17:P:44:ASN:OD1	17:P:65:LEU:HB2	2.05	0.57
22:U:64:ASN:HA	38:U:5927:HOH:O	2.04	0.57
23:V:13:ILE:HG12	23:V:32:CYS:CB	2.34	0.57
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.14	0.57
1:A:449:A:N7	6:E:43:LYS:HG2	2.19	0.57
1:A:1206:U:H6	1:A:1206:U:H5'	1.67	0.57
1:A:1328:A:C8	27:Z:169:ARG:HD3	2.39	0.57
1:A:2015:A:H2'	1:A:2016:U:O4'	2.04	0.57
5:D:49:THR:HG21	5:D:280:VAL:HG23	1.87	0.57
5:D:274:GLU:HA	5:D:292:GLY:O	2.04	0.57
8:G:15:GLN:HG2	8:G:19:ASP:O	2.05	0.57
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.87	0.57
14:M:7:GLN:HB3	14:M:13:HIS:ND1	2.20	0.57
1:A:283:U:H5"	1:A:284:C:P	2.44	0.57
1:A:2135:A:O2'	1:A:2136:G:H5'	2.04	0.57
1:A:2445:U:H2'	1:A:2446:G:H8	1.69	0.57
5:D:74:ILE:HG22	5:D:76:THR:HG23	1.87	0.57
11:J:39:GLY:O	11:J:41:THR:N	2.38	0.57
16:O:64:SER:C	16:O:66:LEU:H	2.09	0.57
19:R:25:PRO:HB2	38:R:4350:HOH:O	2.04	0.57
1:A:187:A:H3'	1:A:188:C:H6	1.69	0.57
1:A:1441:G:O2'	1:A:1442:A:H5'	2.05	0.57
1:A:1701:A:H4'	38:A:6683:HOH:O	2.05	0.57
1:A:2502:C:H2'	1:A:2503:A:H5'	1.85	0.57
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.57
2:B:3051:A:H5'	16:O:160:SER:HB3	1.87	0.57
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.87	0.57
15:N:23:LEU:O	15:N:26:HIS:HB2	2.04	0.57
16:O:5:ARG:HG3	19:R:18:PRO:HB3	1.86	0.57
21:T:57:THR:C	21:T:59:ASP:H	2.08	0.57
1:A:447:A:OP1	22:U:2:LYS:HG2	2.05	0.56
1:A:870:G:C2'	1:A:871:G:H5"	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:74:C:H2'	3:5:75:C:O4'	2.05	0.56
5:D:55:ASN:CB	5:D:63:GLU:HA	2.32	0.56
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.70	0.56
14:M:34:GLY:HA3	14:M:38:HIS:CE1	2.40	0.56
20:S:33:ARG:NH1	38:S:8543:HOH:O	2.37	0.56
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.18	0.56
1:A:241:A:C2	1:A:378:A:H4'	2.39	0.56
1:A:2783:A:H3'	38:A:4717:HOH:O	2.05	0.56
5:D:162:MET:HE2	5:D:310:ARG:HD3	1.88	0.56
6:E:15:GLU:HG3	38:E:8336:HOH:O	2.05	0.56
9:H:96:ALA:HA	38:H:3111:HOH:O	2.04	0.56
18:Q:115:SER:O	18:Q:117:SER:N	2.39	0.56
23:V:52:THR:HG22	23:V:54:THR:HB	1.86	0.56
31:4:48:ASN:ND2	31:4:50:GLY:H	2.03	0.56
1:A:69:A:H5'	1:A:69:A:H8	1.70	0.56
1:A:155:C:O2'	1:A:156:C:H5'	2.05	0.56
1:A:319:A:H4'	1:A:338:C:C5	2.40	0.56
1:A:646:G:H2'	1:A:647:U:H6	1.71	0.56
1:A:702:G:O2'	1:A:703:G:H5'	2.05	0.56
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.30	0.56
1:A:1173:A:H4'	1:A:1174:A:C8	2.40	0.56
1:A:1189:A:H1'	1:A:1209:C:O4'	2.05	0.56
1:A:1654:U:H5"	38:A:6885:HOH:O	2.04	0.56
1:A:2346:C:H4'	7:F:52:THR:CG2	2.34	0.56
1:A:2777:G:O2'	1:A:2778:A:H5'	2.06	0.56
1:A:2786:G:O2'	1:A:2787:C:H5'	2.04	0.56
1:A:2840:A:OP1	5:D:211:THR:HG23	2.06	0.56
1:A:2911:C:H2'	1:A:2912:C:C6	2.41	0.56
2:B:3010:C:C2	16:O:10:MET:HG2	2.40	0.56
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.34	0.56
4:C:188:ASN:HA	38:C:8580:HOH:O	2.05	0.56
6:E:246:ARG:HB3	6:E:246:ARG:HH11	1.69	0.56
7:F:86:THR:C	7:F:89:PRO:HD2	2.24	0.56
8:G:107:PHE:CZ	8:G:152:THR:HB	2.39	0.56
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.86	0.56
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.21	0.56
11:J:69:ASN:O	11:J:72:VAL:HG12	2.04	0.56
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.33	0.56
13:L:37:TYR:CE2	13:L:45:PRO:HA	2.40	0.56
13:L:49:LEU:HD12	13:L:80:ILE:HD13	1.87	0.56
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:134:GLU:HA	14:M:138:GLY:O	2.05	0.56
15:N:149:TRP:O	15:N:152:ARG:HG2	2.05	0.56
16:O:169:PRO:O	16:O:172:PHE:HB3	2.04	0.56
31:4:75:GLY:HA2	38:4:8560:HOH:O	2.05	0.56
1:A:553:G:H5'	38:A:9992:HOH:O	2.04	0.56
1:A:654:A:H4'	38:A:5065:HOH:O	2.05	0.56
1:A:699:C:C2	1:A:744:G:C2	2.93	0.56
1:A:1835:U:C5	1:A:1840:A:N7	2.67	0.56
1:A:2435:U:P	31:4:28:GLY:HA3	2.45	0.56
2:B:3031:C:O2'	2:B:3032:G:H5'	2.06	0.56
5:D:16:ARG:HB3	5:D:217:ARG:HH21	1.71	0.56
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.35	0.56
6:E:236:THR:H	6:E:239:ALA:HB3	1.70	0.56
10:I:64:ASN:N	10:I:64:ASN:ND2	2.53	0.56
15:N:38:VAL:C	15:N:63:VAL:HG13	2.25	0.56
15:N:169:ARG:HD2	38:N:8584:HOH:O	2.06	0.56
1:A:236:A:H8	1:A:236:A:OP1	1.88	0.56
1:A:1305:C:O2'	1:A:1306:U:H5'	2.04	0.56
1:A:2533:C:H5'	1:A:2533:C:C6	2.37	0.56
13:L:87:ARG:NH1	38:L:4066:HOH:O	2.39	0.56
16:O:80:SER:CB	38:O:8534:HOH:O	2.53	0.56
16:O:159:TYR:CE2	16:O:163:PHE:HE2	2.24	0.56
31:4:69:TYR:CB	31:4:78:HIS:CE1	2.89	0.56
1:A:1184:C:H1'	38:A:6934:HOH:O	2.04	0.56
1:A:2316:G:H2'	38:A:4394:HOH:O	2.04	0.56
1:A:2324:G:H4'	1:A:2418:G:O2'	2.05	0.56
5:D:129:ARG:NH2	5:D:176:ASP:OD1	2.38	0.56
7:F:11:HIS:O	7:F:12:GLU:HB3	2.05	0.56
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.87	0.56
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.70	0.56
16:O:73:ALA:HB1	16:O:74:PRO:HD2	1.87	0.56
27:Z:142:SER:OG	38:Z:8618:HOH:O	2.18	0.56
1:A:69:A:H5'	1:A:69:A:C8	2.40	0.56
1:A:1701:A:H4'	1:A:1702:U:C5'	2.35	0.56
1:A:1829:A:N6	28:1:18:TYR:HA	2.21	0.56
1:A:2780:C:C1'	8:G:143:GLN:HE21	2.17	0.56
4:C:132:ASP:OD1	4:C:133:ARG:N	2.38	0.56
7:F:105:SER:CB	7:F:131:THR:HG23	2.31	0.56
16:O:114:LYS:O	16:O:117:ALA:HB3	2.05	0.56
17:P:107:GLU:OE1	17:P:107:GLU:N	2.39	0.56
21:T:51:GLN:NE2	21:T:53:ASN:HD21	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:23:VAL:HG23	22:U:41:ARG:HG3	1.87	0.56
28:1:31:ILE:O	28:1:35:LYS:HG3	2.05	0.56
29:2:28:HIS:HD2	29:2:30:LYS:H	1.54	0.56
1:A:42:C:H1'	38:A:4156:HOH:O	2.05	0.56
1:A:1395:C:H2'	1:A:1396:C:C6	2.41	0.56
1:A:1753:C:O2	5:D:229:ARG:NH2	2.34	0.56
1:A:1773:G:C8	28:1:16:PRO:CA	2.89	0.56
1:A:1829:A:H61	28:1:18:TYR:HA	1.70	0.56
4:C:51:ARG:HB2	38:C:8621:HOH:O	2.05	0.56
5:D:144:THR:HG22	5:D:145:HIS:H	1.71	0.56
6:E:54:LEU:HD21	6:E:87:ARG:HD2	1.86	0.56
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.71	0.56
16:O:151:ASP:O	16:O:154:LEU:HB2	2.06	0.56
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.88	0.56
1:A:195:C:C2'	1:A:196:G:H5'	2.35	0.56
1:A:1168:C:O2'	38:A:5850:HOH:O	2.18	0.56
1:A:1717:A:H5"	18:Q:54:LYS:HB2	1.87	0.56
38:A:3943:HOH:O	15:N:146:GLN:HG2	2.05	0.56
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.71	0.56
12:K:79:PHE:O	12:K:83:ILE:HG13	2.06	0.56
16:O:87:LEU:CD1	16:O:186:LEU:HD21	2.32	0.56
1:A:113:A:OP2	1:A:114:A:H5"	2.06	0.56
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.41	0.56
5:D:254:GLN:HG2	5:D:255:GLY:N	2.21	0.56
5:D:336:GLN:NE2	38:D:8526:HOH:O	2.38	0.56
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.87	0.56
16:O:141:ARG:HB3	38:O:8566:HOH:O	2.06	0.56
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.69	0.56
18:Q:120:ARG:NH2	18:Q:123:TYR:CD2	2.74	0.56
23:V:6:CYS:CA	23:V:13:ILE:HD11	2.34	0.56
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.05	0.56
1:A:201:G:N2	35:A:8505:CL:CL	2.72	0.55
1:A:299:U:H5'	38:A:6805:HOH:O	2.05	0.55
1:A:1118:A:H8	1:A:1119:G:H5"	1.71	0.55
1:A:1127:C:C2'	1:A:1128:U:H5'	2.36	0.55
1:A:2124:G:H2'	1:A:2125:G:C8	2.41	0.55
1:A:2612:A:H4'	38:A:3180:HOH:O	2.06	0.55
5:D:55:ASN:HB3	5:D:64:GLY:H	1.72	0.55
1:A:218:C:P	31:4:39:GLN:NE2	2.79	0.55
1:A:776:A:OP1	29:2:28:HIS:HE1	1.89	0.55
1:A:1330:A:H5"	1:A:1331:A:OP2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3025:G:C3'	2:B:3026:C:H5'	2.32	0.55
16:O:71:TRP:N	38:O:8537:HOH:O	2.38	0.55
16:O:141:ARG:N	38:O:8566:HOH:O	2.38	0.55
22:U:72:ILE:HD13	22:U:93:THR:HG22	1.88	0.55
1:A:545:G:H5'	1:A:545:G:C8	2.34	0.55
1:A:876:A:N3	1:A:876:A:H2'	2.21	0.55
1:A:2453:G:H4'	14:M:50:GLY:C	2.27	0.55
5:D:49:THR:HG21	5:D:280:VAL:CG2	2.36	0.55
7:F:10:PHE:CG	7:F:11:HIS:N	2.74	0.55
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.72	0.55
15:N:37:VAL:HG21	15:N:108:LYS:HG3	1.87	0.55
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.42	0.55
1:A:1116:U:O2'	1:A:1118:A:C2	2.50	0.55
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.20	0.55
6:E:49:ASP:HB3	6:E:52:ALA:HB2	1.87	0.55
1:A:1134:G:H4'	11:J:151:MET:CE	2.29	0.55
1:A:1331:A:OP2	27:Z:142:SER:OG	2.25	0.55
1:A:1379:A:H3'	38:A:8730:HOH:O	2.05	0.55
1:A:2346:C:O5'	1:A:2346:C:H6	1.90	0.55
38:A:8836:HOH:O	25:X:9:GLY:HA3	2.05	0.55
3:5:75:C:N4	36:5:76:PPU:H102	2.22	0.55
8:G:81:GLU:HA	8:G:133:VAL:O	2.07	0.55
9:H:34:ASN:O	9:H:38:LYS:HG3	2.06	0.55
17:P:45:LEU:CD1	17:P:88:LYS:HD2	2.37	0.55
27:Z:130:ARG:HD2	38:Z:8554:HOH:O	2.07	0.55
31:4:24:LYS:HE2	35:4:8504:CL:CL	2.42	0.55
1:A:1191:A:H3'	1:A:1192:A:C5'	2.35	0.55
7:F:69:ILE:HG22	7:F:69:ILE:O	2.07	0.55
8:G:114:ARG:HB3	8:G:151:LEU:HD11	1.89	0.55
11:J:149:ALA:C	11:J:151:MET:H	2.08	0.55
14:M:77:ALA:HB3	38:M:8403:HOH:O	2.06	0.55
31:4:31:THR:HB	31:4:33:MET:HE3	1.85	0.55
1:A:240:C:C5'	15:N:146:GLN:NE2	2.70	0.55
1:A:721:A:H2'	1:A:722:G:H5'	1.87	0.55
1:A:2421:G:H1'	38:A:6491:HOH:O	2.05	0.55
38:A:4026:HOH:O	11:J:151:MET:HE2	2.06	0.55
7:F:23:VAL:HG12	7:F:130:VAL:HG22	1.87	0.55
7:F:58:VAL:HG12	7:F:59:GLY:N	2.22	0.55
13:L:40:THR:O	13:L:41:LYS:C	2.45	0.55
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.36	0.55
16:O:143:ARG:NH1	16:O:173:ASP:OD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1395:C:H2'	1:A:1396:C:H6	1.72	0.55
1:A:2100:A:H5'	38:E:8461:HOH:O	2.07	0.55
38:A:3782:HOH:O	27:Z:208:LYS:HD2	2.06	0.55
4:C:105:VAL:HG12	4:C:106:CYS:H	1.72	0.55
5:D:258:GLY:H	5:D:260:HIS:HE1	1.51	0.55
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.07	0.55
14:M:104:ASP:O	14:M:105:TYR:HB3	2.07	0.55
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.07	0.55
1:A:2385:G:H2'	1:A:2386:U:H6	1.72	0.55
4:C:168:PRO:O	4:C:170:VAL:HG23	2.06	0.55
5:D:85:ARG:NH1	38:D:8642:HOH:O	2.40	0.55
7:F:169:THR:C	7:F:170:TYR:HD1	2.10	0.55
18:Q:41:ARG:O	18:Q:44:VAL:HB	2.07	0.55
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.36	0.55
20:S:132:ARG:CZ	38:S:8582:HOH:O	2.54	0.55
20:S:132:ARG:HG2	20:S:133:ALA:N	2.22	0.55
27:Z:145:LYS:NZ	38:Z:8570:HOH:O	2.35	0.55
1:A:283:U:H5"	1:A:284:C:OP2	2.07	0.55
1:A:332:G:H4'	22:U:2:LYS:O	2.07	0.55
1:A:1589:G:H22	1:A:1605:G:H1'	1.70	0.55
1:A:1942:A:H3'	38:A:6813:HOH:O	2.07	0.55
1:A:2301:A:H5"	1:A:2302:A:H5'	1.89	0.55
38:A:3481:HOH:O	22:U:82:THR:HA	2.07	0.55
4:C:170:VAL:HG11	28:1:14:PHE:CZ	2.42	0.55
6:E:233:THR:HG22	6:E:234:VAL:N	2.22	0.55
17:P:4:ASN:HB3	17:P:7:LEU:HB3	1.87	0.55
25:X:80:ASP:O	25:X:84:VAL:HG23	2.07	0.55
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.07	0.55
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.05	0.55
1:A:245:C:C2'	1:A:246:G:H5'	2.37	0.54
1:A:295:C:O2'	1:A:296:G:H5'	2.07	0.54
1:A:1269:G:H2'	1:A:1270:U:C6	2.42	0.54
1:A:1641:A:C2'	1:A:1642:A:H5'	2.37	0.54
1:A:2276:U:H2'	1:A:2277:U:C6	2.42	0.54
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.40	0.54
5:D:62:ARG:CA	5:D:65:MET:HE3	2.36	0.54
7:F:55:LYS:HA	38:F:6752:HOH:O	2.06	0.54
9:H:36:THR:HG23	9:H:97:ALA:HB2	1.89	0.54
13:L:87:ARG:CZ	38:L:4854:HOH:O	2.55	0.54
15:N:46:LEU:HB2	38:N:8601:HOH:O	2.07	0.54
16:O:119:GLN:O	16:O:123:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:73:LEU:O	25:X:74:GLU:HG3	2.07	0.54
28:1:13:ARG:NH1	38:1:8418:HOH:O	2.40	0.54
31:4:60:LYS:CG	31:4:61:PRO:HD2	2.37	0.54
1:A:558:C:C2'	1:A:559:U:H5"	2.37	0.54
1:A:1321:A:N3	38:A:9722:HOH:O	2.33	0.54
1:A:2421:G:H4'	38:A:4264:HOH:O	2.06	0.54
1:A:2763:G:H5'	38:A:8916:HOH:O	2.07	0.54
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.42	0.54
9:H:101:ALA:HB2	9:H:108:LEU:CD2	2.37	0.54
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.55	0.54
17:P:21:SER:OG	17:P:106:PRO:HB2	2.07	0.54
20:S:34:GLU:OE1	20:S:34:GLU:HA	2.07	0.54
24:W:49:LEU:O	24:W:53:ILE:HG13	2.07	0.54
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.88	0.54
29:2:20:ARG:HB2	38:2:513:HOH:O	2.05	0.54
1:A:78:G:C6	1:A:79:G:C6	2.96	0.54
1:A:714:U:H3'	38:A:6414:HOH:O	2.08	0.54
1:A:1165:G:O2'	1:A:1166:A:OP1	2.23	0.54
1:A:1783:A:O2'	1:A:1784:U:H5'	2.07	0.54
1:A:1804:A:H2'	1:A:1805:G:H8	1.71	0.54
1:A:2011:A:H4'	1:A:2012:U:O5'	2.08	0.54
1:A:2765:C:H2'	1:A:2766:A:H8	1.71	0.54
4:C:105:VAL:CG1	4:C:106:CYS:N	2.70	0.54
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.89	0.54
11:J:139:ASP:N	11:J:140:PRO:CD	2.69	0.54
22:U:25:ALA:O	22:U:39:ASN:CB	2.55	0.54
24:W:64:GLY:O	24:W:65:ASP:HB2	2.07	0.54
26:Y:61:ARG:HH12	26:Y:67:PRO:HD3	1.71	0.54
28:1:53:GLY:HA2	28:1:67:GLY:O	2.07	0.54
1:A:1803:C:O2'	1:A:1804:A:H5'	2.06	0.54
1:A:2338:G:P	7:F:97:GLN:HG3	2.48	0.54
2:B:3076:G:C3'	2:B:3077:A:H5"	2.32	0.54
2:B:3096:C:H2'	2:B:3097:U:C6	2.43	0.54
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.88	0.54
1:A:1308:A:O4'	6:E:226:GLY:HA3	2.07	0.54
1:A:1855:G:H8	4:C:144:GLU:OE2	1.90	0.54
1:A:2044:G:OP1	26:Y:23:HIS:HE1	1.91	0.54
1:A:2252:A:C6	1:A:2253:G:H1'	2.41	0.54
38:A:8540:HOH:O	29:2:15:THR:HG21	2.08	0.54
8:G:23:GLU:HG2	8:G:28:SER:CB	2.38	0.54
26:Y:36:HIS:CE1	26:Y:40:HIS:CD2	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:38:ARG:O	31:4:42:ARG:HB2	2.08	0.54
1:A:1181:A:N1	1:A:1192:A:O2'	2.40	0.54
1:A:2415:A:C2'	1:A:2416:G:H5'	2.38	0.54
12:K:131:THR:HB	12:K:134:GLU:HG3	1.89	0.54
13:L:75:ARG:CZ	38:L:4172:HOH:O	2.55	0.54
15:N:45:ARG:CZ	15:N:48:ARG:HG3	2.37	0.54
15:N:162:GLY:HA2	38:N:8520:HOH:O	2.07	0.54
24:W:39:ALA:N	24:W:40:PRO:CD	2.71	0.54
29:2:22:CYS:HB2	38:2:1159:HOH:O	2.08	0.54
1:A:920:C:H5"	1:A:921:G:O5'	2.07	0.54
1:A:2502:C:C4'	11:J:151:MET:HG2	2.37	0.54
6:E:138:VAL:O	6:E:234:VAL:HA	2.08	0.54
7:F:163:VAL:HA	38:F:6326:HOH:O	2.08	0.54
11:J:118:PRO:HD2	38:J:8327:HOH:O	2.07	0.54
20:S:8:ALA:CB	20:S:13:THR:HG21	2.29	0.54
21:T:11:THR:H	21:T:14:ALA:HB3	1.71	0.54
26:Y:27:ASP:OD2	26:Y:27:ASP:N	2.40	0.54
1:A:485:A:O2'	1:A:487:G:H5'	2.07	0.54
1:A:1687:C:O2	29:2:9:GLY:HA2	2.07	0.54
1:A:2442:G:H3'	38:A:6100:HOH:O	2.07	0.54
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.41	0.54
1:A:2745:C:H5	38:A:5370:HOH:O	1.90	0.54
2:B:3040:C:N4	7:F:51:ARG:HB2	2.22	0.54
5:D:202:VAL:HG11	5:D:301:VAL:HG13	1.88	0.54
7:F:94:ALA:O	7:F:95:THR:O	2.25	0.54
16:O:47:LEU:HD13	16:O:97:VAL:HG11	1.88	0.54
19:R:32:GLU:O	19:R:93:ARG:NH2	2.41	0.54
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.90	0.54
1:A:1058:A:H2'	1:A:1060:C:H5"	1.89	0.54
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.54
1:A:1752:G:H2'	38:A:7018:HOH:O	2.07	0.54
1:A:2408:A:H2	38:4:8518:HOH:O	1.90	0.54
1:A:2769:C:O2'	1:A:2770:G:H5'	2.08	0.54
5:D:81:ALA:HB1	5:D:142:LEU:HD13	1.90	0.54
14:M:146:GLY:C	14:M:148:GLU:H	2.12	0.54
1:A:840:U:H2'	20:S:128:ARG:NH1	2.23	0.54
8:G:125:GLU:O	8:G:132:THR:HG22	2.08	0.54
11:J:53:PRO:HG3	11:J:127:GLY:H	1.73	0.54
17:P:106:PRO:HG2	17:P:107:GLU:OE1	2.08	0.54
18:Q:103:THR:HB	38:Q:4563:HOH:O	2.08	0.54
22:U:41:ARG:HG2	22:U:41:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:14:HIS:HA	38:X:2978:HOH:O	2.07	0.54
27:Z:106:THR:HG23	27:Z:107:PRO:HD2	1.90	0.54
1:A:10:U:H3'	38:A:9833:HOH:O	2.08	0.53
1:A:706:G:HO2'	1:A:707:C:H6	1.55	0.53
1:A:830:G:H2'	1:A:831:U:C6	2.43	0.53
1:A:1972:U:H2'	1:A:1973:A:H5'	1.90	0.53
1:A:2501:G:H1'	38:A:4026:HOH:O	2.08	0.53
4:C:153:ARG:HH11	4:C:153:ARG:CB	2.20	0.53
5:D:43:GLY:O	5:D:308:LEU:HD12	2.07	0.53
7:F:16:PRO:HB2	7:F:165:PHE:CG	2.43	0.53
9:H:46:GLU:OE1	9:H:100:ASP:HA	2.08	0.53
9:H:99:THR:O	9:H:99:THR:HG23	2.07	0.53
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	1.89	0.53
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.08	0.53
22:U:40:VAL:HG23	22:U:119:ALA:C	2.28	0.53
1:A:514:G:O5'	1:A:514:G:C8	2.61	0.53
1:A:1187:U:H5"	38:A:5672:HOH:O	2.07	0.53
1:A:1594:C:O2'	1:A:1607:A:H4'	2.08	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.09	0.53
1:A:2729:C:O2'	1:A:2730:G:H5'	2.08	0.53
6:E:22:PHE:HA	6:E:116:ALA:HA	1.90	0.53
15:N:46:LEU:HD22	15:N:50:ARG:HG3	1.90	0.53
1:A:67:A:H5"	1:A:69:A:C8	2.43	0.53
1:A:245:C:H2'	1:A:246:G:H5'	1.90	0.53
1:A:646:G:H2'	1:A:647:U:C6	2.44	0.53
1:A:1423:C:O2'	1:A:1424:A:H5'	2.07	0.53
1:A:2272:G:H5"	38:C:8519:HOH:O	2.08	0.53
38:A:6925:HOH:O	6:E:188:ARG:HD2	2.08	0.53
5:D:175:LEU:C	5:D:175:LEU:CD2	2.76	0.53
7:F:45:THR:CG2	7:F:75:LEU:HD11	2.38	0.53
20:S:106:GLY:HA2	20:S:109:MET:CE	2.38	0.53
24:W:58:THR:O	24:W:62:GLU:HG3	2.08	0.53
25:X:90:TYR:N	25:X:90:TYR:CD1	2.75	0.53
31:4:11:CYS:HB2	31:4:20:HIS:HE1	1.72	0.53
1:A:820:G:O2'	1:A:856:G:H4'	2.08	0.53
1:A:1086:A:C6	25:X:11:VAL:HG11	2.42	0.53
1:A:1305:C:H5'	38:A:9338:HOH:O	2.09	0.53
1:A:1484:G:H2'	38:A:8623:HOH:O	2.08	0.53
1:A:1552:G:H2'	1:A:1553:C:C6	2.42	0.53
1:A:1589:G:C2	1:A:1605:G:N3	2.77	0.53
1:A:2263:G:H5'	38:N:8617:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:31:ARG:HH12	8:G:68:HIS:CE1	2.27	0.53
8:G:145:ALA:HB1	8:G:168:ILE:HD11	1.89	0.53
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.43	0.53
16:O:82:TYR:HD2	16:O:83:LEU:N	2.06	0.53
16:O:139:TRP:O	16:O:142:THR:HB	2.09	0.53
25:X:72:PRO:O	25:X:74:GLU:N	2.42	0.53
27:Z:131:GLN:HB3	27:Z:153:GLN:OE1	2.07	0.53
1:A:111:C:O2'	1:A:112:G:H5'	2.09	0.53
1:A:902:G:N7	14:M:18:HIS:HD2	2.07	0.53
1:A:1161:A:O5'	1:A:1161:A:C8	2.60	0.53
1:A:1209:C:C2	1:A:1210:G:C8	2.96	0.53
1:A:1730:G:H5'	1:A:1731:C:C5	2.44	0.53
2:B:3031:C:H2'	2:B:3032:G:O4'	2.08	0.53
4:C:29:HIS:CE1	4:C:107:ASN:ND2	2.77	0.53
5:D:41:PHE:HB3	5:D:190:MET:HE3	1.89	0.53
6:E:141:SER:HA	38:E:8380:HOH:O	2.07	0.53
10:I:12:ILE:N	10:I:13:PRO:CD	2.72	0.53
15:N:89:ASN:HA	38:N:8549:HOH:O	2.07	0.53
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.90	0.53
20:S:4:TYR:HA	20:S:144:GLU:OE2	2.09	0.53
20:S:91:LEU:HD21	20:S:145:LEU:HB2	1.90	0.53
25:X:38:THR:HG22	38:X:3580:HOH:O	2.09	0.53
1:A:751:U:H5"	6:E:100:LEU:HD22	1.90	0.53
6:E:133:ARG:HD2	38:E:8409:HOH:O	2.08	0.53
6:E:196:THR:HG23	38:E:8399:HOH:O	2.09	0.53
7:F:101:THR:HG22	38:F:7400:HOH:O	2.08	0.53
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.43	0.53
11:J:111:MET:O	11:J:114:PRO:HD3	2.08	0.53
13:L:1:MET:HE1	38:L:6646:HOH:O	2.07	0.53
13:L:37:TYR:HE2	13:L:45:PRO:HA	1.72	0.53
15:N:77:PHE:CE2	15:N:86:MET:HG2	2.43	0.53
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.90	0.53
16:O:75:THR:HA	16:O:80:SER:OG	2.08	0.53
1:A:515:C:H3'	38:A:5127:HOH:O	2.09	0.53
1:A:695:C:H2'	1:A:696:C:C6	2.44	0.53
1:A:932:U:H2'	1:A:933:C:C6	2.44	0.53
1:A:945:U:H2'	1:A:946:C:H6	1.74	0.53
1:A:1834:C:H2'	1:A:1840:A:N6	2.24	0.53
2:B:3035:C:H5"	38:B:8458:HOH:O	2.06	0.53
5:D:177:HIS:O	5:D:181:ILE:HG13	2.09	0.53
11:J:26:LYS:HD2	11:J:28:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:A:C2'	1:A:205:U:H5'	2.39	0.53
1:A:1890:U:H4'	1:A:2010:A:C6	2.44	0.53
1:A:2607:U:O5'	1:A:2609:G:H4'	2.08	0.53
2:B:3013:A:O2'	2:B:3014:G:H5"	2.08	0.53
7:F:84:LEU:C	7:F:86:THR:H	2.12	0.53
9:H:33:THR:HG21	9:H:59:ILE:O	2.09	0.53
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	2.05	0.53
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.44	0.53
1:A:1462:C:H2'	1:A:1463:A:C8	2.44	0.53
1:A:1516:C:H2'	1:A:1517:U:C6	2.44	0.53
38:A:7053:HOH:O	28:1:31:ILE:HG13	2.08	0.53
38:A:7151:HOH:O	15:N:154:ARG:HB2	2.08	0.53
38:A:8917:HOH:O	15:N:52:LEU:HD23	2.08	0.53
6:E:127:ARG:HG2	6:E:127:ARG:NH1	2.22	0.53
22:U:20:HIS:HB3	22:U:41:ARG:HD2	1.91	0.53
1:A:666:A:H2'	1:A:667:C:O4'	2.09	0.53
1:A:1930:A:H1'	1:A:2128:G:H5'	1.91	0.53
1:A:2001:G:O2'	1:A:2002:C:H5'	2.09	0.53
1:A:2281:C:H2'	1:A:2282:U:H5'	1.89	0.53
1:A:2379:G:H4'	1:A:2380:A:H5"	1.91	0.53
1:A:2815:G:OP2	12:K:99:GLU:HG2	2.10	0.53
6:E:156:LEU:HD12	6:E:156:LEU:O	2.08	0.53
8:G:11:VAL:HG11	8:G:22:VAL:CG1	2.39	0.53
9:H:99:THR:O	9:H:100:ASP:HB2	2.08	0.53
12:K:19:MET:HE2	12:K:79:PHE:CA	2.35	0.53
16:O:114:LYS:O	16:O:118:ILE:HG13	2.08	0.53
22:U:25:ALA:O	22:U:39:ASN:HB2	2.09	0.53
25:X:130:HIS:O	25:X:136:GLY:HA3	2.09	0.53
28:1:19:GLY:O	28:1:23:ARG:HG2	2.09	0.53
1:A:21:G:H5"	20:S:1:GLY:O	2.09	0.52
1:A:431:G:P	15:N:48:ARG:HH12	2.31	0.52
1:A:1029:U:O2'	1:A:1273:C:OP1	2.25	0.52
1:A:1269:G:H2'	1:A:1270:U:H6	1.74	0.52
1:A:1908:G:N1	1:A:1930:A:OP2	2.39	0.52
1:A:2755:G:H1'	38:A:4163:HOH:O	2.09	0.52
4:C:93:THR:C	4:C:94:LEU:HD23	2.28	0.52
5:D:232:TRP:CD1	5:D:235:ARG:HD2	2.44	0.52
8:G:7:ILE:CG2	8:G:45:ASP:O	2.56	0.52
12:K:59:LYS:O	12:K:63:ILE:HG13	2.08	0.52
13:L:18:ILE:HG22	13:L:93:ASN:HB2	1.91	0.52
17:P:106:PRO:HG2	17:P:107:GLU:CD	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:C:H2'	1:A:669:G:H8	1.73	0.52
7:F:153:THR:HG22	38:F:5234:HOH:O	2.09	0.52
8:G:146:ALA:O	8:G:150:GLN:HG2	2.10	0.52
12:K:60:ARG:HA	12:K:63:ILE:HD12	1.90	0.52
16:O:86:LEU:HD12	16:O:125:ALA:CB	2.33	0.52
17:P:107:GLU:N	17:P:107:GLU:CD	2.63	0.52
18:Q:50:GLN:HB3	38:Q:5440:HOH:O	2.09	0.52
20:S:18:LEU:HB2	20:S:143:VAL:HG13	1.91	0.52
1:A:2316:G:H8	38:A:5135:HOH:O	1.91	0.52
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.24	0.52
4:C:51:ARG:NH2	38:C:8555:HOH:O	2.43	0.52
5:D:87:TYR:OH	5:D:163:GLU:OE2	2.15	0.52
6:E:156:LEU:HD11	6:E:160:LEU:HD11	1.92	0.52
11:J:139:ASP:HA	38:J:8359:HOH:O	2.08	0.52
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.33	0.52
25:X:6:GLN:HA	25:X:52:VAL:HG23	1.90	0.52
1:A:1377:C:H5'	1:A:1377:C:C6	2.38	0.52
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.74	0.52
1:A:2433:A:H2	38:A:7393:HOH:O	1.92	0.52
1:A:2768:A:H3'	38:A:3906:HOH:O	2.09	0.52
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.91	0.52
17:P:21:SER:HB3	17:P:106:PRO:O	2.09	0.52
19:R:42:LYS:NZ	19:R:43:ILE:O	2.36	0.52
20:S:82:GLU:O	20:S:86:LYS:HG3	2.09	0.52
21:T:22:ASN:HD21	21:T:68:LEU:HB2	1.75	0.52
25:X:60:GLU:O	25:X:63:GLU:HB2	2.09	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.52
1:A:668:C:H2'	1:A:669:G:C8	2.44	0.52
1:A:1555:G:H4'	1:A:1630:A:H2	1.74	0.52
1:A:2691:A:H8	1:A:2691:A:OP1	1.92	0.52
38:A:4456:HOH:O	11:J:57:ARG:HG3	2.09	0.52
2:B:3056:A:H2'	2:B:3057:A:C5'	2.25	0.52
5:D:51:VAL:HG23	5:D:329:TYR:O	2.09	0.52
6:E:84:VAL:O	6:E:85:LYS:HB2	2.09	0.52
10:I:69:ARG:NH1	38:I:3513:HOH:O	2.43	0.52
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.91	0.52
14:M:90:ARG:HA	14:M:119:THR:HB	1.91	0.52
15:N:94:LYS:CE	38:N:8578:HOH:O	2.50	0.52
22:U:19:ARG:NH1	22:U:68:ASP:O	2.43	0.52
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.23	0.52
28:1:39:CYS:HB2	28:1:57:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:G:H1	1:A:1208:C:H42	1.56	0.52
1:A:2348:C:H5'	7:F:22:VAL:HG11	1.92	0.52
4:C:164:ARG:NE	38:C:8602:HOH:O	2.43	0.52
8:G:157:LYS:NZ	38:G:2401:HOH:O	2.42	0.52
12:K:126:ASN:HA	35:K:8501:CL:CL	2.47	0.52
23:V:6:CYS:SG	23:V:32:CYS:N	2.81	0.52
1:A:840:U:H2'	20:S:128:ARG:HH12	1.74	0.52
1:A:1003:U:O2'	11:J:90:PHE:HE1	1.92	0.52
1:A:2389:U:OP1	19:R:82:LYS:NZ	2.38	0.52
1:A:2407:G:O2'	1:A:2408:A:H5'	2.10	0.52
1:A:2543:G:H2'	1:A:2544:G:O4'	2.09	0.52
2:B:3056:A:N1	7:F:13:MET:HE3	2.25	0.52
5:D:266:ASN:OD1	5:D:317:PRO:HA	2.10	0.52
11:J:47:GLU:OE2	11:J:162:SER:OG	2.28	0.52
15:N:36:ALA:HB1	38:N:8546:HOH:O	2.09	0.52
20:S:39:THR:HG22	20:S:42:GLU:HG3	1.92	0.52
27:Z:187:VAL:HB	27:Z:203:VAL:CG2	2.40	0.52
1:A:1025:C:H5'	25:X:23:MET:O	2.10	0.52
1:A:1095:U:O2	25:X:120:PRO:HG2	2.10	0.52
1:A:1169:U:C5	1:A:1170:U:C4	2.98	0.52
1:A:1192:A:H3'	1:A:1193:A:H5'	1.92	0.52
1:A:1205:U:H2'	1:A:1206:U:H5'	1.91	0.52
1:A:1442:A:H1'	38:A:6486:HOH:O	2.09	0.52
1:A:1505:U:H6	1:A:1505:U:H5'	1.74	0.52
1:A:2466:G:H5"	38:A:3142:HOH:O	2.10	0.52
38:A:5805:HOH:O	7:F:55:LYS:HB2	2.10	0.52
2:B:3023:U:C3'	2:B:3024:U:H5"	2.39	0.52
6:E:140:VAL:HB	38:E:8450:HOH:O	2.09	0.52
13:L:86:THR:HG22	13:L:87:ARG:N	2.25	0.52
15:N:61:ILE:HD12	15:N:61:ILE:N	2.24	0.52
16:O:155:GLU:O	16:O:156:GLU:HG3	2.10	0.52
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.30	0.52
22:U:101:LEU:HD13	22:U:112:LEU:HD11	1.91	0.52
26:Y:29:ALA:O	26:Y:32:LEU:N	2.42	0.52
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.13	0.52
1:A:407:A:H3'	38:A:3938:HOH:O	2.09	0.52
1:A:1162:G:H2'	1:A:1162:G:N3	2.24	0.52
1:A:2121:G:O2'	31:4:47:GLY:HA2	2.10	0.52
5:D:82:VAL:O	5:D:82:VAL:HG12	2.10	0.52
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.09	0.52
8:G:15:GLN:HG3	8:G:20:ILE:CG1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:48:LEU:CG	11:J:157:ILE:HG21	2.40	0.52
16:O:154:LEU:HD12	16:O:156:GLU:O	2.09	0.52
21:T:58:MET:SD	30:3:8:LYS:HE3	2.50	0.52
28:1:50:ALA:HB3	28:1:54:ILE:HG22	1.92	0.52
1:A:1015:C:H2'	1:A:1016:U:H6	1.74	0.52
1:A:1422:U:H2'	1:A:1423:C:C6	2.45	0.52
1:A:1635:U:O2'	1:A:1636:G:H5'	2.10	0.52
1:A:2878:U:H2'	1:A:2879:A:O4'	2.09	0.52
5:D:41:PHE:HD2	5:D:190:MET:HE3	1.71	0.52
27:Z:117:LEU:HA	27:Z:174:VAL:HG11	1.91	0.52
31:4:39:GLN:CA	31:4:42:ARG:NH2	2.73	0.52
1:A:853:C:H2'	1:A:854:G:O4'	2.10	0.51
1:A:945:U:H2'	1:A:946:C:C6	2.44	0.51
1:A:1189:A:H1'	1:A:1209:C:H1'	1.92	0.51
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.51
1:A:2013:G:C2	1:A:2014:G:N7	2.78	0.51
2:B:3057:A:N3	2:B:3057:A:H5'	2.25	0.51
5:D:79:MET:HE1	38:D:8631:HOH:O	2.09	0.51
6:E:25:PRO:HD2	38:E:8427:HOH:O	2.10	0.51
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.92	0.51
14:M:73:VAL:HG23	14:M:74:THR:H	1.75	0.51
17:P:7:LEU:HD22	38:P:5650:HOH:O	2.09	0.51
20:S:29:LYS:HD3	38:S:8540:HOH:O	2.09	0.51
20:S:39:THR:HB	20:S:42:GLU:OE1	2.10	0.51
24:W:64:GLY:O	24:W:65:ASP:CB	2.58	0.51
25:X:121:PRO:CA	25:X:153:MET:HG2	2.40	0.51
1:A:2432:C:O5'	1:A:2432:C:H6	1.93	0.51
2:B:3044:A:O4'	7:F:76:ARG:NE	2.44	0.51
7:F:86:THR:O	7:F:90:LEU:HG	2.11	0.51
10:I:12:ILE:HD12	38:I:692:HOH:O	2.09	0.51
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.24	0.51
1:A:1878:G:O2'	1:A:1879:U:C6	2.62	0.51
1:A:2467:A:H2'	38:A:4937:HOH:O	2.09	0.51
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.90	0.51
7:F:70:GLY:N	38:F:5576:HOH:O	2.44	0.51
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.39	0.51
9:H:57:GLU:O	9:H:61:MET:HG3	2.10	0.51
12:K:107:ASN:ND2	12:K:109:TYR:H	2.09	0.51
16:O:69:TYR:HE2	16:O:183:ASP:OD2	1.93	0.51
18:Q:7:LYS:HD2	18:Q:21:VAL:HG21	1.93	0.51
1:A:810:G:H2'	1:A:811:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1979:G:O2'	1:A:1980:U:OP1	2.24	0.51
1:A:2499:U:O2'	1:A:2500:C:H5'	2.09	0.51
2:B:3055:U:H4'	2:B:3056:A:H8	1.75	0.51
4:C:192:VAL:O	4:C:192:VAL:HG12	2.11	0.51
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.40	0.51
9:H:56:PRO:CG	15:N:44:THR:HA	2.40	0.51
11:J:44:ALA:HA	11:J:163:PRO:O	2.10	0.51
11:J:44:ALA:HB3	11:J:136:VAL:O	2.11	0.51
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.27	0.51
15:N:172:GLY:C	15:N:183:VAL:HG11	2.31	0.51
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.45	0.51
28:1:49:ARG:HD2	38:1:8425:HOH:O	2.11	0.51
1:A:24:G:N2	1:A:518:G:H1'	2.25	0.51
1:A:396:U:H2'	1:A:397:A:N7	2.26	0.51
1:A:474:C:O3'	6:E:73:LEU:HD21	2.10	0.51
1:A:1377:C:H1'	38:A:6740:HOH:O	2.11	0.51
1:A:1513:C:O2'	1:A:1514:C:H5'	2.10	0.51
1:A:2346:C:O3'	7:F:52:THR:CG2	2.59	0.51
2:B:3039:U:H3	2:B:3042:C:H5"	1.74	0.51
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.32	0.51
6:E:95:GLU:H	6:E:95:GLU:CD	2.13	0.51
11:J:93:ILE:HG12	11:J:120:GLY:O	2.11	0.51
26:Y:22:ASN:O	26:Y:25:ARG:HG3	2.10	0.51
1:A:371:U:H2'	1:A:372:A:H8	1.75	0.51
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.41	0.51
1:A:2890:A:H2'	38:A:4674:HOH:O	2.10	0.51
7:F:64:ARG:O	7:F:67:ASP:OD2	2.28	0.51
7:F:144:ARG:NH2	38:F:3839:HOH:O	2.38	0.51
9:H:104:ALA:O	9:H:108:LEU:HB3	2.10	0.51
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.92	0.51
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.11	0.51
25:X:122:ARG:NH2	38:X:4276:HOH:O	2.43	0.51
1:A:428:G:H5'	38:A:7116:HOH:O	2.11	0.51
38:A:4320:HOH:O	12:K:47:THR:HB	2.10	0.51
4:C:149:ASP:OD1	4:C:151:GLN:HB2	2.11	0.51
7:F:52:THR:HG22	7:F:52:THR:O	2.09	0.51
11:J:31:PHE:HE2	11:J:87:LYS:O	1.93	0.51
19:R:32:GLU:HA	19:R:71:TYR:OH	2.11	0.51
20:S:29:LYS:HD2	20:S:62:HIS:NE2	2.26	0.51
26:Y:43:VAL:HG12	26:Y:44:ASP:O	2.11	0.51
30:3:48:ASP:O	30:3:49:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:C:H2'	1:A:102:A:H8	1.75	0.51
1:A:2506:A:C1'	38:A:3244:HOH:O	2.57	0.51
1:A:2768:A:C2'	1:A:2769:C:O4'	2.58	0.51
2:B:3078:G:N2	2:B:3103:A:OP2	2.38	0.51
4:C:125:ASN:HB3	4:C:158:VAL:HG12	1.93	0.51
11:J:144:GLU:HG3	38:J:8333:HOH:O	2.10	0.51
11:J:154:THR:HB	11:J:155:PRO:HD3	1.93	0.51
16:O:104:ILE:O	16:O:107:ASN:HB2	2.11	0.51
24:W:50:ARG:HD3	38:W:2826:HOH:O	2.10	0.51
27:Z:115:ARG:NE	38:Z:8558:HOH:O	2.44	0.51
28:1:47:LEU:HA	28:1:56:MET:O	2.11	0.51
1:A:514:G:OP1	1:A:514:G:H2'	2.11	0.51
1:A:1657:A:H2'	1:A:1658:A:C8	2.45	0.51
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.76	0.51
1:A:1805:G:H2'	1:A:1806:G:H8	1.76	0.51
1:A:2010:A:H2'	38:A:5444:HOH:O	2.11	0.51
1:A:2064:U:H5'	1:A:2652:U:O3'	2.11	0.51
1:A:2329:C:O2'	1:A:2330:U:H5'	2.11	0.51
1:A:2768:A:O2'	1:A:2769:C:H5'	2.11	0.51
2:B:3049:G:O2'	2:B:3050:G:H5'	2.11	0.51
4:C:153:ARG:HB2	4:C:153:ARG:NH1	2.24	0.51
7:F:57:THR:HG23	7:F:63:ILE:CB	2.40	0.51
15:N:99:ARG:CD	15:N:167:GLY:HA2	2.38	0.51
17:P:99:GLU:HG2	38:P:6044:HOH:O	2.10	0.51
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.26	0.51
20:S:34:GLU:HG2	20:S:46:TYR:OH	2.10	0.51
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.92	0.51
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.25	0.51
1:A:282:C:H1'	1:A:368:C:H42	1.74	0.51
1:A:450:C:H4'	6:E:46:TYR:CE1	2.46	0.51
1:A:818:A:H5"	38:A:6062:HOH:O	2.10	0.51
1:A:2073:G:OP2	1:A:2490:A:H5'	2.11	0.51
1:A:2597:U:C2'	1:A:2598:U:H5'	2.40	0.51
38:A:6114:HOH:O	17:P:24:ALA:N	2.43	0.51
2:B:3002:U:OP2	2:B:3002:U:H4'	2.11	0.51
6:E:16:VAL:HG12	6:E:17:ASP:H	1.75	0.51
7:F:93:LEU:HB2	38:F:5198:HOH:O	2.10	0.51
17:P:39:THR:O	17:P:115:ARG:NH2	2.44	0.51
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.93	0.51
27:Z:200:THR:HG22	27:Z:201:GLU:HG2	1.92	0.51
1:A:544:G:H2'	1:A:545:G:C5'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:A:H2'	1:A:1133:A:C8	2.46	0.50
1:A:1209:C:O2'	1:A:1210:G:H5'	2.11	0.50
1:A:2437:A:H2'	1:A:2438:G:C8	2.46	0.50
2:B:3039:U:H1'	2:B:3044:A:N6	2.24	0.50
5:D:41:PHE:CE1	5:D:79:MET:HG3	2.45	0.50
7:F:40:ILE:HG23	38:F:5583:HOH:O	2.12	0.50
8:G:11:VAL:CG1	8:G:12:ASP:N	2.74	0.50
8:G:84:MET:HB2	8:G:131:LEU:HB2	1.92	0.50
14:M:22:ARG:HG2	38:M:8397:HOH:O	2.11	0.50
18:Q:27:ARG:HA	38:Q:3969:HOH:O	2.11	0.50
25:X:137:GLN:NE2	25:X:141:HIS:HE1	2.09	0.50
1:A:1180:U:H2'	1:A:1181:A:O4'	2.12	0.50
1:A:2039:A:H2'	1:A:2040:C:C6	2.46	0.50
1:A:2505:G:O2'	1:A:2506:A:H5'	2.11	0.50
2:B:3025:G:H5"	2:B:3026:C:C6	2.47	0.50
4:C:105:VAL:CG1	4:C:106:CYS:H	2.24	0.50
5:D:146:THR:C	5:D:148:PRO:HD3	2.31	0.50
6:E:194:PHE:HA	6:E:234:VAL:HG13	1.93	0.50
16:O:163:PHE:HA	38:O:8564:HOH:O	2.11	0.50
26:Y:18:ARG:HA	38:Y:5356:HOH:O	2.10	0.50
1:A:559:U:H2'	1:A:560:C:O4'	2.11	0.50
1:A:1785:G:OP1	18:Q:76:GLY:HA3	2.11	0.50
1:A:2754:G:O2'	1:A:2755:G:H5'	2.11	0.50
38:A:8694:HOH:O	31:4:48:ASN:HB2	2.11	0.50
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.46	0.50
6:E:233:THR:HG21	6:E:235:PHE:CE1	2.47	0.50
13:L:20:CYS:HB3	13:L:26:ALA:O	2.12	0.50
16:O:115:VAL:HG22	38:O:8551:HOH:O	2.10	0.50
16:O:120:GLU:HG3	16:O:136:LEU:HD13	1.92	0.50
1:A:285:A:H2'	1:A:286:U:O4'	2.11	0.50
1:A:518:G:H4'	38:A:5551:HOH:O	2.10	0.50
1:A:820:G:C6	4:C:171:LYS:HB2	2.46	0.50
1:A:825:U:H5"	1:A:826:U:OP1	2.11	0.50
1:A:952:G:OP1	19:R:42:LYS:HE2	2.11	0.50
1:A:1166:A:N3	1:A:1166:A:H2'	2.26	0.50
1:A:1352:A:N1	6:E:48:SER:HB3	2.26	0.50
1:A:1666:C:C2'	1:A:1667:A:C5'	2.90	0.50
1:A:2456:A:H5'	38:A:5177:HOH:O	2.11	0.50
4:C:190:ARG:NH2	4:C:207:GLN:OE1	2.45	0.50
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.42	0.50
16:O:35:VAL:HB	16:O:46:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:1:MET:N	25:X:103:GLU:OE2	2.39	0.50
4:C:55:VAL:CG1	4:C:67:LEU:HD22	2.40	0.50
20:S:39:THR:HB	20:S:42:GLU:CD	2.32	0.50
22:U:4:PRO:O	22:U:8:ARG:HG3	2.11	0.50
24:W:29:ASN:O	24:W:33:VAL:HG23	2.11	0.50
25:X:8:ARG:HD3	25:X:51:PHE:HA	1.94	0.50
1:A:960:G:N3	1:A:960:G:C2'	2.74	0.50
1:A:1052:G:N3	1:A:1052:G:H2'	2.26	0.50
1:A:1666:C:H2'	1:A:1667:A:C5'	2.41	0.50
1:A:2115:U:H2'	1:A:2116:U:C6	2.47	0.50
1:A:2715:G:O2'	5:D:262:ARG:HD2	2.12	0.50
38:A:4213:HOH:O	16:O:21:HIS:HD2	1.94	0.50
38:A:9955:HOH:O	12:K:46:ILE:HD12	2.11	0.50
4:C:65:ARG:C	4:C:66:ARG:HG3	2.31	0.50
5:D:55:ASN:HB3	5:D:64:GLY:N	2.26	0.50
5:D:190:MET:HE2	5:D:194:PHE:HD1	1.75	0.50
7:F:92:GLU:O	7:F:93:LEU:O	2.29	0.50
15:N:169:ARG:HB3	38:N:8584:HOH:O	2.11	0.50
22:U:37:GLN:OE1	22:U:118:SER:HA	2.12	0.50
1:A:530:C:H4'	1:A:612:U:H4'	1.92	0.50
1:A:1545:C:H2'	1:A:1546:G:O4'	2.12	0.50
1:A:2440:C:H5"	38:A:3313:HOH:O	2.12	0.50
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.77	0.50
1:A:2869:G:H2'	1:A:2870:C:C6	2.46	0.50
5:D:54:VAL:O	5:D:55:ASN:C	2.49	0.50
7:F:25:MET:CE	7:F:37:ALA:HB1	2.38	0.50
11:J:48:LEU:CD1	11:J:157:ILE:HG21	2.42	0.50
12:K:42:GLU:HG3	12:K:145:TRP:CD1	2.47	0.50
16:O:37:ARG:CZ	38:O:8532:HOH:O	2.59	0.50
17:P:47:ARG:HG3	17:P:47:ARG:NH1	2.24	0.50
17:P:96:VAL:HA	38:P:4258:HOH:O	2.12	0.50
22:U:48:VAL:HG22	22:U:97:ARG:O	2.12	0.50
27:Z:112:GLU:OE1	27:Z:112:GLU:HA	2.12	0.50
30:3:9:LYS:O	30:3:12:ALA:HB3	2.11	0.50
30:3:36:ASN:O	30:3:39:ARG:HG3	2.12	0.50
31:4:7:PHE:CE2	31:4:22:VAL:CG2	2.93	0.50
31:4:91:GLN:O	31:4:92:GLU:HB2	2.11	0.50
1:A:512:G:O3'	1:A:513:A:H8	1.94	0.50
1:A:585:C:H5"	38:A:4353:HOH:O	2.10	0.50
1:A:602:A:O2'	1:A:605:C:H4'	2.12	0.50
1:A:832:U:H2'	1:A:833:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:G:H5'	2:B:3081:C:H4'	1.94	0.50
1:A:2348:C:C5'	7:F:22:VAL:HG21	2.42	0.50
1:A:2737:C:H3'	1:A:2738:G:H5"	1.93	0.50
38:A:6925:HOH:O	6:E:188:ARG:CD	2.60	0.50
5:D:49:THR:CG2	5:D:280:VAL:CG2	2.89	0.50
11:J:26:LYS:CD	11:J:28:ILE:HB	2.42	0.50
15:N:46:LEU:CD2	15:N:50:ARG:HG3	2.41	0.50
15:N:63:VAL:HG21	15:N:109:PHE:CZ	2.46	0.50
18:Q:7:LYS:HD2	18:Q:21:VAL:CG2	2.42	0.50
25:X:83:TRP:CZ3	25:X:112:LEU:HD21	2.46	0.50
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.12	0.50
28:1:81:LYS:O	28:1:82:ALA:O	2.30	0.50
1:A:177:A:H2'	1:A:178:U:O4'	2.12	0.50
1:A:283:U:H5	1:A:284:C:N4	2.10	0.50
1:A:621:C:H5'	27:Z:132:ASP:OD2	2.11	0.50
1:A:860:U:H2'	1:A:861:A:C8	2.47	0.50
1:A:1086:A:N6	25:X:11:VAL:HG11	2.27	0.50
1:A:1629:G:N2	1:A:1632:A:OP2	2.43	0.50
1:A:1762:C:H4'	38:A:4135:HOH:O	2.12	0.50
1:A:1885:A:H2'	1:A:1886:A:H5'	1.94	0.50
1:A:2815:G:H2'	38:A:5199:HOH:O	2.12	0.50
38:A:6763:HOH:O	15:N:152:ARG:HB3	2.12	0.50
11:J:136:VAL:HG22	11:J:137:ASN:O	2.12	0.50
11:J:150:LYS:O	11:J:150:LYS:HG2	2.10	0.50
13:L:75:ARG:NH1	13:L:112:PRO:HD2	2.27	0.50
16:O:43:VAL:HG11	16:O:81:ALA:HA	1.94	0.50
16:O:182:GLY:O	16:O:183:ASP:O	2.30	0.50
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.77	0.50
19:R:35:ASP:HA	19:R:63:VAL:O	2.12	0.50
25:X:3:ALA:O	25:X:54:PHE:HA	2.12	0.50
28:1:30:GLU:HB2	38:1:8414:HOH:O	2.12	0.50
31:4:23:GLU:HG2	31:4:24:LYS:N	2.27	0.50
1:A:286:U:H2'	1:A:287:C:C6	2.46	0.49
1:A:832:U:H2'	1:A:833:G:H8	1.76	0.49
1:A:962:C:C1'	16:O:5:ARG:NH1	2.65	0.49
1:A:1139:U:H2'	1:A:1140:C:C6	2.47	0.49
1:A:1159:G:P	38:A:3777:HOH:O	2.69	0.49
1:A:1190:G:H5'	1:A:1208:C:O2'	2.12	0.49
1:A:1289:C:H3'	38:A:5891:HOH:O	2.11	0.49
1:A:1565:C:O4'	1:A:2738:G:H1'	2.12	0.49
1:A:2626:C:H2'	1:A:2627:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:226:LYS:HG2	5:D:230:GLN:HE21	1.77	0.49
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.93	0.49
7:F:103:ASN:ND2	7:F:134:LEU:H	2.09	0.49
9:H:28:ALA:HB3	9:H:99:THR:HG23	1.94	0.49
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.47	0.49
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.27	0.49
25:X:47:LYS:NZ	38:X:3920:HOH:O	2.26	0.49
1:A:701:U:OP2	1:A:701:U:H2'	2.13	0.49
1:A:2672:C:P	5:D:25:ARG:HH11	2.35	0.49
1:A:2719:A:H2'	1:A:2720:C:H5'	1.94	0.49
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.93	0.49
15:N:32:ARG:NH2	38:N:8590:HOH:O	2.44	0.49
16:O:67:ALA:HA	16:O:71:TRP:HB3	1.94	0.49
21:T:8:PRO:HD2	24:W:32:ALA:HA	1.94	0.49
21:T:80:ARG:NH1	38:T:8342:HOH:O	2.44	0.49
22:U:53:GLY:HA3	38:U:6384:HOH:O	2.11	0.49
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.42	0.49
28:1:58:GLY:HA3	38:1:8436:HOH:O	2.12	0.49
1:A:370:G:O2'	1:A:371:U:H5'	2.12	0.49
1:A:1986:G:H2'	1:A:1987:C:C6	2.47	0.49
1:A:2064:U:H5'	1:A:2652:U:H4'	1.94	0.49
1:A:2433:A:H4'	31:4:30:GLN:OE1	2.12	0.49
2:B:3108:C:O2'	2:B:3109:G:H5'	2.13	0.49
4:C:84:VAL:O	4:C:98:GLU:HG3	2.13	0.49
7:F:169:THR:O	7:F:170:TYR:HB2	2.12	0.49
9:H:63:ILE:HB	9:H:64:PRO:CD	2.39	0.49
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.58	0.49
14:M:93:VAL:HG21	14:M:122:ALA:HB2	1.94	0.49
15:N:48:ARG:NH1	15:N:52:LEU:HD21	2.26	0.49
17:P:54:GLU:O	17:P:55:ASP:HB2	2.12	0.49
21:T:81:ILE:HG12	38:T:8334:HOH:O	2.13	0.49
22:U:71:VAL:CG1	22:U:90:PRO:HB3	2.28	0.49
23:V:8:TYR:CD2	23:V:36:CYS:HB3	2.48	0.49
26:Y:71:ARG:HB2	38:Y:6590:HOH:O	2.12	0.49
1:A:65:C:O2'	1:A:66:G:H5'	2.12	0.49
1:A:240:C:H5'	15:N:146:GLN:NE2	2.27	0.49
1:A:820:G:H5'	1:A:821:U:H5'	1.93	0.49
1:A:872:U:O2'	1:A:873:G:H5'	2.13	0.49
1:A:1416:G:H2'	1:A:1417:G:H5'	1.94	0.49
1:A:2125:G:O6	38:A:9913:HOH:O	2.20	0.49
1:A:2325:C:H2'	1:A:2326:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3052:A:N7	38:B:8492:HOH:O	2.35	0.49
6:E:130:GLU:HA	6:E:130:GLU:OE1	2.13	0.49
8:G:69:ILE:HA	8:G:72:MET:CE	2.42	0.49
11:J:59:ASN:N	11:J:59:ASN:ND2	2.55	0.49
20:S:18:LEU:HG	20:S:91:LEU:HD13	1.94	0.49
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.45	0.49
28:1:11:THR:HG21	28:1:23:ARG:HB2	1.93	0.49
1:A:87:C:H2'	30:3:28:LYS:O	2.13	0.49
1:A:100:C:H4'	22:U:16:LEU:HB2	1.95	0.49
1:A:107:U:C2'	1:A:108:U:H5'	2.43	0.49
1:A:677:C:O2'	1:A:678:G:H5'	2.13	0.49
1:A:1114:A:H2'	1:A:1115:U:H6	1.77	0.49
1:A:1166:A:H61	1:A:1180:U:H3	1.60	0.49
1:A:1512:G:N2	1:A:1513:C:H1'	2.26	0.49
1:A:2134:G:N2	1:A:2242:U:C2	2.81	0.49
1:A:2506:A:O2'	1:A:2507:G:O5'	2.30	0.49
1:A:2587:U:H2'	1:A:2589:U:H5"	1.94	0.49
4:C:188:ASN:HB3	38:C:8613:HOH:O	2.13	0.49
7:F:86:THR:HG23	38:F:7477:HOH:O	2.12	0.49
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.11	0.49
9:H:49:PHE:HE1	9:H:98:VAL:HG23	1.78	0.49
9:H:117:GLU:C	9:H:119:ARG:H	2.15	0.49
16:O:154:LEU:O	16:O:155:GLU:CB	2.61	0.49
18:Q:63:ARG:NH2	38:Q:5642:HOH:O	2.40	0.49
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.95	0.49
1:A:1073:A:H1'	1:A:1088:A:C2	2.47	0.49
1:A:1209:C:O2	1:A:1210:G:C8	2.65	0.49
1:A:1353:C:N3	14:M:5:LYS:NZ	2.60	0.49
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.13	0.49
1:A:1918:U:OP2	38:A:3514:HOH:O	2.20	0.49
38:A:4838:HOH:O	4:C:215:ILE:HD12	2.12	0.49
5:D:223:ARG:O	5:D:228:ALA:HB2	2.13	0.49
8:G:45:ASP:OD2	8:G:46:THR:HG23	2.13	0.49
13:L:9:THR:HA	38:L:1611:HOH:O	2.11	0.49
15:N:137:ASP:HA	15:N:142:LYS:HE3	1.93	0.49
16:O:152:GLU:C	16:O:154:LEU:H	2.15	0.49
31:4:34:LYS:HB2	31:4:37:ASP:OD2	2.13	0.49
1:A:281:U:O2'	1:A:282:C:H5'	2.12	0.49
1:A:1118:A:C8	1:A:1118:A:C3'	2.90	0.49
1:A:1407:A:O2'	1:A:1408:U:H3'	2.13	0.49
1:A:1464:U:O2'	1:A:1465:A:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:A:H1'	38:A:3600:HOH:O	2.11	0.49
1:A:2124:G:H2'	1:A:2125:G:H8	1.77	0.49
1:A:2577:A:H5'	38:A:7221:HOH:O	2.12	0.49
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.48	0.49
5:D:2:GLN:HA	38:D:8626:HOH:O	2.12	0.49
5:D:148:PRO:HD2	38:D:8588:HOH:O	2.11	0.49
7:F:152:PRO:O	7:F:156:ARG:HG2	2.12	0.49
11:J:110:GLY:HA2	38:J:8379:HOH:O	2.12	0.49
1:A:2860:G:H1'	38:A:6055:HOH:O	2.13	0.49
4:C:153:ARG:HD3	38:C:8534:HOH:O	2.12	0.49
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.43	0.49
9:H:100:ASP:O	9:H:101:ALA:O	2.31	0.49
11:J:148:ARG:NE	38:J:8333:HOH:O	2.37	0.49
15:N:77:PHE:HD2	38:N:8528:HOH:O	1.96	0.49
19:R:66:LYS:HB2	19:R:70:ALA:O	2.13	0.49
20:S:39:THR:O	20:S:42:GLU:N	2.46	0.49
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.11	0.49
27:Z:189:ASN:HD22	27:Z:192:ASP:H	1.60	0.49
1:A:338:C:H5"	38:A:5320:HOH:O	2.11	0.49
1:A:1815:A:H4'	1:A:2751:C:O4'	2.13	0.49
1:A:2382:A:C1'	31:4:10:TYR:CD2	2.95	0.49
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.48	0.49
4:C:188:ASN:HA	38:C:8564:HOH:O	2.13	0.49
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.43	0.49
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.94	0.49
27:Z:187:VAL:HB	38:Z:8572:HOH:O	2.11	0.49
1:A:97:G:C2	22:U:107:LYS:HD2	2.48	0.49
1:A:138:U:OP2	1:A:139:C:H5	1.96	0.49
1:A:292:G:H2'	1:A:358:G:N2	2.28	0.49
1:A:1186:C:N4	1:A:1187:U:C4	2.81	0.49
38:A:5430:HOH:O	18:Q:87:ARG:HG2	2.13	0.49
4:C:69:LEU:HB3	38:C:8588:HOH:O	2.13	0.49
7:F:84:LEU:HA	7:F:87:ALA:HB3	1.94	0.49
9:H:32:GLY:N	38:H:3111:HOH:O	2.45	0.49
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.94	0.49
14:M:35:ARG:HB2	14:M:43:HIS:CD2	2.47	0.49
1:A:170:U:H5'	31:4:48:ASN:HB3	1.95	0.48
1:A:690:G:H4'	1:A:741:C:O2	2.13	0.48
1:A:696:C:O2'	1:A:697:G:H5'	2.13	0.48
1:A:1123:A:N6	1:A:1238:C:H5'	2.28	0.48
1:A:2121:G:O2'	15:N:83:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2403:C:H2'	1:A:2404:G:O5'	2.12	0.48
38:A:9645:HOH:O	31:4:46:ILE:HG12	2.11	0.48
2:B:3023:U:H6	2:B:3023:U:C5'	2.26	0.48
2:B:3053:G:O2'	2:B:3054:A:H5'	2.13	0.48
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.95	0.48
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.95	0.48
5:D:205:VAL:O	5:D:307:ARG:NE	2.45	0.48
6:E:197:SER:OG	6:E:242:GLU:OE2	2.28	0.48
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.93	0.48
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.48	0.48
12:K:45:VAL:HG22	12:K:46:ILE:N	2.28	0.48
25:X:14:HIS:HB2	25:X:17:ILE:HG13	1.94	0.48
1:A:10:U:H1'	1:A:532:A:H62	1.78	0.48
1:A:585:C:H2'	1:A:586:C:C6	2.47	0.48
1:A:639:A:H2'	1:A:640:G:H8	1.73	0.48
1:A:734:U:O2'	1:A:737:A:N6	2.46	0.48
1:A:1187:U:C3'	38:A:6366:HOH:O	2.61	0.48
1:A:1192:A:O2'	1:A:1193:A:OP1	2.31	0.48
1:A:1244:U:OP1	12:K:18:ILE:HD13	2.13	0.48
1:A:1278:A:H4'	1:A:1279:U:C4	2.48	0.48
1:A:1396:C:H1'	18:Q:1:THR:O	2.13	0.48
1:A:1477:C:O2'	1:A:1478:U:H5'	2.13	0.48
1:A:1500:U:P	18:Q:41:ARG:HH22	2.36	0.48
1:A:1852:A:H4'	4:C:230:SER:HB2	1.95	0.48
1:A:2492:U:H5	38:A:6490:HOH:O	1.95	0.48
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.94	0.48
38:A:5966:HOH:O	15:N:189:VAL:HA	2.11	0.48
4:C:200:PRO:HG2	4:C:225:VAL:HG21	1.95	0.48
11:J:57:ARG:HG3	11:J:57:ARG:NH1	2.29	0.48
13:L:63:GLU:HG3	38:L:6344:HOH:O	2.12	0.48
13:L:118:ALA:HA	13:L:125:ALA:HB2	1.94	0.48
14:M:133:VAL:HB	38:M:8433:HOH:O	2.12	0.48
15:N:14:ARG:CB	15:N:17:GLU:HG3	2.41	0.48
25:X:11:VAL:O	25:X:12:ASN:HB2	2.13	0.48
25:X:52:VAL:HG13	25:X:53:ALA:N	2.27	0.48
1:A:710:G:P	17:P:24:ALA:HB3	2.53	0.48
1:A:1084:C:O5'	1:A:1084:C:H6	1.95	0.48
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.48	0.48
1:A:1743:G:H1'	38:A:4373:HOH:O	2.13	0.48
1:A:2084:C:H2'	1:A:2085:A:H8	1.78	0.48
38:A:5527:HOH:O	31:4:62:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.42	0.48
6:E:214:THR:HG23	38:E:8436:HOH:O	2.12	0.48
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.95	0.48
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.78	0.48
15:N:63:VAL:HG21	15:N:109:PHE:CE1	2.48	0.48
15:N:184:ARG:HB2	15:N:184:ARG:CZ	2.44	0.48
17:P:22:GLY:O	38:P:2823:HOH:O	2.20	0.48
25:X:19:ASP:O	25:X:23:MET:HG3	2.13	0.48
25:X:122:ARG:HH22	25:X:154:ARG:C	2.16	0.48
27:Z:186:ARG:HG2	27:Z:186:ARG:NH1	2.28	0.48
27:Z:187:VAL:HG23	27:Z:192:ASP:HB3	1.94	0.48
31:4:55:VAL:HG22	38:4:8511:HOH:O	2.13	0.48
1:A:412:C:O2'	1:A:413:G:H5'	2.14	0.48
1:A:481:U:H5'	38:A:5127:HOH:O	2.13	0.48
1:A:894:A:H1'	38:A:4712:HOH:O	2.13	0.48
1:A:2460:A:OP1	31:4:60:LYS:CB	2.62	0.48
2:B:3026:C:H1'	38:B:8421:HOH:O	2.12	0.48
2:B:3056:A:C4	7:F:13:MET:HB3	2.49	0.48
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.48	0.48
11:J:26:LYS:HG2	11:J:28:ILE:N	2.27	0.48
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.95	0.48
30:3:18:ASN:ND2	30:3:40:ARG:H	2.11	0.48
31:4:11:CYS:SG	31:4:71:CYS:HB2	2.53	0.48
1:A:716:G:H2'	1:A:717:C:O5'	2.14	0.48
1:A:735:C:OP1	1:A:735:C:C6	2.66	0.48
1:A:1333:U:H2'	1:A:1334:C:H6	1.78	0.48
1:A:2338:G:OP1	7:F:97:GLN:HG3	2.12	0.48
1:A:2346:C:H4'	7:F:52:THR:HG22	1.94	0.48
2:B:3055:U:H4'	2:B:3056:A:C8	2.49	0.48
5:D:81:ALA:CB	5:D:142:LEU:HD13	2.43	0.48
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.49	0.48
6:E:12:THR:HB	38:E:8440:HOH:O	2.13	0.48
6:E:103:ASN:HB2	6:E:106:GLU:HB2	1.96	0.48
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.43	0.48
16:O:180:LEU:O	16:O:181:ASP:HB3	2.12	0.48
22:U:52:ARG:O	22:U:53:GLY:O	2.32	0.48
23:V:20:MET:HE1	38:V:7438:HOH:O	2.14	0.48
28:1:55:TRP:CZ2	28:1:70:GLN:C	2.87	0.48
1:A:101:C:H2'	1:A:102:A:C8	2.48	0.48
1:A:319:A:H4'	1:A:338:C:C4	2.49	0.48
1:A:1555:G:H4'	1:A:1630:A:C2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:C:H3'	38:A:7279:HOH:O	2.12	0.48
1:A:1768:C:H2'	1:A:1769:C:O4'	2.12	0.48
1:A:1772:C:O4'	1:A:1773:G:C2	2.67	0.48
1:A:1873:G:H2'	1:A:1874:U:H5'	1.96	0.48
1:A:2638:G:H5'	38:A:4413:HOH:O	2.13	0.48
1:A:2737:C:H2'	38:A:5632:HOH:O	2.14	0.48
38:A:3146:HOH:O	17:P:3:THR:HG21	2.12	0.48
38:A:4225:HOH:O	16:O:21:HIS:HB2	2.14	0.48
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.78	0.48
4:C:135:VAL:N	38:C:8609:HOH:O	2.45	0.48
5:D:144:THR:CG2	5:D:145:HIS:N	2.77	0.48
5:D:305:ASP:O	5:D:306:LYS:HB2	2.14	0.48
6:E:20:ASP:O	6:E:23:GLU:HB2	2.12	0.48
6:E:153:VAL:O	6:E:157:LEU:HG	2.14	0.48
7:F:16:PRO:HB2	7:F:165:PHE:CD1	2.48	0.48
7:F:159:PRO:O	7:F:163:VAL:HG23	2.13	0.48
9:H:58:GLU:CD	15:N:27:ARG:HH22	2.15	0.48
9:H:79:GLN:HB2	9:H:82:ASP:OD2	2.13	0.48
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.28	0.48
13:L:125:ALA:C	13:L:127:ALA:H	2.16	0.48
15:N:48:ARG:NH2	38:N:8556:HOH:O	2.45	0.48
22:U:45:GLY:HA3	22:U:102:ASP:CB	2.44	0.48
25:X:72:PRO:CG	25:X:77:ALA:HB3	2.32	0.48
26:Y:7:GLU:HA	26:Y:74:ALA:O	2.13	0.48
31:4:69:TYR:O	31:4:77:ALA:HA	2.13	0.48
1:A:187:A:OP1	15:N:154:ARG:NE	2.47	0.48
1:A:1554:U:O2'	1:A:1631:A:N3	2.43	0.48
1:A:1741:U:O2'	1:A:2723:G:H4'	2.13	0.48
1:A:1878:G:C1'	38:A:5611:HOH:O	2.53	0.48
1:A:2106:C:H1'	1:A:2484:U:O2	2.14	0.48
1:A:2812:A:H1'	38:A:5270:HOH:O	2.13	0.48
1:A:2913:A:OP2	38:A:5856:HOH:O	2.20	0.48
4:C:48:ASP:HB3	38:C:8621:HOH:O	2.14	0.48
6:E:5:ILE:HG23	38:E:8429:HOH:O	2.14	0.48
6:E:218:VAL:HG12	38:E:8422:HOH:O	2.13	0.48
8:G:11:VAL:HG12	8:G:12:ASP:H	1.77	0.48
8:G:132:THR:O	8:G:132:THR:HG23	2.13	0.48
8:G:156:ASP:OD2	8:G:157:LYS:NZ	2.37	0.48
13:L:22:ASP:CG	13:L:24:THR:HG23	2.34	0.48
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.49	0.48
28:1:46:LYS:HB2	28:1:57:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:C:O2'	1:A:1484:G:H5'	2.14	0.48
1:A:1598:A:N6	35:A:8515:CL:CL	2.84	0.48
1:A:2029:C:O2'	1:A:2030:A:H5'	2.14	0.48
1:A:2468:A:H61	31:4:48:ASN:HD21	1.62	0.48
1:A:2716:G:H5"	5:D:206:THR:CG2	2.32	0.48
9:H:58:GLU:HG3	9:H:61:MET:HE1	1.95	0.48
10:I:71:LEU:C	10:I:73:ASP:N	2.66	0.48
12:K:40:ASN:HA	12:K:106:GLY:H	1.79	0.48
13:L:28:GLU:HG2	13:L:58:THR:HB	1.94	0.48
1:A:349:U:O2'	1:A:350:C:H5'	2.14	0.48
1:A:485:A:N3	1:A:487:G:H5"	2.29	0.48
1:A:539:G:H2'	1:A:540:A:C8	2.49	0.48
1:A:894:A:C2	6:E:87:ARG:NH2	2.82	0.48
1:A:1266:U:O3'	27:Z:115:ARG:NH2	2.46	0.48
1:A:1874:U:P	4:C:51:ARG:HD2	2.54	0.48
1:A:2765:C:H2'	1:A:2766:A:C8	2.48	0.48
4:C:36:ASP:HB2	4:C:83:GLY:HA3	1.96	0.48
5:D:294:TYR:HE2	38:D:8659:HOH:O	1.96	0.48
7:F:140:ARG:HH11	7:F:140:ARG:HG3	1.78	0.48
11:J:17:ARG:HD3	11:J:23:ILE:CD1	2.43	0.48
11:J:166:ASN:N	11:J:166:ASN:HD22	2.11	0.48
12:K:36:VAL:HG12	12:K:37:ALA:N	2.29	0.48
16:O:75:THR:CG2	38:O:8536:HOH:O	2.61	0.48
16:O:78:MET:CB	16:O:79:PRO:HD3	2.44	0.48
25:X:35:VAL:CG2	25:X:41:TYR:CD2	2.96	0.48
1:A:184:G:H5"	15:N:153:THR:HG22	1.96	0.48
1:A:694:A:C2'	1:A:695:C:H5'	2.42	0.48
1:A:1342:C:C2'	1:A:1343:C:H5'	2.44	0.48
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.78	0.48
1:A:2852:A:H5"	38:A:4718:HOH:O	2.14	0.48
5:D:325:PRO:HD2	38:D:8570:HOH:O	2.14	0.48
11:J:161:SER:HB3	38:J:8351:HOH:O	2.14	0.48
12:K:12:VAL:HG11	12:K:116:LEU:HD11	1.96	0.48
12:K:77:GLY:O	12:K:78:ILE:C	2.52	0.48
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.44	0.48
31:4:84:ARG:HB2	38:4:8514:HOH:O	2.13	0.48
1:A:968:G:O2'	1:A:969:G:H5'	2.14	0.47
1:A:1023:C:O2'	1:A:1024:G:H5'	2.15	0.47
1:A:1517:U:C2	1:A:1670:G:N2	2.82	0.47
38:A:5661:HOH:O	5:D:216:LYS:HB2	2.12	0.47
2:B:3114:G:O6	16:O:11:ARG:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:81:ALA:O	5:D:186:GLY:HA3	2.14	0.47
9:H:26:THR:HG21	9:H:103:ALA:CB	2.43	0.47
11:J:82:LYS:NZ	11:J:82:LYS:CB	2.77	0.47
14:M:65:ASP:CG	14:M:111:ALA:HB3	2.34	0.47
15:N:81:ARG:HG3	15:N:85:ARG:HB2	1.96	0.47
17:P:33:LEU:HA	17:P:40:HIS:CE1	2.49	0.47
19:R:21:ARG:HG2	19:R:22:GLY:N	2.29	0.47
24:W:16:ARG:NH1	24:W:65:ASP:O	2.47	0.47
28:1:75:ALA:O	28:1:79:VAL:HG23	2.14	0.47
1:A:242:A:N6	1:A:269:G:H1'	2.29	0.47
1:A:251:C:O2'	1:A:252:C:H5'	2.14	0.47
1:A:558:C:H5'	38:A:4742:HOH:O	2.13	0.47
1:A:622:G:P	27:Z:148:GLY:HA3	2.54	0.47
1:A:661:G:C4	1:A:686:A:C2	3.02	0.47
1:A:1097:A:H5"	25:X:125:HIS:NE2	2.29	0.47
1:A:1132:A:N6	1:A:1229:C:H2'	2.29	0.47
1:A:1994:A:P	13:L:66:ARG:HH22	2.37	0.47
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.47	0.47
1:A:2650:U:O2'	1:A:2651:C:H5'	2.15	0.47
38:A:9998:HOH:O	18:Q:133:SER:HA	2.13	0.47
4:C:112:PRO:HB3	4:C:151:GLN:HB3	1.96	0.47
13:L:14:LYS:NZ	13:L:32:ILE:O	2.42	0.47
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.29	0.47
13:L:87:ARG:NE	38:L:4854:HOH:O	2.46	0.47
14:M:94:ARG:NH1	14:M:143:THR:HG21	2.29	0.47
1:A:1751:G:C3'	1:A:1752:G:H5"	2.44	0.47
1:A:2362:A:H2'	1:A:2363:G:C8	2.49	0.47
1:A:2488:A:H61	1:A:2534:C:H42	1.62	0.47
4:C:171:LYS:HE3	38:C:8570:HOH:O	2.14	0.47
5:D:195:ARG:NH1	5:D:324:ASP:OD1	2.41	0.47
15:N:47:ASP:O	15:N:51:SER:HB2	2.15	0.47
1:A:581:G:O2'	1:A:582:C:H5'	2.14	0.47
1:A:1808:C:O2'	1:A:1809:G:H5'	2.14	0.47
1:A:1823:G:C2	1:A:2027:U:C2	3.02	0.47
1:A:2327:A:H2'	1:A:2328:U:C6	2.48	0.47
1:A:2334:C:O2'	1:A:2335:C:H5'	2.14	0.47
9:H:22:VAL:HG21	9:H:104:ALA:HB2	1.96	0.47
12:K:93:ARG:O	12:K:96:GLU:HB2	2.15	0.47
20:S:111:ILE:O	20:S:111:ILE:HG22	2.14	0.47
22:U:71:VAL:HG12	22:U:72:ILE:N	2.29	0.47
27:Z:187:VAL:HB	27:Z:203:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:A:H5"	1:A:1353:C:OP2	2.14	0.47
1:A:1450:C:O2'	1:A:1494:A:H5'	2.14	0.47
1:A:1754:A:H2'	1:A:1755:A:O4'	2.14	0.47
1:A:2111:G:H5"	38:A:4327:HOH:O	2.14	0.47
1:A:2424:U:H5'	38:A:6755:HOH:O	2.15	0.47
1:A:2775:A:C6	1:A:2799:A:C8	3.02	0.47
4:C:36:ASP:O	4:C:38:ILE:N	2.47	0.47
8:G:126:ILE:HB	8:G:131:LEU:HD21	1.95	0.47
14:M:93:VAL:CG2	14:M:122:ALA:HB2	2.44	0.47
23:V:4:ARG:N	38:V:5334:HOH:O	2.48	0.47
1:A:371:U:H2'	1:A:372:A:C8	2.50	0.47
1:A:392:U:C5'	15:N:193:LYS:HB3	2.44	0.47
1:A:790:A:H1'	1:A:1710:A:H2'	1.96	0.47
1:A:875:A:H5'	1:A:876:A:N7	2.29	0.47
1:A:2431:C:O2'	1:A:2432:C:H5'	2.15	0.47
1:A:2502:C:H4'	11:J:151:MET:CG	2.42	0.47
1:A:2526:C:HO2'	1:A:2527:U:H5'	1.79	0.47
1:A:2866:U:C5	23:V:50:GLU:HB2	2.49	0.47
5:D:243:ASN:HA	5:D:244:PRO:C	2.34	0.47
5:D:297:VAL:HB	38:D:8611:HOH:O	2.14	0.47
16:O:58:LEU:N	16:O:58:LEU:CD1	2.78	0.47
28:1:44:PHE:HD2	28:1:46:LYS:HD2	1.80	0.47
29:2:30:LYS:HD3	38:2:3205:HOH:O	2.15	0.47
1:A:111:C:O2'	29:2:20:ARG:HG2	2.15	0.47
1:A:161:A:OP1	15:N:81:ARG:HA	2.14	0.47
1:A:716:G:C2'	1:A:717:C:O5'	2.63	0.47
1:A:721:A:C2'	1:A:722:G:H5'	2.45	0.47
1:A:819:A:H5"	38:1:8418:HOH:O	2.15	0.47
1:A:947:U:H2'	1:A:948:G:C8	2.50	0.47
1:A:1014:A:H5"	2:B:3101:G:O2'	2.14	0.47
1:A:1204:C:H6	1:A:1204:C:O5'	1.98	0.47
1:A:1329:A:H2	38:A:4164:HOH:O	1.97	0.47
1:A:1565:C:O2'	1:A:1566:C:H5'	2.14	0.47
1:A:1819:G:H2'	1:A:1820:G:C4'	2.41	0.47
1:A:1882:C:H2'	1:A:1883:U:H6	1.78	0.47
1:A:1997:A:N1	38:A:6441:HOH:O	2.35	0.47
1:A:2415:A:N3	16:O:26:LEU:HD13	2.30	0.47
2:B:3012:C:H5'	2:B:3070:U:O4'	2.14	0.47
3:5:74:C:O2'	3:5:75:C:H5'	2.14	0.47
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.95	0.47
4:C:215:ILE:HG13	4:C:216:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:140:VAL:HG12	6:E:141:SER:N	2.29	0.47
6:E:162:VAL:HG12	6:E:192:ILE:CD1	2.44	0.47
7:F:45:THR:HB	7:F:75:LEU:HD21	1.95	0.47
7:F:95:THR:C	7:F:97:GLN:N	2.66	0.47
8:G:22:VAL:O	8:G:28:SER:HA	2.15	0.47
8:G:58:THR:O	8:G:59:MET:C	2.53	0.47
8:G:101:GLU:OE2	8:G:115:ARG:HD3	2.14	0.47
8:G:167:TYR:N	8:G:167:TYR:CD1	2.83	0.47
10:I:64:ASN:ND2	10:I:64:ASN:H	2.13	0.47
11:J:140:PRO:HA	11:J:142:VAL:HG12	1.95	0.47
12:K:93:ARG:HH11	12:K:93:ARG:CB	2.23	0.47
17:P:85:ALA:O	17:P:89:ILE:HG13	2.14	0.47
18:Q:5:ALA:HB3	38:Q:1715:HOH:O	2.15	0.47
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.97	0.47
23:V:8:TYR:O	23:V:46:ALA:CB	2.63	0.47
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.14	0.47
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.79	0.47
28:1:56:MET:CE	28:1:63:LYS:HG3	2.44	0.47
31:4:70:ARG:HB3	38:4:8571:HOH:O	2.14	0.47
1:A:111:C:C2'	1:A:112:G:H5'	2.44	0.47
1:A:517:U:H2'	1:A:518:G:H5'	1.97	0.47
1:A:934:C:H1'	38:A:9848:HOH:O	2.15	0.47
1:A:1734:C:OP1	5:D:234:ARG:NH1	2.46	0.47
1:A:2842:G:H2'	1:A:2843:A:H5'	1.96	0.47
6:E:21:VAL:C	6:E:23:GLU:H	2.18	0.47
7:F:65:GLU:HG3	38:F:6752:HOH:O	2.14	0.47
7:F:155:HIS:NE2	38:F:7597:HOH:O	2.36	0.47
11:J:74:ASN:ND2	11:J:141:ASN:OD1	2.48	0.47
11:J:112:ARG:O	11:J:113:ALA:C	2.52	0.47
22:U:27:LEU:HD21	22:U:40:VAL:CG1	2.45	0.47
31:4:17:HIS:O	31:4:18:GLN:HG3	2.15	0.47
1:A:262:A:OP2	9:H:91:VAL:HG11	2.15	0.47
1:A:797:A:C4'	28:1:10:ARG:N	2.78	0.47
1:A:820:G:H5'	1:A:821:U:C5'	2.45	0.47
1:A:1191:A:C2	1:A:1207:A:C2	3.03	0.47
1:A:1730:G:H5'	1:A:1731:C:C6	2.50	0.47
1:A:1804:A:O2'	1:A:1805:G:H5'	2.15	0.47
1:A:2072:G:C6	1:A:2533:C:H1'	2.50	0.47
1:A:2432:C:H1'	38:A:3570:HOH:O	2.14	0.47
2:B:3114:G:H2'	2:B:3115:C:C6	2.50	0.47
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:190:MET:HE2	5:D:194:PHE:CD1	2.50	0.47
14:M:73:VAL:HG21	14:M:116:HIS:CD2	2.50	0.47
15:N:63:VAL:O	15:N:130:GLU:HA	2.15	0.47
16:O:163:PHE:O	16:O:164:ASP:O	2.32	0.47
17:P:25:VAL:HG23	17:P:26:TRP:H	1.79	0.47
18:Q:91:LYS:O	18:Q:95:GLU:HG3	2.15	0.47
20:S:6:VAL:HG23	20:S:113:HIS:CE1	2.50	0.47
25:X:40:ALA:O	25:X:44:MET:HG3	2.14	0.47
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.50	0.47
25:X:121:PRO:HA	25:X:153:MET:HG2	1.96	0.47
26:Y:78:GLU:CG	26:Y:79:GLU:N	2.77	0.47
29:2:29:THR:O	29:2:32:LYS:HE2	2.15	0.47
1:A:136:C:H2'	1:A:137:U:O4'	2.15	0.47
1:A:218:C:OP1	31:4:39:GLN:NE2	2.36	0.47
1:A:697:G:H4'	1:A:730:G:O3'	2.15	0.47
1:A:1187:U:H3'	38:A:6366:HOH:O	2.14	0.47
1:A:1314:U:H5"	1:A:1316:G:O4'	2.14	0.47
1:A:1477:C:H5'	1:A:1868:G:C5'	2.45	0.47
1:A:1527:A:H1'	1:A:1528:A:C8	2.49	0.47
1:A:1878:G:HO2'	1:A:1879:U:H6	1.57	0.47
1:A:2432:C:H2'	1:A:2433:A:H8	1.80	0.47
38:A:9682:HOH:O	15:N:9:ARG:HG3	2.14	0.47
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.74	0.47
38:G:2512:HOH:O	12:K:127:ILE:HD11	2.14	0.47
11:J:43:PRO:HD2	11:J:137:ASN:HA	1.97	0.47
11:J:113:ALA:N	11:J:114:PRO:HD3	2.29	0.47
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.96	0.47
16:O:165:ALA:HA	38:O:8518:HOH:O	2.14	0.47
20:S:114:VAL:O	20:S:114:VAL:HG13	2.14	0.47
31:4:65:THR:HB	31:4:83:TRP:H	1.79	0.47
1:A:1023:C:H2'	1:A:1024:G:O4'	2.14	0.46
1:A:1855:G:H4'	1:A:1856:C:O5'	2.15	0.46
1:A:2748:G:H1'	38:A:7371:HOH:O	2.15	0.46
38:A:4192:HOH:O	19:R:48:PRO:HG3	2.15	0.46
4:C:211:LYS:NZ	38:C:8584:HOH:O	2.43	0.46
5:D:157:LYS:HG2	38:D:8668:HOH:O	2.15	0.46
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.28	0.46
11:J:112:ARG:HB3	38:J:8383:HOH:O	2.15	0.46
11:J:141:ASN:CA	38:J:8355:HOH:O	2.62	0.46
12:K:37:ALA:HA	12:K:102:ARG:O	2.15	0.46
14:M:75:LEU:N	14:M:75:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:93:VAL:HG12	14:M:97:VAL:HG23	1.95	0.46
25:X:122:ARG:NE	38:X:5817:HOH:O	2.48	0.46
1:A:185:G:H4'	1:A:186:A:OP1	2.15	0.46
1:A:558:C:C2'	1:A:559:U:C5'	2.92	0.46
1:A:830:G:O2'	1:A:831:U:H5'	2.16	0.46
1:A:1309:U:O2'	1:A:1310:U:H5'	2.15	0.46
1:A:2039:A:H2'	1:A:2040:C:H6	1.80	0.46
1:A:2241:C:O2'	1:A:2242:U:H5'	2.15	0.46
1:A:2353:A:H4'	1:A:2354:A:O5'	2.15	0.46
1:A:2819:C:H2'	1:A:2820:A:C8	2.50	0.46
8:G:36:PRO:HD3	12:K:127:ILE:HD12	1.97	0.46
9:H:26:THR:HG21	9:H:103:ALA:HB2	1.96	0.46
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.45	0.46
12:K:90:LYS:HB2	35:K:8502:CL:CL	2.53	0.46
16:O:184:ILE:HG22	16:O:185:GLU:N	2.30	0.46
18:Q:6:GLN:OE1	18:Q:6:GLN:N	2.35	0.46
22:U:92:ASP:C	22:U:94:SER:H	2.18	0.46
28:1:41:VAL:HG12	28:1:42:CYS:N	2.28	0.46
1:A:396:U:H4'	38:A:3916:HOH:O	2.14	0.46
1:A:834:G:H4'	1:A:835:U:OP2	2.15	0.46
1:A:861:A:H2'	1:A:862:U:C6	2.50	0.46
1:A:2430:A:H2'	1:A:2431:C:C6	2.50	0.46
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.46
2:B:3019:G:O2'	2:B:3020:G:H5'	2.16	0.46
5:D:44:TYR:OH	5:D:148:PRO:HG3	2.14	0.46
5:D:51:VAL:CG2	5:D:330:VAL:HG22	2.45	0.46
7:F:64:ARG:HB3	7:F:67:ASP:OD2	2.15	0.46
9:H:21:GLU:O	9:H:24:ARG:HG3	2.14	0.46
9:H:56:PRO:HG2	15:N:44:THR:HA	1.95	0.46
11:J:65:ARG:CZ	38:J:8373:HOH:O	2.62	0.46
11:J:82:LYS:HB2	11:J:82:LYS:HZ2	1.81	0.46
12:K:122:ASP:OD1	12:K:124:LEU:HB2	2.15	0.46
13:L:32:ILE:CD1	13:L:56:SER:HB3	2.43	0.46
13:L:98:VAL:HG13	13:L:99:ASP:N	2.29	0.46
19:R:40:HIS:CE1	19:R:94:GLN:HA	2.51	0.46
20:S:47:LEU:O	20:S:51:ILE:HG13	2.16	0.46
22:U:20:HIS:CE1	22:U:67:LEU:HD11	2.50	0.46
1:A:107:U:H2'	1:A:108:U:H5'	1.97	0.46
1:A:710:G:OP1	17:P:24:ALA:HB3	2.16	0.46
1:A:731:U:H2'	1:A:732:C:C6	2.51	0.46
1:A:858:U:H2'	1:A:859:C:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:G:C2'	1:A:1417:G:H5'	2.45	0.46
38:A:3833:HOH:O	27:Z:214:ARG:CZ	2.62	0.46
4:C:199:HIS:HD2	4:C:201:PHE:H	1.62	0.46
5:D:98:THR:HG22	5:D:99:GLU:H	1.81	0.46
6:E:129:HIS:HE1	6:E:231:ARG:HA	1.80	0.46
7:F:154:LYS:H	7:F:154:LYS:CD	2.21	0.46
9:H:34:ASN:ND2	9:H:38:LYS:HE2	2.30	0.46
12:K:48:GLY:CA	12:K:53:ILE:HD11	2.45	0.46
12:K:56:LYS:HE2	12:K:60:ARG:NH2	2.30	0.46
14:M:66:VAL:CG2	14:M:67:ARG:N	2.77	0.46
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.30	0.46
26:Y:25:ARG:HG2	38:Y:5356:HOH:O	2.13	0.46
27:Z:106:THR:HG22	27:Z:107:PRO:O	2.15	0.46
1:A:306:A:P	22:U:38:ARG:HH21	2.38	0.46
1:A:567:U:H6	1:A:567:U:O5'	1.99	0.46
1:A:573:A:P	38:A:6516:HOH:O	2.74	0.46
1:A:936:C:O2'	1:A:937:C:H5'	2.16	0.46
1:A:941:G:O2'	1:A:942:U:H5'	2.15	0.46
1:A:1044:C:H5"	38:A:8543:HOH:O	2.15	0.46
1:A:1187:U:C2'	38:A:6366:HOH:O	2.53	0.46
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.15	0.46
1:A:1669:A:C2	38:A:3200:HOH:O	2.56	0.46
1:A:1827:G:C6	1:A:1828:G:C6	3.04	0.46
5:D:171:VAL:HG23	5:D:172:SER:N	2.30	0.46
8:G:20:ILE:O	8:G:30:THR:HA	2.16	0.46
9:H:34:ASN:HA	15:N:4:ALA:HB2	1.98	0.46
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.45	0.46
11:J:12:PRO:HD2	38:J:8341:HOH:O	2.16	0.46
14:M:7:GLN:HB3	14:M:13:HIS:CE1	2.51	0.46
16:O:157:PRO:HA	38:O:8526:HOH:O	2.15	0.46
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.79	0.46
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.45	0.46
21:T:81:ILE:HG23	38:T:8334:HOH:O	2.16	0.46
24:W:42:ASN:HB3	38:W:7247:HOH:O	2.16	0.46
26:Y:86:GLU:O	26:Y:87:ALA:O	2.32	0.46
1:A:151:A:C2	1:A:442:A:C8	3.04	0.46
1:A:221:G:H2'	1:A:222:A:C8	2.50	0.46
1:A:322:G:O2'	1:A:323:C:H5'	2.16	0.46
1:A:645:U:O2	1:A:761:A:H2	1.99	0.46
1:A:1151:G:P	10:I:16:LYS:HZ1	2.34	0.46
1:A:2291:A:N9	1:A:2309:C:H5'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2906:A:H5'	1:A:2907:C:O4'	2.15	0.46
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.96	0.46
4:C:100:PRO:HG2	4:C:103:VAL:CG2	2.46	0.46
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.51	0.46
16:O:48:VAL:HG12	16:O:49:THR:N	2.30	0.46
16:O:149:GLU:O	16:O:152:GLU:HB2	2.16	0.46
1:A:514:G:H2'	1:A:514:G:P	2.56	0.46
1:A:1215:A:O3'	1:A:1216:G:C4'	2.63	0.46
1:A:1426:C:H2'	38:A:9094:HOH:O	2.16	0.46
1:A:1659:A:H2'	1:A:1660:G:O4'	2.16	0.46
1:A:2256:G:C2'	1:A:2257:G:C5'	2.87	0.46
1:A:2364:A:H5"	19:R:15:LYS:HD3	1.97	0.46
1:A:2493:C:H2'	38:A:4158:HOH:O	2.16	0.46
1:A:2507:G:H2'	1:A:2510:C:N4	2.30	0.46
1:A:2673:U:C2	1:A:2817:G:N2	2.84	0.46
2:B:3095:C:O2'	2:B:3096:C:H5'	2.15	0.46
5:D:76:THR:N	5:D:77:PRO:HD3	2.30	0.46
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.15	0.46
6:E:136:VAL:HG22	6:E:137:PRO:HA	1.98	0.46
8:G:69:ILE:O	8:G:72:MET:HB2	2.15	0.46
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.50	0.46
11:J:163:PRO:O	11:J:164:ALA:HB2	2.15	0.46
15:N:104:ARG:O	15:N:108:LYS:HE2	2.16	0.46
17:P:99:GLU:CG	38:P:6044:HOH:O	2.63	0.46
30:3:18:ASN:HD21	30:3:40:ARG:H	1.64	0.46
31:4:40:ARG:HA	31:4:52:PHE:CE1	2.51	0.46
1:A:506:G:N2	1:A:509:A:H5'	2.21	0.46
1:A:1168:C:H2'	1:A:1169:U:O4'	2.15	0.46
1:A:1497:G:O2'	1:A:1498:G:H5'	2.16	0.46
1:A:1592:G:O2'	1:A:1593:C:O4'	2.32	0.46
1:A:2717:C:H5'	5:D:302:PRO:HA	1.97	0.46
2:B:3049:G:H2'	2:B:3050:G:O4'	2.16	0.46
4:C:101:GLU:HG2	4:C:131:HIS:ND1	2.31	0.46
9:H:101:ALA:HA	38:H:5413:HOH:O	2.15	0.46
11:J:74:ASN:HD22	11:J:141:ASN:CG	2.18	0.46
15:N:35:PRO:HD2	15:N:38:VAL:CG2	2.46	0.46
15:N:184:ARG:HG3	15:N:185:PRO:HA	1.98	0.46
16:O:34:LEU:HD22	16:O:129:ILE:HD13	1.98	0.46
18:Q:115:SER:O	18:Q:118:GLN:N	2.48	0.46
27:Z:100:ARG:HE	27:Z:234:VAL:HG21	1.80	0.46
28:1:47:LEU:HD23	28:1:57:CYS:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:G:H21	20:S:117:HIS:CD2	2.25	0.46
1:A:204:A:H2'	1:A:205:U:H5'	1.96	0.46
1:A:282:C:H2'	1:A:283:U:O4'	2.15	0.46
1:A:1299:G:N2	38:A:4164:HOH:O	2.48	0.46
1:A:2416:G:H2'	1:A:2417:C:C6	2.51	0.46
1:A:2453:G:H2'	1:A:2454:C:C6	2.51	0.46
1:A:2457:U:H1'	31:4:79:LEU:HD13	1.98	0.46
2:B:3036:C:C5	2:B:3037:C:C5	3.04	0.46
38:B:8478:HOH:O	16:O:23:ARG:NH1	2.49	0.46
4:C:228:ILE:HG13	38:C:8516:HOH:O	2.16	0.46
5:D:27:ASN:HD22	5:D:27:ASN:H	1.64	0.46
8:G:118:ILE:HG23	8:G:144:THR:CG2	2.46	0.46
10:I:23:ILE:HG22	10:I:70:ALA:CB	2.46	0.46
11:J:53:PRO:HA	11:J:125:VAL:O	2.14	0.46
11:J:157:ILE:CG2	11:J:158:ASN:N	2.79	0.46
12:K:40:ASN:OD1	12:K:106:GLY:HA2	2.16	0.46
13:L:115:ARG:HG3	13:L:116:GLU:H	1.81	0.46
15:N:35:PRO:CD	15:N:38:VAL:HG23	2.45	0.46
17:P:113:VAL:O	17:P:114:ILE:HD13	2.15	0.46
20:S:100:ASP:O	20:S:102:GLN:N	2.49	0.46
23:V:31:PHE:CE2	23:V:37:GLU:HA	2.51	0.46
25:X:4:LEU:HD23	25:X:4:LEU:HA	1.79	0.46
1:A:257:G:O2'	1:A:258:G:H5'	2.15	0.46
1:A:821:U:H5"	38:A:9553:HOH:O	2.14	0.46
1:A:1314:U:C2	1:A:1316:G:N2	2.84	0.46
1:A:1380:U:OP2	1:A:2747:C:N4	2.49	0.46
1:A:1512:G:O2'	1:A:1513:C:H5'	2.16	0.46
1:A:2269:C:H2'	1:A:2270:G:O4'	2.15	0.46
1:A:2434:A:H4'	31:4:28:GLY:O	2.16	0.46
1:A:2438:G:H2'	1:A:2439:C:C6	2.50	0.46
1:A:2514:U:H6	1:A:2514:U:O5'	2.00	0.46
1:A:2897:C:H2'	1:A:2898:G:C8	2.50	0.46
2:B:3057:A:N6	38:B:8447:HOH:O	2.49	0.46
4:C:217:ARG:HH11	4:C:217:ARG:CG	2.28	0.46
5:D:215:VAL:HG11	5:D:234:ARG:NH2	2.31	0.46
6:E:15:GLU:CG	38:E:8336:HOH:O	2.64	0.46
6:E:224:ALA:HB1	6:E:228:ALA:O	2.15	0.46
7:F:99:ASP:CB	7:F:103:ASN:H	2.29	0.46
13:L:118:ALA:O	13:L:120:ARG:N	2.49	0.46
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.99	0.46
28:1:58:GLY:CA	38:1:8436:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:C:C3'	1:A:246:G:H5'	2.46	0.45
1:A:1245:C:H5"	1:A:1246:A:H8	1.80	0.45
1:A:1771:U:O2'	28:1:23:ARG:NH2	2.44	0.45
1:A:1825:U:O4'	1:A:1999:C:H5"	2.16	0.45
1:A:2673:U:C2'	1:A:2674:G:H5'	2.46	0.45
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.81	0.45
38:A:9101:HOH:O	15:N:165:SER:HB3	2.16	0.45
5:D:305:ASP:O	5:D:306:LYS:CB	2.63	0.45
6:E:246:ARG:NH2	38:E:8422:HOH:O	2.49	0.45
8:G:11:VAL:CG1	8:G:22:VAL:HG13	2.45	0.45
8:G:107:PHE:CD2	8:G:108:LEU:HD13	2.51	0.45
9:H:23:ALA:O	9:H:27:GLY:N	2.49	0.45
11:J:127:GLY:O	11:J:128:ALA:CB	2.63	0.45
11:J:151:MET:CE	11:J:151:MET:HA	2.46	0.45
12:K:6:PHE:CD1	12:K:102:ARG:HD2	2.51	0.45
12:K:51:GLU:O	12:K:55:GLU:HG3	2.16	0.45
14:M:124:ASP:OD1	14:M:149:ARG:NH2	2.49	0.45
28:1:30:GLU:HB3	28:1:34:LYS:CE	2.40	0.45
1:A:942:U:O4	38:A:9250:HOH:O	2.20	0.45
1:A:1245:C:H5"	1:A:1246:A:C8	2.51	0.45
9:H:37:THR:O	9:H:41:GLU:HG3	2.15	0.45
15:N:67:ILE:HD13	15:N:104:ARG:HH11	1.81	0.45
17:P:21:SER:HB2	17:P:106:PRO:O	2.17	0.45
22:U:79:LEU:HG	22:U:89:ARG:HB2	1.97	0.45
27:Z:216:ARG:NH1	38:Z:8532:HOH:O	2.48	0.45
28:1:77:LYS:HA	28:1:80:MET:CE	2.46	0.45
28:1:77:LYS:HA	28:1:80:MET:HE3	1.98	0.45
31:4:14:CYS:SG	31:4:18:GLN:NE2	2.89	0.45
1:A:40:C:H6	1:A:40:C:O5'	1.99	0.45
1:A:212:A:O4'	1:A:214:U:C6	2.69	0.45
1:A:394:G:O6	15:N:182:LYS:NZ	2.44	0.45
1:A:482:G:H4'	1:A:508:A:N1	2.32	0.45
1:A:588:G:O6	25:X:154:ARG:NH1	2.49	0.45
1:A:627:G:H2'	1:A:2071:C:C5	2.51	0.45
1:A:797:A:O4'	28:1:10:ARG:N	2.49	0.45
1:A:1253:C:H5'	38:A:7201:HOH:O	2.15	0.45
1:A:1767:A:O2'	1:A:1768:C:H5'	2.16	0.45
1:A:2239:C:H6	38:A:6143:HOH:O	1.99	0.45
1:A:2718:C:H6	1:A:2718:C:H5'	1.82	0.45
3:5:75:C:H42	36:5:76:PPU:H102	1.79	0.45
5:D:190:MET:CE	5:D:194:PHE:CD1	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:95:GLU:HG3	38:E:8474:HOH:O	2.15	0.45
12:K:4:ALA:O	12:K:5:GLU:O	2.34	0.45
13:L:3:ALA:HB1	38:L:581:HOH:O	2.17	0.45
13:L:84:ASP:O	23:V:16:GLY:HA2	2.16	0.45
14:M:146:GLY:O	14:M:148:GLU:N	2.48	0.45
16:O:139:TRP:HH2	16:O:176:ARG:HH11	1.64	0.45
17:P:80:ASP:CG	17:P:81:PHE:N	2.69	0.45
19:R:93:ARG:NH1	19:R:93:ARG:CG	2.80	0.45
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.77	0.45
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.46	0.45
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.97	0.45
1:A:162:C:C2'	1:A:163:U:H5'	2.46	0.45
1:A:475:G:C5'	6:E:73:LEU:HD23	2.47	0.45
1:A:661:G:C6	1:A:686:A:C2	3.05	0.45
1:A:876:A:N3	1:A:876:A:C2'	2.80	0.45
1:A:2251:G:H2'	1:A:2252:A:C8	2.52	0.45
1:A:2355:G:H2'	38:A:5117:HOH:O	2.15	0.45
1:A:2433:A:C2	1:A:2459:G:C2	3.04	0.45
1:A:2436:U:H5'	31:4:68:LYS:HE2	1.98	0.45
1:A:2607:U:H4'	38:A:8940:HOH:O	2.16	0.45
1:A:2766:A:H5'	38:A:9065:HOH:O	2.15	0.45
1:A:2815:G:H4'	1:A:2816:A:OP2	2.16	0.45
1:A:2860:G:N2	1:A:2898:G:C4	2.84	0.45
4:C:192:VAL:HG13	38:C:8563:HOH:O	2.16	0.45
4:C:212:PRO:HB2	38:C:8568:HOH:O	2.15	0.45
5:D:132:HIS:CE1	5:D:171:VAL:CG2	3.00	0.45
6:E:79:ARG:O	6:E:87:ARG:HG2	2.15	0.45
11:J:140:PRO:HA	11:J:142:VAL:CG1	2.45	0.45
11:J:166:ASN:N	11:J:166:ASN:ND2	2.65	0.45
13:L:122:GLY:O	13:L:125:ALA:N	2.49	0.45
15:N:18:GLY:O	15:N:21:ALA:HB3	2.15	0.45
18:Q:143:ALA:CA	38:Q:5521:HOH:O	2.60	0.45
24:W:23:LEU:HD12	24:W:56:ILE:HD12	1.98	0.45
27:Z:154:ARG:HH12	27:Z:155:ARG:CG	2.30	0.45
27:Z:174:VAL:HG12	27:Z:174:VAL:O	2.16	0.45
28:1:27:ALA:HA	38:1:8414:HOH:O	2.17	0.45
1:A:23:G:C6	1:A:24:G:N1	2.85	0.45
1:A:1652:C:H5"	28:1:52:THR:OG1	2.16	0.45
1:A:1656:A:H2'	1:A:1657:A:O4'	2.16	0.45
1:A:2361:A:H5"	38:A:8523:HOH:O	2.15	0.45
38:A:3280:HOH:O	15:N:189:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.31	0.45
5:D:280:VAL:C	38:D:8567:HOH:O	2.53	0.45
16:O:86:LEU:O	16:O:90:LEU:HG	2.17	0.45
22:U:71:VAL:CG1	22:U:72:ILE:N	2.78	0.45
25:X:122:ARG:HG2	25:X:122:ARG:NH1	2.31	0.45
31:4:84:ARG:HG3	31:4:84:ARG:HH11	1.81	0.45
1:A:236:A:H4'	1:A:237:G:OP1	2.16	0.45
1:A:240:C:H4'	15:N:146:GLN:NE2	2.30	0.45
1:A:566:A:H2	1:A:1094:G:O4'	1.99	0.45
1:A:724:G:O2'	1:A:725:C:H5'	2.17	0.45
1:A:1557:G:O2'	1:A:1558:C:H5'	2.17	0.45
1:A:1636:G:O2'	1:A:1637:A:H5'	2.17	0.45
1:A:1921:A:C6	1:A:1922:A:C2	3.04	0.45
1:A:1934:A:C8	1:A:1935:C:C5	3.05	0.45
1:A:2272:G:H5'	4:C:223:ARG:HB2	1.98	0.45
1:A:2338:G:H2'	7:F:129:ASP:OD1	2.16	0.45
1:A:2405:C:H5'	38:A:6070:HOH:O	2.16	0.45
1:A:2699:A:H2'	1:A:2700:G:O4'	2.17	0.45
4:C:95:PRO:HA	4:C:153:ARG:HA	1.99	0.45
5:D:129:ARG:O	5:D:133:GLU:HG3	2.17	0.45
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.98	0.45
11:J:72:VAL:O	11:J:72:VAL:HG13	2.15	0.45
13:L:49:LEU:HD21	13:L:74:VAL:O	2.16	0.45
16:O:43:VAL:HG13	16:O:118:ILE:HD11	1.97	0.45
20:S:17:MET:HG2	20:S:144:GLU:HA	1.98	0.45
25:X:41:TYR:O	25:X:45:VAL:HG13	2.16	0.45
25:X:65:VAL:HA	25:X:68:THR:CG2	2.46	0.45
1:A:481:U:C5'	38:A:5127:HOH:O	2.65	0.45
1:A:585:C:H6	38:A:5586:HOH:O	1.98	0.45
1:A:871:G:H5"	1:A:871:G:H8	1.74	0.45
1:A:1615:A:H5'	38:A:3673:HOH:O	2.17	0.45
1:A:1768:C:C2'	1:A:1769:C:H5'	2.46	0.45
1:A:1796:A:H2'	1:A:1797:A:C8	2.51	0.45
1:A:1983:C:O5'	1:A:1983:C:H6	2.00	0.45
1:A:2381:C:H2'	1:A:2382:A:H8	1.82	0.45
5:D:88:GLU:HA	5:D:136:ASP:O	2.17	0.45
5:D:279:THR:OG1	5:D:290:VAL:HB	2.16	0.45
6:E:246:ARG:NE	38:E:8422:HOH:O	2.50	0.45
7:F:19:GLU:O	7:F:133:ASN:HB3	2.17	0.45
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.32	0.45
11:J:45:GLN:NE2	11:J:135:TRP:HE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:39:ALA:C	24:W:41:GLU:N	2.70	0.45
1:A:10:U:O4	1:A:532:A:OP2	2.35	0.45
1:A:710:G:N2	1:A:719:C:C2	2.84	0.45
1:A:795:G:N3	1:A:817:G:C2	2.85	0.45
1:A:936:C:C2'	1:A:937:C:H5'	2.47	0.45
1:A:2524:G:N2	1:A:2526:C:H41	2.13	0.45
2:B:3025:G:N2	38:B:8513:HOH:O	2.49	0.45
2:B:3063:C:O2'	2:B:3064:C:H5'	2.17	0.45
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.99	0.45
5:D:248:ARG:O	5:D:251:VAL:CG1	2.49	0.45
8:G:38:ILE:HG21	8:G:65:PHE:CE1	2.51	0.45
11:J:65:ARG:NH1	38:J:8373:HOH:O	2.50	0.45
15:N:113:ARG:NH1	15:N:150:ILE:O	2.48	0.45
17:P:10:LEU:HD13	17:P:99:GLU:HG3	1.98	0.45
22:U:24:ARG:HH21	22:U:39:ASN:ND2	2.14	0.45
25:X:5:VAL:O	25:X:52:VAL:HG22	2.16	0.45
27:Z:184:GLU:OE2	27:Z:204:ARG:HD2	2.17	0.45
28:1:38:LYS:HA	28:1:45:LYS:HA	1.99	0.45
1:A:1183:C:N4	38:A:3883:HOH:O	2.50	0.45
1:A:1811:A:C2	1:A:2752:C:H1'	2.52	0.45
1:A:1878:G:O2'	1:A:1879:U:H6	1.98	0.45
1:A:2608:C:H2'	38:A:3069:HOH:O	2.15	0.45
1:A:2730:G:O2'	1:A:2731:G:H5'	2.17	0.45
1:A:2759:C:O5'	1:A:2759:C:H6	2.00	0.45
1:A:2912:C:H3'	38:A:5856:HOH:O	2.15	0.45
38:A:6071:HOH:O	31:4:79:LEU:HD12	2.17	0.45
38:A:6107:HOH:O	4:C:1:GLY:N	2.50	0.45
38:A:9199:HOH:O	5:D:254:GLN:HG3	2.16	0.45
7:F:36:ASN:HA	38:F:7500:HOH:O	2.15	0.45
9:H:28:ALA:HB1	9:H:99:THR:HG23	1.99	0.45
9:H:110:GLU:HG2	38:H:6926:HOH:O	2.16	0.45
11:J:82:LYS:NZ	11:J:82:LYS:HB2	2.31	0.45
12:K:93:ARG:HB3	12:K:93:ARG:NH1	2.26	0.45
17:P:39:THR:CB	38:P:3360:HOH:O	2.61	0.45
25:X:48:VAL:CG1	25:X:48:VAL:O	2.63	0.45
25:X:65:VAL:CG1	25:X:116:LEU:HD13	2.46	0.45
27:Z:214:ARG:NH2	27:Z:232:THR:OG1	2.49	0.45
1:A:475:G:OP1	6:E:73:LEU:HD22	2.16	0.45
1:A:656:G:H2'	1:A:657:G:H8	1.82	0.45
1:A:892:G:H5"	29:2:54:ALA:HB2	1.98	0.45
1:A:1925:G:OP1	31:4:29:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2276:U:H2'	1:A:2277:U:H6	1.81	0.45
1:A:2781:U:O2'	1:A:2782:G:H5'	2.17	0.45
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.47	0.45
7:F:169:THR:C	7:F:170:TYR:CD1	2.91	0.45
8:G:15:GLN:NE2	8:G:40:VAL:O	2.50	0.45
11:J:71:TYR:C	11:J:73:GLN:N	2.69	0.45
12:K:131:THR:HG22	12:K:133:GLY:N	2.31	0.45
15:N:84:LYS:O	15:N:87:MET:HG2	2.17	0.45
16:O:47:LEU:HD23	16:O:47:LEU:HA	1.70	0.45
16:O:181:ASP:HA	38:O:8568:HOH:O	2.17	0.45
17:P:112:ARG:HG3	17:P:114:ILE:HD11	1.99	0.45
17:P:112:ARG:CG	17:P:114:ILE:HD11	2.47	0.45
20:S:16:ALA:HB2	20:S:95:ALA:HB2	1.99	0.45
27:Z:187:VAL:HG12	27:Z:205:ILE:HA	1.98	0.45
1:A:324:G:O2'	1:A:325:U:H5'	2.17	0.44
1:A:736:A:H2'	1:A:737:A:O4'	2.17	0.44
1:A:1109:U:O4	12:K:21:ARG:HA	2.17	0.44
1:A:1234:U:O2	1:A:2066:C:H5"	2.17	0.44
1:A:1736:A:H8	1:A:1736:A:O5'	2.00	0.44
1:A:2118:A:H2'	1:A:2119:C:H6	1.82	0.44
1:A:2271:G:P	38:A:8934:HOH:O	2.75	0.44
1:A:2910:A:H5"	38:A:3620:HOH:O	2.16	0.44
38:A:4048:HOH:O	6:E:50:GLU:HG2	2.16	0.44
14:M:10:SER:O	14:M:11:ARG:HB3	2.17	0.44
16:O:82:TYR:CD2	16:O:83:LEU:N	2.84	0.44
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.82	0.44
17:P:32:ARG:O	17:P:35:LYS:HB2	2.16	0.44
27:Z:105:LYS:NZ	27:Z:225:GLY:O	2.48	0.44
1:A:1162:G:C2	1:A:1163:G:C8	3.06	0.44
1:A:1803:C:H2'	1:A:1804:A:C8	2.52	0.44
1:A:1815:A:H5'	38:A:3652:HOH:O	2.16	0.44
1:A:1853:C:H5'	4:C:228:ILE:O	2.18	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.17	0.44
1:A:2403:C:O2'	19:R:67:GLN:O	2.29	0.44
4:C:1:GLY:HA2	4:C:197:VAL:HG23	1.99	0.44
4:C:29:HIS:HB2	4:C:153:ARG:HH12	1.82	0.44
4:C:182:ARG:O	4:C:184:THR:N	2.51	0.44
4:C:184:THR:HG22	4:C:185:LYS:N	2.32	0.44
5:D:280:VAL:CG1	5:D:334:SER:HA	2.47	0.44
7:F:154:LYS:HD3	38:F:1796:HOH:O	2.17	0.44
38:L:1387:HOH:O	23:V:20:MET:HE3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:90:ARG:HH11	14:M:119:THR:HG21	1.80	0.44
15:N:164:THR:HG22	15:N:167:GLY:CA	2.46	0.44
16:O:3:GLY:HA3	38:O:8512:HOH:O	2.17	0.44
16:O:132:ASN:O	16:O:135:VAL:HG12	2.17	0.44
20:S:89:LEU:HD23	20:S:89:LEU:HA	1.87	0.44
31:4:87:ARG:HG3	38:4:8572:HOH:O	2.16	0.44
1:A:182:G:O2'	1:A:183:A:H5'	2.18	0.44
1:A:553:G:O4'	1:A:1325:G:H5'	2.17	0.44
1:A:711:G:N2	1:A:718:C:C2	2.86	0.44
1:A:1497:G:H2'	1:A:1498:G:C8	2.50	0.44
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.49	0.44
1:A:1603:A:C5'	1:A:1605:G:H5'	2.47	0.44
1:A:1819:G:H2'	1:A:1820:G:C5'	2.47	0.44
1:A:2769:C:H2'	1:A:2770:G:C5'	2.46	0.44
2:B:3056:A:C3'	2:B:3057:A:H5"	2.44	0.44
5:D:66:GLU:HG2	38:D:8656:HOH:O	2.17	0.44
5:D:171:VAL:HG23	5:D:172:SER:H	1.83	0.44
14:M:35:ARG:HH12	14:M:43:HIS:HB3	1.82	0.44
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.98	0.44
15:N:122:GLU:OE2	15:N:127:LYS:HE2	2.17	0.44
16:O:19:ASP:OD1	16:O:22:GLN:N	2.31	0.44
16:O:47:LEU:HD12	16:O:92:ALA:HB1	1.99	0.44
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.17	0.44
16:O:92:ALA:O	16:O:95:ALA:HB3	2.17	0.44
25:X:122:ARG:CG	25:X:152:ALA:O	2.66	0.44
27:Z:189:ASN:ND2	27:Z:192:ASP:N	2.64	0.44
27:Z:198:GLY:HA3	27:Z:225:GLY:O	2.17	0.44
28:1:47:LEU:CD2	28:1:57:CYS:HB2	2.47	0.44
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.99	0.44
1:A:152:A:C2	1:A:153:C:C2	3.05	0.44
1:A:168:C:C2'	1:A:169:A:H5'	2.47	0.44
1:A:814:G:H2'	1:A:815:U:O4'	2.17	0.44
1:A:840:U:C5	1:A:2648:U:C5	3.06	0.44
1:A:1380:U:H5'	38:A:8730:HOH:O	2.16	0.44
1:A:1503:U:H2'	1:A:1504:A:O4'	2.18	0.44
1:A:1790:C:H2'	1:A:1791:U:H6	1.83	0.44
1:A:1931:A:H8	1:A:1931:A:O5'	2.00	0.44
1:A:2281:C:O2'	1:A:2282:U:H5'	2.18	0.44
1:A:2382:A:C1'	31:4:10:TYR:HD2	2.31	0.44
1:A:2431:C:N3	38:A:3182:HOH:O	2.36	0.44
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:4433:HOH:O	15:N:82:ARG:HD3	2.17	0.44
2:B:3081:C:O5'	2:B:3081:C:H6	2.01	0.44
4:C:58:VAL:O	4:C:65:ARG:HD2	2.18	0.44
5:D:7:ARG:CD	5:D:9:GLY:O	2.66	0.44
5:D:115:VAL:HA	5:D:116:PRO:HD3	1.90	0.44
5:D:224:LYS:HA	5:D:224:LYS:HD3	1.88	0.44
13:L:123:SER:HA	13:L:126:SER:OG	2.18	0.44
14:M:59:GLU:HG2	14:M:104:ASP:OD2	2.17	0.44
15:N:82:ARG:NH2	38:N:8615:HOH:O	2.51	0.44
17:P:44:ASN:HA	17:P:65:LEU:O	2.17	0.44
22:U:96:VAL:CG1	22:U:97:ARG:N	2.81	0.44
1:A:402:U:H2'	1:A:403:C:C6	2.52	0.44
1:A:1215:A:O3'	1:A:1216:G:H4'	2.17	0.44
1:A:1574:C:H6	1:A:1574:C:O5'	2.00	0.44
1:A:1862:C:H1'	38:A:6685:HOH:O	2.16	0.44
1:A:2408:A:O2'	31:4:16:GLU:HA	2.18	0.44
1:A:2413:A:H2'	1:A:2414:A:O4'	2.18	0.44
1:A:2769:C:H2'	1:A:2770:G:H5'	2.00	0.44
38:A:4909:HOH:O	31:4:25:VAL:HG21	2.18	0.44
8:G:57:LYS:O	8:G:60:SER:HB2	2.18	0.44
8:G:61:THR:O	8:G:64:THR:N	2.51	0.44
11:J:57:ARG:O	11:J:60:ALA:N	2.51	0.44
13:L:82:ARG:HD2	13:L:88:VAL:HG21	1.99	0.44
14:M:40:PHE:C	14:M:40:PHE:CD1	2.90	0.44
14:M:114:VAL:N	38:M:8440:HOH:O	2.46	0.44
16:O:79:PRO:HB3	16:O:172:PHE:CD1	2.53	0.44
17:P:25:VAL:HG23	17:P:26:TRP:CD2	2.53	0.44
17:P:97:SER:HB3	17:P:100:GLN:HE21	1.82	0.44
25:X:38:THR:HB	38:X:5390:HOH:O	2.16	0.44
28:1:18:TYR:HB3	28:1:22:ILE:HG21	1.98	0.44
1:A:603:A:H4'	1:A:604:G:O5'	2.17	0.44
1:A:1118:A:C8	1:A:1119:G:H5"	2.52	0.44
1:A:1189:A:N3	38:A:7152:HOH:O	2.48	0.44
1:A:1311:G:C2	1:A:1312:G:C8	3.06	0.44
1:A:1552:G:H2'	1:A:1553:C:H6	1.82	0.44
1:A:1562:C:N4	38:A:5350:HOH:O	2.39	0.44
1:A:2821:C:O2'	5:D:114:ASP:O	2.34	0.44
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.18	0.44
6:E:168:ARG:NH2	6:E:190:ALA:O	2.51	0.44
7:F:58:VAL:CG1	7:F:59:GLY:N	2.79	0.44
12:K:17:CYS:HA	12:K:119:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:130:ARG:O	14:M:131:GLU:C	2.54	0.44
15:N:174:ARG:HG3	38:N:8522:HOH:O	2.18	0.44
16:O:74:PRO:HD3	16:O:159:TYR:CE2	2.52	0.44
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.99	0.44
25:X:79:VAL:HG13	25:X:83:TRP:CE3	2.53	0.44
1:A:827:A:H2'	1:A:828:G:O4'	2.17	0.44
1:A:864:U:H4'	38:A:8869:HOH:O	2.17	0.44
1:A:1164:U:N3	1:A:1192:A:H2	2.06	0.44
1:A:1609:C:H2'	1:A:1610:G:C8	2.53	0.44
1:A:1840:A:H4'	1:A:1841:C:O5'	2.18	0.44
1:A:2064:U:H4'	1:A:2653:A:OP1	2.17	0.44
1:A:2385:G:C4	1:A:2386:U:C5	3.06	0.44
1:A:2610:U:H4'	38:D:8531:HOH:O	2.16	0.44
38:A:3254:HOH:O	22:U:9:LYS:HD2	2.16	0.44
4:C:74:VAL:H	28:1:65:ALA:HB3	1.83	0.44
4:C:217:ARG:HG2	4:C:229:ALA:HB2	1.99	0.44
7:F:95:THR:OG1	7:F:174:VAL:HG22	2.18	0.44
7:F:147:ALA:HA	16:O:15:GLU:O	2.18	0.44
11:J:131:ILE:HG23	11:J:132:PHE:CD1	2.53	0.44
11:J:139:ASP:H	11:J:140:PRO:HD3	1.78	0.44
13:L:90:PHE:N	13:L:90:PHE:CD1	2.86	0.44
15:N:65:VAL:HG21	15:N:105:ALA:HB2	2.00	0.44
15:N:87:MET:H	15:N:87:MET:HG3	1.38	0.44
15:N:137:ASP:C	15:N:142:LYS:HE3	2.38	0.44
15:N:157:LEU:HD22	15:N:160:PHE:CD1	2.53	0.44
17:P:70:LEU:O	17:P:92:VAL:HG21	2.16	0.44
22:U:38:ARG:HH11	22:U:38:ARG:CG	2.27	0.44
24:W:12:THR:O	24:W:13:PRO:C	2.56	0.44
27:Z:99:ALA:HB2	27:Z:233:TYR:CE1	2.53	0.44
27:Z:115:ARG:CZ	38:Z:8558:HOH:O	2.65	0.44
30:3:49:GLU:HB2	38:3:719:HOH:O	2.18	0.44
1:A:366:U:H2'	1:A:367:G:O4'	2.18	0.44
1:A:517:U:C2'	1:A:518:G:H5'	2.47	0.44
1:A:795:G:H1'	1:A:817:G:N2	2.32	0.44
1:A:1273:C:O2'	1:A:1274:A:H5'	2.18	0.44
1:A:1398:G:O2'	1:A:1399:A:H5'	2.17	0.44
1:A:1985:U:H5"	38:A:4682:HOH:O	2.18	0.44
1:A:2133:U:H4'	1:A:2134:G:H5'	2.00	0.44
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.82	0.44
6:E:219:ASN:O	6:E:223:LEU:HB2	2.18	0.44
7:F:174:VAL:HG21	38:F:2195:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:80:TRP:O	8:G:134:SER:HA	2.17	0.44
11:J:57:ARG:C	11:J:59:ASN:N	2.69	0.44
11:J:81:TYR:CD1	11:J:81:TYR:C	2.91	0.44
12:K:52:GLN:CG	12:K:53:ILE:N	2.70	0.44
19:R:21:ARG:HG2	19:R:22:GLY:H	1.83	0.44
20:S:39:THR:O	20:S:40:ALA:C	2.56	0.44
25:X:48:VAL:O	25:X:48:VAL:HG12	2.16	0.44
25:X:54:PHE:C	25:X:146:ILE:HD11	2.38	0.44
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.48	0.44
28:1:37:HIS:O	28:1:45:LYS:HA	2.17	0.44
1:A:226:A:H1'	1:A:393:G:C5	2.53	0.44
1:A:290:C:O2'	1:A:291:C:H5'	2.16	0.44
1:A:316:A:H1'	1:A:336:G:N3	2.33	0.44
1:A:553:G:P	27:Z:204:ARG:NH2	2.86	0.44
1:A:564:G:H1'	38:A:5796:HOH:O	2.18	0.44
1:A:1008:C:OP1	11:J:16:ARG:NH2	2.47	0.44
1:A:1195:G:C2	1:A:1205:U:O2	2.71	0.44
1:A:1852:A:H5"	4:C:232:ARG:O	2.18	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.82	0.44
38:A:4739:HOH:O	6:E:73:LEU:HD11	2.17	0.44
7:F:44:ILE:HG12	7:F:83:PHE:CE1	2.48	0.44
7:F:55:LYS:O	7:F:56:ARG:HB2	2.18	0.44
9:H:79:GLN:HB2	9:H:82:ASP:CG	2.39	0.44
11:J:84:ARG:CZ	11:J:135:TRP:CH2	3.01	0.44
15:N:38:VAL:O	15:N:38:VAL:HG12	2.17	0.44
15:N:61:ILE:HA	38:N:8619:HOH:O	2.18	0.44
16:O:42:HIS:HD1	16:O:75:THR:HG1	1.64	0.44
16:O:113:SER:HB3	38:O:8551:HOH:O	2.18	0.44
19:R:3:SER:HB3	38:R:5998:HOH:O	2.18	0.44
26:Y:76:ARG:NH1	26:Y:76:ARG:CG	2.81	0.44
1:A:263:U:C2	9:H:59:ILE:CD1	3.01	0.43
1:A:558:C:H2'	1:A:559:U:H5"	1.98	0.43
1:A:920:C:H4'	1:A:921:G:N2	2.33	0.43
1:A:963:C:O5'	1:A:963:C:H6	2.01	0.43
1:A:1226:G:H2'	1:A:1227:C:H6	1.83	0.43
1:A:1603:A:H5"	1:A:1605:G:H5'	2.00	0.43
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.17	0.43
1:A:2505:G:C2'	1:A:2506:A:H5'	2.47	0.43
5:D:72:THR:HB	38:D:8611:HOH:O	2.18	0.43
5:D:101:TRP:HB2	5:D:119:HIS:CD2	2.53	0.43
5:D:130:ASP:HB2	38:D:8603:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:162:VAL:HG12	6:E:162:VAL:O	2.18	0.43
8:G:118:ILE:HG22	8:G:119:HIS:N	2.32	0.43
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.99	0.43
11:J:55:GLN:HE21	11:J:124:ARG:NE	2.01	0.43
11:J:150:LYS:HE2	38:J:8371:HOH:O	2.17	0.43
21:T:17:ASP:HB3	21:T:23:LYS:HB2	1.99	0.43
25:X:72:PRO:C	25:X:74:GLU:N	2.70	0.43
1:A:77:G:O2'	1:A:78:G:H5'	2.17	0.43
1:A:683:G:O2'	1:A:684:G:H5'	2.18	0.43
1:A:821:U:O2'	1:A:822:C:H5'	2.18	0.43
1:A:1566:C:O2'	1:A:1567:A:H5'	2.17	0.43
1:A:1682:A:H5"	38:A:8955:HOH:O	2.18	0.43
1:A:1789:G:H2'	1:A:1790:C:O5'	2.18	0.43
1:A:1878:G:O2'	1:A:1879:U:P	2.76	0.43
1:A:2312:G:H2'	1:A:2313:C:H5'	2.00	0.43
4:C:81:GLN:H	4:C:92:ASN:ND2	2.16	0.43
6:E:2:GLN:HB3	38:E:8336:HOH:O	2.18	0.43
9:H:107:VAL:O	9:H:111:ILE:HG13	2.17	0.43
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.54	0.43
17:P:36:PRO:O	17:P:39:THR:OG1	2.32	0.43
22:U:41:ARG:NH1	22:U:42:VAL:O	2.51	0.43
23:V:31:PHE:CG	23:V:37:GLU:HG2	2.53	0.43
25:X:13:MET:HE3	25:X:17:ILE:CG2	2.47	0.43
26:Y:41:PHE:CZ	26:Y:74:ALA:HB3	2.53	0.43
1:A:794:U:H3	1:A:819:A:H61	1.65	0.43
1:A:1069:C:H2'	1:A:1070:A:O4'	2.18	0.43
1:A:1149:U:H5"	1:A:1151:G:O4'	2.19	0.43
1:A:1942:A:HO2'	1:A:1943:C:H5'	1.83	0.43
38:A:6475:HOH:O	4:C:220:PRO:HB3	2.17	0.43
6:E:35:VAL:HG21	6:E:227:GLY:HA2	2.00	0.43
6:E:115:LEU:O	6:E:118:THR:HB	2.18	0.43
8:G:61:THR:O	8:G:62:ILE:C	2.56	0.43
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.48	0.43
15:N:39:ARG:NH2	38:N:8619:HOH:O	2.51	0.43
15:N:48:ARG:O	15:N:52:LEU:HG	2.19	0.43
17:P:26:TRP:HE3	17:P:26:TRP:HA	1.83	0.43
20:S:33:ARG:HA	38:S:8548:HOH:O	2.17	0.43
20:S:132:ARG:NH1	38:S:8582:HOH:O	2.51	0.43
24:W:42:ASN:N	24:W:43:PRO:HD3	2.33	0.43
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.82	0.43
1:A:1066:U:H2'	1:A:1067:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:C:C2	1:A:1445:G:N2	2.87	0.43
1:A:1803:C:H2'	1:A:1804:A:H8	1.83	0.43
1:A:2323:G:H5'	38:A:6491:HOH:O	2.18	0.43
1:A:2634:G:OP2	4:C:204:GLY:N	2.37	0.43
1:A:2756:U:H3	1:A:2896:A:H2	1.64	0.43
38:A:6825:HOH:O	4:C:177:HIS:HE1	2.02	0.43
5:D:41:PHE:HB3	5:D:190:MET:CE	2.48	0.43
5:D:41:PHE:CG	5:D:190:MET:HE3	2.53	0.43
5:D:98:THR:C	5:D:99:GLU:HG3	2.38	0.43
9:H:31:LYS:HG3	38:H:5719:HOH:O	2.19	0.43
15:N:74:ARG:CD	15:N:91:ILE:CD1	2.96	0.43
15:N:137:ASP:O	15:N:142:LYS:HE3	2.19	0.43
20:S:72:VAL:CG1	20:S:75:TRP:HB3	2.48	0.43
20:S:92:LEU:HD23	20:S:145:LEU:HD21	2.00	0.43
21:T:73:ASP:O	21:T:77:VAL:HG23	2.18	0.43
22:U:92:ASP:O	22:U:94:SER:N	2.52	0.43
25:X:4:LEU:CD2	25:X:54:PHE:HB3	2.46	0.43
1:A:638:C:H2'	1:A:639:A:C8	2.53	0.43
1:A:1439:C:H6	1:A:1439:C:O5'	2.01	0.43
1:A:1829:A:C8	1:A:1885:A:C8	3.06	0.43
1:A:2120:U:H2'	1:A:2121:G:O4'	2.18	0.43
1:A:2300:A:C2	1:A:2306:U:C5	3.07	0.43
1:A:2424:U:H1'	19:R:7:LEU:HD12	1.99	0.43
1:A:2458:U:OP1	31:4:82:GLY:N	2.47	0.43
1:A:2548:C:H2'	1:A:2549:C:H6	1.84	0.43
38:A:4730:HOH:O	15:N:29:GLN:HA	2.19	0.43
2:B:3045:A:H4'	7:F:143:LYS:O	2.19	0.43
5:D:23:THR:HA	5:D:24:PRO:HD3	1.73	0.43
6:E:13:ASP:OD1	6:E:13:ASP:O	2.36	0.43
10:I:67:LEU:O	10:I:71:LEU:HG	2.18	0.43
11:J:56:ILE:O	11:J:61:LEU:HD21	2.18	0.43
12:K:108:PRO:HG2	12:K:109:TYR:CD1	2.54	0.43
15:N:175:GLY:O	15:N:184:ARG:NH2	2.46	0.43
16:O:18:THR:HA	38:O:8525:HOH:O	2.17	0.43
16:O:165:ALA:HB1	38:O:8526:HOH:O	2.19	0.43
21:T:10:VAL:CG1	24:W:35:ALA:O	2.66	0.43
26:Y:47:ALA:HB1	26:Y:82:GLU:HA	1.99	0.43
27:Z:133:HIS:HE1	38:Z:8617:HOH:O	2.02	0.43
28:1:33:HIS:HA	28:1:69:TYR:O	2.18	0.43
1:A:222:A:H2'	1:A:223:G:O4'	2.18	0.43
1:A:278:A:H2'	1:A:279:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:U:H2'	1:A:910:C:O4'	2.19	0.43
1:A:1213:C:C2'	1:A:1214:G:H5'	2.47	0.43
1:A:2296:C:H5	38:R:5998:HOH:O	2.00	0.43
1:A:2719:A:H5"	38:A:3181:HOH:O	2.18	0.43
1:A:2761:A:C4	1:A:2763:G:C8	3.05	0.43
5:D:168:GLY:O	5:D:169:GLY:O	2.36	0.43
6:E:3:ALA:O	6:E:15:GLU:HB2	2.19	0.43
6:E:3:ALA:N	6:E:16:VAL:O	2.51	0.43
8:G:20:ILE:HD12	8:G:33:LEU:HD12	2.00	0.43
11:J:154:THR:HB	11:J:155:PRO:CD	2.48	0.43
12:K:77:GLY:O	12:K:80:LYS:N	2.51	0.43
14:M:98:GLU:O	14:M:99:GLU:CB	2.67	0.43
15:N:48:ARG:HH11	15:N:52:LEU:HD21	1.82	0.43
15:N:78:ASN:ND2	38:N:8640:HOH:O	2.44	0.43
18:Q:31:ILE:HG12	18:Q:43:LEU:HD13	2.01	0.43
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.52	0.43
24:W:5:VAL:HG23	38:W:2271:HOH:O	2.18	0.43
29:2:28:HIS:O	29:2:32:LYS:N	2.48	0.43
1:A:183:A:H5'	15:N:157:LEU:HD12	2.01	0.43
1:A:200:U:O2'	1:A:201:G:H5'	2.18	0.43
1:A:283:U:H5	1:A:284:C:H42	1.67	0.43
1:A:458:G:H4'	38:A:9202:HOH:O	2.18	0.43
1:A:475:G:H5'	6:E:73:LEU:HD23	1.99	0.43
1:A:593:A:H1'	38:A:3303:HOH:O	2.19	0.43
1:A:877:G:H1'	38:C:8513:HOH:O	2.19	0.43
1:A:1044:C:C5'	38:A:8543:HOH:O	2.66	0.43
1:A:1067:A:O2'	25:X:12:ASN:OD1	2.35	0.43
1:A:1175:G:H1'	1:A:1193:A:H2'	2.01	0.43
1:A:1209:C:H2'	1:A:1210:G:C8	2.50	0.43
1:A:2382:A:H1'	31:4:10:TYR:HE2	1.82	0.43
1:A:2519:C:H5"	11:J:59:ASN:HB3	2.01	0.43
2:B:3091:C:H2'	2:B:3092:G:O4'	2.18	0.43
4:C:42:VAL:HG21	4:C:74:VAL:CG1	2.49	0.43
5:D:41:PHE:N	38:D:8657:HOH:O	2.52	0.43
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.49	0.43
11:J:47:GLU:CB	11:J:133:ILE:CD1	2.94	0.43
12:K:19:MET:HE1	12:K:132:LEU:HD11	1.99	0.43
14:M:21:ARG:N	38:M:8404:HOH:O	2.52	0.43
15:N:187:LEU:CD2	15:N:194:ALA:HB3	2.48	0.43
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.54	0.43
17:P:96:VAL:HG12	17:P:97:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:41:ARG:HG2	22:U:41:ARG:NH1	2.33	0.43
23:V:6:CYS:CB	23:V:13:ILE:HD11	2.48	0.43
25:X:128:VAL:O	25:X:138:LEU:HD11	2.18	0.43
31:4:1:MET:HE2	31:4:83:TRP:HZ2	1.83	0.43
1:A:390:G:H5"	38:A:9051:HOH:O	2.17	0.43
1:A:401:C:P	38:A:5274:HOH:O	2.76	0.43
1:A:445:U:H2'	1:A:446:G:H8	1.84	0.43
1:A:567:U:H5"	38:X:5817:HOH:O	2.19	0.43
1:A:672:G:O6	6:E:217:GLU:HG3	2.18	0.43
1:A:1164:U:O4'	1:A:1165:G:OP1	2.36	0.43
1:A:1973:A:H5'	1:A:1973:A:H8	1.83	0.43
1:A:2589:U:H2'	1:A:2590:U:C6	2.53	0.43
38:A:5661:HOH:O	5:D:216:LYS:HD2	2.18	0.43
6:E:123:LEU:HD23	6:E:123:LEU:HA	1.88	0.43
7:F:11:HIS:C	7:F:13:MET:N	2.71	0.43
7:F:56:ARG:N	38:F:6752:HOH:O	2.50	0.43
7:F:104:PHE:CE2	7:F:132:VAL:HB	2.53	0.43
13:L:27:ARG:HD2	38:L:4747:HOH:O	2.18	0.43
14:M:143:THR:CG2	14:M:144:ASP:N	2.79	0.43
17:P:37:ARG:HG2	38:P:3002:HOH:O	2.19	0.43
18:Q:59:ARG:O	18:Q:63:ARG:HG3	2.19	0.43
23:V:9:CYS:SG	23:V:11:THR:HG23	2.59	0.43
24:W:16:ARG:CZ	24:W:63:GLU:HG3	2.47	0.43
25:X:125:HIS:CD2	25:X:127:GLY:H	2.37	0.43
27:Z:141:THR:HG23	38:Z:8592:HOH:O	2.17	0.43
31:4:22:VAL:HG12	31:4:90:PHE:HE2	1.84	0.43
1:A:818:A:C5'	38:A:6062:HOH:O	2.67	0.43
1:A:830:G:H2'	1:A:831:U:H6	1.83	0.43
1:A:952:G:N3	1:A:2302:A:H2'	2.34	0.43
1:A:1200:A:H4'	38:A:6809:HOH:O	2.19	0.43
1:A:1600:G:H8	1:A:1600:G:OP2	2.02	0.43
1:A:1603:A:H5"	1:A:1604:G:H3'	2.01	0.43
1:A:1707:G:N1	1:A:1710:A:OP2	2.47	0.43
1:A:2434:A:C1'	38:A:3009:HOH:O	2.65	0.43
1:A:2559:C:H4'	38:A:6723:HOH:O	2.18	0.43
1:A:2719:A:C2'	1:A:2720:C:H5'	2.49	0.43
1:A:2869:G:H2'	1:A:2870:C:H6	1.83	0.43
7:F:67:ASP:HA	7:F:68:PRO:HD3	1.86	0.43
7:F:169:THR:O	7:F:169:THR:HG22	2.19	0.43
12:K:19:MET:HE1	12:K:132:LEU:CD1	2.48	0.43
12:K:74:ARG:HH12	12:K:76:ASP:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:63:VAL:HG12	15:N:64:ARG:N	2.32	0.43
16:O:162:ASP:HB3	16:O:163:PHE:H	1.63	0.43
18:Q:28:GLN:O	18:Q:32:ALA:HB2	2.19	0.43
24:W:12:THR:O	24:W:15:GLU:N	2.52	0.43
31:4:6:ARG:HG2	31:4:6:ARG:HH11	1.84	0.43
1:A:133:U:H5'	1:A:1465:A:OP1	2.19	0.43
1:A:1110:G:O2'	1:A:1111:U:H5'	2.18	0.43
1:A:1163:G:H3'	1:A:1164:U:H2'	2.01	0.43
1:A:1865:A:H2'	1:A:1866:A:C8	2.54	0.43
1:A:2038:A:O2'	1:A:2039:A:H5'	2.19	0.43
1:A:2487:C:C1'	36:5:76:PPU:HD2	2.49	0.43
2:B:3097:U:H2'	2:B:3098:C:C6	2.54	0.43
4:C:125:ASN:CB	4:C:158:VAL:HG12	2.49	0.43
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.64	0.43
9:H:38:LYS:HZ3	15:N:3:SER:HA	1.81	0.43
11:J:162:SER:CB	11:J:163:PRO:CD	2.75	0.43
13:L:124:VAL:O	13:L:127:ALA:HB3	2.19	0.43
14:M:145:LEU:O	14:M:145:LEU:HD23	2.19	0.43
15:N:67:ILE:CD1	15:N:104:ARG:HD2	2.49	0.43
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.54	0.43
20:S:39:THR:N	20:S:42:GLU:OE1	2.50	0.43
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.83	0.43
26:Y:70:ILE:O	26:Y:70:ILE:HG23	2.19	0.43
1:A:116:G:H5"	1:A:131:A:H5'	2.01	0.42
1:A:317:A:OP1	22:U:52:ARG:O	2.37	0.42
1:A:396:U:H2'	1:A:397:A:C8	2.54	0.42
1:A:508:A:H2'	1:A:509:A:H5"	2.00	0.42
1:A:653:C:H2'	1:A:654:A:C8	2.54	0.42
1:A:1593:C:O2'	1:A:1594:C:H5'	2.19	0.42
1:A:1942:A:OP1	4:C:234:GLY:N	2.49	0.42
1:A:2055:A:H4'	20:S:132:ARG:NH2	2.34	0.42
1:A:2243:C:C5'	38:A:3248:HOH:O	2.60	0.42
1:A:2512:U:H3'	38:A:4829:HOH:O	2.19	0.42
1:A:2656:G:H1'	38:A:6842:HOH:O	2.19	0.42
2:B:3048:C:OP1	16:O:114:LYS:HG3	2.18	0.42
6:E:98:ARG:NH1	38:E:8358:HOH:O	2.44	0.42
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.83	0.42
7:F:29:HIS:C	38:F:5858:HOH:O	2.57	0.42
7:F:57:THR:CG2	7:F:63:ILE:HG22	2.46	0.42
7:F:94:ALA:HB3	7:F:174:VAL:HA	2.01	0.42
9:H:56:PRO:HG2	15:N:43:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:80:ILE:O	13:L:80:ILE:HG13	2.19	0.42
18:Q:16:VAL:CG1	18:Q:20:ARG:HB2	2.49	0.42
18:Q:27:ARG:CD	38:Q:5262:HOH:O	2.67	0.42
19:R:86:VAL:HG13	19:R:91:LEU:HD11	2.01	0.42
20:S:39:THR:HB	20:S:42:GLU:HG3	2.01	0.42
21:T:23:LYS:HE2	38:T:8329:HOH:O	2.19	0.42
21:T:33:SER:O	21:T:37:VAL:HG23	2.19	0.42
23:V:47:ARG:HG3	38:V:4381:HOH:O	2.18	0.42
1:A:1182:C:H1'	1:A:1192:A:C8	2.52	0.42
1:A:1525:G:H5'	1:A:1526:A:OP2	2.19	0.42
1:A:1609:C:H2'	1:A:1610:G:H8	1.84	0.42
1:A:1755:A:O2'	1:A:1756:G:H5'	2.18	0.42
1:A:1878:G:O2'	1:A:1879:U:OP2	2.36	0.42
1:A:2809:G:H2'	1:A:2810:G:O4'	2.19	0.42
1:A:2823:G:H4'	1:A:2827:A:O4'	2.19	0.42
1:A:2896:A:H2'	1:A:2896:A:N3	2.34	0.42
38:A:9457:HOH:O	6:E:78:ARG:HD3	2.19	0.42
2:B:3020:G:C2'	2:B:3021:G:H5'	2.49	0.42
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.34	0.42
6:E:27:ARG:HG2	6:E:30:LEU:HG	2.00	0.42
16:O:75:THR:HG21	38:O:8536:HOH:O	2.18	0.42
25:X:4:LEU:O	25:X:32:CYS:HA	2.19	0.42
25:X:13:MET:CE	25:X:17:ILE:CG2	2.97	0.42
31:4:9:THR:OG1	31:4:80:ARG:NH2	2.43	0.42
1:A:160:A:C4	1:A:177:A:C2	3.08	0.42
1:A:293:A:C4	1:A:360:A:C2	3.07	0.42
1:A:329:A:C5	1:A:347:A:C2	3.08	0.42
1:A:401:C:H2'	1:A:402:U:C6	2.54	0.42
1:A:470:U:O2'	29:2:16:HIS:HD2	2.02	0.42
1:A:921:G:H4'	1:A:924:G:C6	2.53	0.42
1:A:1013:A:C2	1:A:1014:A:H1'	2.55	0.42
1:A:1505:U:H5'	1:A:1505:U:C6	2.54	0.42
1:A:1771:U:O2'	1:A:1773:G:N7	2.49	0.42
1:A:2025:G:C6	1:A:2026:C:C4	3.08	0.42
1:A:2320:U:OP2	31:4:2:GLN:N	2.51	0.42
1:A:2690:U:H2'	1:A:2703:A:N6	2.34	0.42
1:A:2836:G:C6	1:A:2838:A:C2	3.06	0.42
2:B:3041:C:H2'	2:B:3042:C:H6	1.84	0.42
2:B:3059:C:H2'	2:B:3060:C:C6	2.55	0.42
2:B:3096:C:H2'	2:B:3097:U:H6	1.80	0.42
5:D:48:MET:O	5:D:49:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.33	0.42
7:F:59:GLY:O	7:F:61:PHE:N	2.42	0.42
8:G:64:THR:HG22	8:G:68:HIS:CD2	2.54	0.42
10:I:23:ILE:O	10:I:27:ILE:HG13	2.19	0.42
11:J:156:THR:C	11:J:157:ILE:HG13	2.39	0.42
16:O:50:LEU:HD12	16:O:50:LEU:HA	1.85	0.42
16:O:71:TRP:HB2	38:O:8537:HOH:O	2.17	0.42
16:O:74:PRO:HG2	16:O:159:TYR:CZ	2.53	0.42
16:O:93:GLN:HG2	38:O:8554:HOH:O	2.19	0.42
16:O:108:SER:HA	16:O:109:PRO:HD3	1.82	0.42
16:O:171:HIS:HA	16:O:174:GLU:OE1	2.18	0.42
23:V:6:CYS:C	23:V:8:TYR:H	2.23	0.42
24:W:45:ARG:O	24:W:48:GLU:N	2.52	0.42
25:X:119:HIS:HD2	25:X:120:PRO:O	2.02	0.42
31:4:70:ARG:CA	38:4:8571:HOH:O	2.67	0.42
1:A:90:A:H2'	1:A:91:G:O4'	2.19	0.42
1:A:151:A:H2'	1:A:152:A:O4'	2.19	0.42
1:A:169:A:HO2'	1:A:170:U:H6	1.65	0.42
1:A:324:G:C6	1:A:325:U:C5	3.07	0.42
1:A:706:G:H4'	38:A:6853:HOH:O	2.19	0.42
1:A:797:A:H4'	28:1:10:ARG:N	2.35	0.42
1:A:1098:A:H2'	1:A:1099:G:O4'	2.20	0.42
1:A:1154:A:H2'	1:A:1155:G:C8	2.54	0.42
1:A:1345:A:H2'	1:A:1346:U:C6	2.54	0.42
1:A:1787:C:O2'	1:A:1788:U:H5'	2.20	0.42
1:A:2134:G:C6	1:A:2258:A:C8	3.08	0.42
4:C:94:LEU:N	4:C:94:LEU:CD2	2.80	0.42
5:D:144:THR:CG2	5:D:145:HIS:H	2.32	0.42
5:D:146:THR:O	5:D:148:PRO:HD3	2.19	0.42
5:D:195:ARG:O	5:D:198:GLU:HG3	2.19	0.42
5:D:224:LYS:O	5:D:225:GLY:C	2.57	0.42
12:K:107:ASN:HD22	12:K:108:PRO:HD2	1.84	0.42
13:L:115:ARG:CG	13:L:116:GLU:N	2.80	0.42
16:O:163:PHE:H	16:O:163:PHE:HD2	1.66	0.42
20:S:100:ASP:C	20:S:102:GLN:H	2.21	0.42
23:V:49:LEU:O	23:V:55:ALA:CB	2.68	0.42
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.82	0.42
27:Z:144:ARG:CZ	38:Z:8618:HOH:O	2.66	0.42
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.33	0.42
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.68	0.42
29:2:5:THR:N	29:2:6:PRO:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:G:O2'	1:A:14:C:H5'	2.19	0.42
1:A:382:U:O2'	1:A:430:A:H1'	2.20	0.42
1:A:401:C:O2'	15:N:92:THR:HB	2.19	0.42
1:A:639:A:C2	1:A:1363:G:C2	3.07	0.42
1:A:1242:A:OP2	12:K:60:ARG:NH1	2.51	0.42
1:A:2004:U:O2	1:A:2004:U:H2'	2.19	0.42
1:A:2084:C:H2'	1:A:2085:A:C8	2.54	0.42
38:A:4185:HOH:O	28:1:51:GLY:HA3	2.19	0.42
5:D:226:LYS:HG2	5:D:230:GLN:NE2	2.34	0.42
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.37	0.42
9:H:26:THR:HB	9:H:102:GLY:O	2.20	0.42
11:J:139:ASP:HB3	38:J:8380:HOH:O	2.17	0.42
12:K:6:PHE:CZ	12:K:102:ARG:HG3	2.53	0.42
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.19	0.42
16:O:161:GLY:O	16:O:162:ASP:C	2.57	0.42
20:S:16:ALA:CB	20:S:95:ALA:HB2	2.49	0.42
22:U:26:THR:HA	22:U:39:ASN:HB3	2.00	0.42
1:A:171:C:C2'	1:A:172:U:H5'	2.50	0.42
1:A:398:U:H2'	1:A:399:C:C6	2.53	0.42
1:A:740:G:C6	1:A:741:C:C4	3.08	0.42
1:A:745:G:H4'	38:A:4633:HOH:O	2.19	0.42
1:A:1174:A:C5	1:A:1201:C:H4'	2.54	0.42
1:A:1471:A:H2'	1:A:1472:C:C6	2.55	0.42
1:A:1562:C:O2	1:A:1562:C:H2'	2.19	0.42
1:A:2408:A:H4'	31:4:15:ASN:O	2.20	0.42
1:A:2430:A:H2'	1:A:2431:C:H6	1.83	0.42
1:A:2909:G:O2'	1:A:2910:A:H5'	2.19	0.42
5:D:51:VAL:CG2	5:D:329:TYR:O	2.68	0.42
5:D:62:ARG:CB	5:D:65:MET:HE3	2.50	0.42
11:J:26:LYS:NZ	11:J:31:PHE:CZ	2.85	0.42
13:L:31:VAL:HG22	13:L:53:ILE:HD12	2.01	0.42
13:L:98:VAL:HG13	13:L:102:GLU:HA	2.01	0.42
17:P:32:ARG:O	17:P:32:ARG:HD3	2.19	0.42
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.19	0.42
23:V:49:LEU:HD13	23:V:51:TRP:HE1	1.84	0.42
1:A:1573:A:H2'	1:A:1574:C:O4'	2.19	0.42
1:A:1602:C:H5'	38:A:5962:HOH:O	2.20	0.42
1:A:1778:A:H2'	1:A:1779:A:H5'	2.00	0.42
1:A:1819:G:H5'	38:A:4194:HOH:O	2.18	0.42
1:A:2105:C:H2'	1:A:2106:C:C6	2.55	0.42
1:A:2133:U:H4'	1:A:2134:G:C5'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2478:U:O2'	1:A:2479:A:H5'	2.19	0.42
1:A:2673:U:H2'	1:A:2674:G:H5'	2.01	0.42
2:B:3092:G:H2'	2:B:3093:A:H8	1.81	0.42
2:B:3092:G:C6	2:B:3093:A:C6	3.08	0.42
5:D:162:MET:HE3	5:D:308:LEU:CD2	2.31	0.42
7:F:156:ARG:HH11	7:F:156:ARG:HG3	1.83	0.42
8:G:1:PRO:HG2	8:G:59:MET:SD	2.60	0.42
8:G:11:VAL:CG1	8:G:12:ASP:H	2.33	0.42
8:G:81:GLU:N	38:G:6931:HOH:O	2.45	0.42
11:J:60:ALA:CB	38:J:8338:HOH:O	2.67	0.42
15:N:27:ARG:O	15:N:30:GLU:N	2.53	0.42
19:R:16:ASN:HD22	19:R:16:ASN:HA	1.66	0.42
31:4:60:LYS:HG3	31:4:61:PRO:HD2	2.00	0.42
1:A:290:C:N3	1:A:363:A:C2	2.87	0.42
1:A:665:A:C6	1:A:666:A:C6	3.08	0.42
1:A:807:A:H2'	1:A:808:A:C8	2.54	0.42
1:A:869:G:OP1	15:N:79:LYS:HE2	2.18	0.42
1:A:947:U:H2'	1:A:948:G:H8	1.81	0.42
1:A:1276:U:H2'	1:A:1278:A:OP2	2.20	0.42
1:A:1474:C:O2'	1:A:1475:G:H5'	2.19	0.42
1:A:1810:C:N3	1:A:1811:A:C5	2.88	0.42
1:A:1847:A:OP1	4:C:175:LYS:HG3	2.20	0.42
1:A:1885:A:H8	1:A:1885:A:O5'	2.02	0.42
1:A:1915:U:C2	1:A:1925:G:N2	2.88	0.42
1:A:2387:U:H2'	1:A:2388:C:H6	1.84	0.42
1:A:2634:G:H2'	1:A:2635:A:H8	1.85	0.42
1:A:2766:A:O2'	1:A:2767:C:H5'	2.20	0.42
1:A:2812:A:C2	1:A:2814:A:N6	2.72	0.42
38:A:3094:HOH:O	27:Z:115:ARG:HB2	2.19	0.42
2:B:3004:G:O2'	16:O:44:ARG:NH2	2.53	0.42
4:C:170:VAL:HG22	28:1:22:ILE:HG23	2.01	0.42
5:D:156:LYS:HE3	38:D:8638:HOH:O	2.19	0.42
6:E:4:THR:HB	6:E:135:GLU:OE1	2.20	0.42
9:H:105:ALA:HB2	38:H:5522:HOH:O	2.19	0.42
13:L:48:GLY:O	13:L:73:VAL:HB	2.20	0.42
13:L:101:ASN:O	13:L:102:GLU:HB2	2.20	0.42
18:Q:59:ARG:HG2	18:Q:59:ARG:HH11	1.85	0.42
19:R:23:THR:HG23	38:R:4792:HOH:O	2.19	0.42
22:U:64:ASN:HB3	22:U:73:HIS:HB2	2.00	0.42
29:2:13:THR:HG22	29:2:14:THR:N	2.34	0.42
1:A:695:C:H2'	1:A:696:C:H6	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:G:N2	1:A:1246:A:H2	2.11	0.42
1:A:1157:C:H2'	1:A:1158:G:H8	1.85	0.42
1:A:1789:G:C2'	1:A:1790:C:O5'	2.68	0.42
1:A:1857:A:C6	1:A:2247:C:H1'	2.55	0.42
1:A:1916:C:N4	1:A:1917:G:C6	2.88	0.42
1:A:2247:C:C5'	38:A:6811:HOH:O	2.67	0.42
1:A:2526:C:H3'	1:A:2526:C:H6	1.85	0.42
1:A:2613:G:O2'	1:A:2614:C:H5'	2.20	0.42
1:A:2672:C:OP2	5:D:25:ARG:NH1	2.53	0.42
1:A:2853:U:C4	1:A:2906:A:N6	2.87	0.42
2:B:3038:A:H2	2:B:3043:G:H5"	1.85	0.42
4:C:95:PRO:O	4:C:99:ILE:HG12	2.20	0.42
7:F:11:HIS:O	7:F:13:MET:N	2.44	0.42
8:G:158:ASP:HA	38:G:2712:HOH:O	2.20	0.42
9:H:48:VAL:HG23	9:H:74:PHE:HB3	2.01	0.42
11:J:47:GLU:N	11:J:160:ASP:O	2.42	0.42
11:J:151:MET:HA	11:J:151:MET:HE3	2.01	0.42
12:K:130:VAL:HG12	12:K:131:THR:N	2.33	0.42
25:X:132:VAL:C	25:X:134:GLU:H	2.22	0.42
1:A:171:C:H2'	1:A:172:U:H5'	2.02	0.42
1:A:212:A:C8	1:A:214:U:C2	3.08	0.42
1:A:472:A:O4'	1:A:774:C:H4'	2.20	0.42
1:A:489:A:C8	22:U:82:THR:HG22	2.55	0.42
1:A:678:G:OP2	6:E:107:ARG:NH2	2.53	0.42
1:A:1181:A:H2'	1:A:1182:C:O4'	2.19	0.42
1:A:1188:A:C5	1:A:1189:A:C2	3.08	0.42
1:A:1325:G:O2'	1:A:1326:U:H5'	2.19	0.42
1:A:1477:C:H4'	1:A:1868:G:OP1	2.19	0.42
1:A:1494:A:C6	1:A:1512:G:C6	3.08	0.42
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.42
1:A:1666:C:C2'	1:A:1667:A:H5"	2.49	0.42
1:A:1702:U:H1'	38:A:5255:HOH:O	2.20	0.42
1:A:1820:G:C6	1:A:2030:A:C2	3.08	0.42
1:A:1922:A:H3'	1:A:1923:G:H8	1.84	0.42
1:A:2005:G:H3'	1:A:2005:G:OP2	2.19	0.42
1:A:2035:C:O5'	1:A:2035:C:H6	2.03	0.42
1:A:2813:A:H2'	38:A:3400:HOH:O	2.18	0.42
38:A:5734:HOH:O	23:V:56:ARG:HB3	2.19	0.42
38:A:6071:HOH:O	31:4:79:LEU:HB2	2.19	0.42
2:B:3029:C:H5"	7:F:140:ARG:HD3	2.02	0.42
4:C:37:VAL:HG22	38:C:8610:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:54:VAL:HB	38:D:8618:HOH:O	2.20	0.42
5:D:154:VAL:HA	5:D:155:PRO:HD3	1.89	0.42
5:D:316:ARG:N	5:D:317:PRO:HD3	2.35	0.42
8:G:69:ILE:HA	8:G:72:MET:HE2	2.01	0.42
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.92	0.42
10:I:71:LEU:O	10:I:73:ASP:N	2.53	0.42
11:J:31:PHE:HD2	11:J:85:ILE:O	2.03	0.42
11:J:58:HIS:CE1	11:J:59:ASN:ND2	2.87	0.42
15:N:169:ARG:CB	38:N:8584:HOH:O	2.67	0.42
18:Q:16:VAL:CG1	18:Q:17:GLY:H	2.33	0.42
20:S:100:ASP:C	20:S:102:GLN:N	2.73	0.42
22:U:48:VAL:HG13	22:U:49:GLU:N	2.34	0.42
24:W:27:LEU:HA	24:W:49:LEU:HD13	2.01	0.42
25:X:7:LEU:HD12	25:X:53:ALA:HB2	2.01	0.42
26:Y:20:GLU:O	26:Y:21:PRO:C	2.57	0.42
28:1:10:ARG:HG3	28:1:11:THR:N	2.35	0.42
1:A:820:G:C5	4:C:171:LYS:HB2	2.54	0.41
1:A:1056:U:H2'	1:A:1057:A:O4'	2.20	0.41
1:A:1086:A:P	25:X:9:GLY:H	2.42	0.41
1:A:1308:A:H5'	38:A:6406:HOH:O	2.20	0.41
1:A:1409:G:H5'	38:A:3222:HOH:O	2.19	0.41
1:A:1665:G:C6	1:A:1666:C:C4	3.08	0.41
1:A:1727:G:H1'	38:A:4153:HOH:O	2.20	0.41
1:A:1755:A:H2'	1:A:1756:G:O4'	2.20	0.41
1:A:1838:U:H2'	1:A:1839:A:H5'	2.01	0.41
1:A:1886:A:O2'	28:1:20:LEU:HB2	2.20	0.41
1:A:2433:A:H2'	1:A:2434:A:C8	2.55	0.41
1:A:2673:U:C2	1:A:2817:G:C2	3.08	0.41
1:A:2694:A:H5"	8:G:90:HIS:CE1	2.55	0.41
1:A:2761:A:H4'	38:A:3968:HOH:O	2.19	0.41
1:A:2821:C:H4'	5:D:116:PRO:HG3	2.01	0.41
2:B:3097:U:H2'	2:B:3098:C:H6	1.85	0.41
4:C:83:GLY:O	4:C:94:LEU:HB3	2.19	0.41
4:C:109:GLU:HG2	4:C:116:GLY:N	2.35	0.41
5:D:57:GLU:HA	5:D:58:PRO:HD2	1.92	0.41
5:D:105:PHE:CD1	5:D:115:VAL:CG1	3.03	0.41
5:D:329:TYR:CE2	23:V:15:PRO:CG	3.02	0.41
7:F:101:THR:HG22	7:F:101:THR:O	2.19	0.41
7:F:170:TYR:CD1	7:F:170:TYR:N	2.88	0.41
9:H:78:GLU:HG3	38:H:5966:HOH:O	2.21	0.41
12:K:41:ALA:O	12:K:43:ARG:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:170:GLU:HA	16:O:173:ASP:OD2	2.20	0.41
21:T:39:ASP:O	21:T:43:GLU:HG3	2.20	0.41
24:W:27:LEU:CA	24:W:49:LEU:HD13	2.50	0.41
25:X:125:HIS:HE1	38:X:3071:HOH:O	2.02	0.41
1:A:84:G:O2'	1:A:85:C:H5'	2.21	0.41
1:A:418:C:O5'	1:A:418:C:H6	2.03	0.41
1:A:445:U:C1'	38:A:6805:HOH:O	2.68	0.41
1:A:449:A:C8	6:E:43:LYS:HG2	2.54	0.41
1:A:858:U:H2'	1:A:859:C:C6	2.54	0.41
1:A:902:G:N7	14:M:18:HIS:CD2	2.87	0.41
1:A:1352:A:P	6:E:92:PRO:HG3	2.60	0.41
1:A:1474:C:H6	1:A:1474:C:C5'	2.26	0.41
1:A:1483:C:C2'	1:A:1484:G:H5'	2.49	0.41
1:A:1523:G:H2'	1:A:1524:U:C6	2.55	0.41
1:A:1667:A:H2'	1:A:1668:U:C6	2.55	0.41
1:A:1687:C:H2'	1:A:1688:G:O4'	2.20	0.41
1:A:1705:C:P	18:Q:59:ARG:HH12	2.42	0.41
1:A:2324:G:C2	1:A:2377:U:O2	2.73	0.41
1:A:2455:A:H2'	1:A:2456:A:O4'	2.19	0.41
1:A:2594:C:O2'	1:A:2595:U:H5'	2.20	0.41
1:A:2785:C:H4'	1:A:2786:G:OP2	2.21	0.41
5:D:215:VAL:HA	5:D:220:VAL:HG22	2.03	0.41
7:F:73:VAL:HG21	38:F:5828:HOH:O	2.20	0.41
7:F:173:GLU:O	7:F:174:VAL:C	2.59	0.41
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.50	0.41
14:M:120:LEU:HD12	14:M:133:VAL:HG21	2.00	0.41
15:N:37:VAL:CB	15:N:108:LYS:HG3	2.50	0.41
18:Q:103:THR:O	18:Q:106:ARG:HB3	2.20	0.41
19:R:35:ASP:OD1	19:R:35:ASP:N	2.53	0.41
21:T:57:THR:HG22	21:T:58:MET:N	2.35	0.41
23:V:20:MET:HE2	23:V:30:HIS:CD2	2.55	0.41
26:Y:23:HIS:CD2	26:Y:24:LYS:HG3	2.55	0.41
1:A:699:C:C2	1:A:743:G:N2	2.89	0.41
1:A:791:A:H4'	1:A:1709:G:H4'	2.02	0.41
1:A:793:A:C5'	18:Q:83:LYS:HG2	2.51	0.41
1:A:812:A:H2'	1:A:813:C:C6	2.56	0.41
1:A:1174:A:C8	1:A:1201:C:OP1	2.73	0.41
1:A:1342:C:O2'	1:A:1343:C:H5'	2.20	0.41
1:A:1425:G:O2'	1:A:1426:C:H5'	2.20	0.41
1:A:1452:G:H1'	35:A:8503:CL:CL	2.56	0.41
1:A:1542:G:C2	1:A:1644:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1761:U:H5'	18:Q:81:LYS:O	2.20	0.41
1:A:2437:A:C6	1:A:2438:G:C6	3.09	0.41
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.48	0.41
5:D:204:GLY:HA3	38:D:8662:HOH:O	2.20	0.41
5:D:320:GLN:HG3	5:D:321:PRO:HD2	2.01	0.41
6:E:39:GLN:O	6:E:43:LYS:CD	2.62	0.41
7:F:23:VAL:HG22	7:F:73:VAL:HB	2.02	0.41
9:H:72:VAL:HA	9:H:73:PRO:HD3	1.84	0.41
14:M:53:ARG:O	14:M:58:GLN:NE2	2.54	0.41
23:V:8:TYR:HD2	23:V:36:CYS:HB3	1.85	0.41
25:X:29:VAL:O	25:X:30:ASN:HB2	2.20	0.41
27:Z:98:GLN:HA	38:Z:8538:HOH:O	2.21	0.41
28:1:56:MET:HE3	28:1:63:LYS:HG3	2.01	0.41
1:A:13:G:H2'	1:A:14:C:H6	1.85	0.41
1:A:56:G:H5"	24:W:50:ARG:HH12	1.82	0.41
1:A:240:C:O2	1:A:240:C:H2'	2.21	0.41
1:A:401:C:C5'	38:A:5274:HOH:O	2.67	0.41
1:A:550:C:H2'	1:A:551:A:O4'	2.20	0.41
1:A:796:A:H5'	38:A:5989:HOH:O	2.20	0.41
1:A:1516:C:H2'	1:A:1517:U:H6	1.85	0.41
1:A:1730:G:C5'	1:A:1731:C:C6	3.03	0.41
1:A:1815:A:O2'	1:A:2750:G:H1'	2.20	0.41
1:A:2038:A:H5"	5:D:222:LYS:HG3	2.02	0.41
1:A:2820:A:H2'	1:A:2821:C:O4'	2.21	0.41
2:B:3023:U:H3'	2:B:3024:U:C5'	2.47	0.41
2:B:3082:U:H2'	2:B:3083:G:C8	2.55	0.41
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.34	0.41
5:D:337:GLY:C	38:D:8558:HOH:O	2.59	0.41
7:F:27:ILE:CG2	38:F:5858:HOH:O	2.68	0.41
7:F:99:ASP:HB3	7:F:103:ASN:H	1.85	0.41
8:G:71:ASN:HA	8:G:80:TRP:HZ2	1.84	0.41
8:G:92:PRO:HB2	38:G:4917:HOH:O	2.19	0.41
11:J:75:SER:O	11:J:79:ALA:CB	2.65	0.41
15:N:52:LEU:HD13	15:N:116:ASN:HB3	2.02	0.41
15:N:186:SER:OG	15:N:189:VAL:CG1	2.69	0.41
17:P:44:ASN:HB3	17:P:67:SER:O	2.20	0.41
20:S:61:GLN:CD	38:S:8540:HOH:O	2.59	0.41
25:X:65:VAL:CA	25:X:68:THR:HG22	2.49	0.41
25:X:110:GLN:HE21	25:X:110:GLN:CA	2.23	0.41
1:A:152:A:H1'	1:A:440:C:O2'	2.20	0.41
1:A:192:A:H5"	38:A:5708:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:C:O2'	1:A:401:C:H5'	2.20	0.41
1:A:445:U:H2'	1:A:446:G:C8	2.56	0.41
1:A:463:A:O3'	1:A:464:G:H4'	2.20	0.41
1:A:694:A:H4'	1:A:2441:U:OP1	2.20	0.41
1:A:786:G:O2'	1:A:787:G:H5'	2.21	0.41
1:A:1064:U:H2'	1:A:1065:G:C8	2.56	0.41
1:A:1398:G:C4'	18:Q:25:PRO:HG3	2.51	0.41
1:A:1500:U:C2	1:A:1503:U:O4	2.74	0.41
1:A:1576:G:H2'	1:A:1577:U:O4'	2.20	0.41
1:A:1730:G:C5'	1:A:1731:C:H6	2.33	0.41
1:A:1816:C:O5'	1:A:1816:C:H6	2.04	0.41
1:A:2372:A:H2'	1:A:2373:U:C6	2.56	0.41
1:A:2408:A:O2'	31:4:17:HIS:N	2.53	0.41
1:A:2428:G:H1'	1:A:2461:U:O4	2.21	0.41
1:A:2621:U:H2'	1:A:2622:A:O4'	2.21	0.41
4:C:30:ARG:HE	4:C:30:ARG:HB3	1.71	0.41
4:C:37:VAL:HG13	38:C:8624:HOH:O	2.20	0.41
4:C:109:GLU:HG3	4:C:153:ARG:O	2.21	0.41
5:D:7:ARG:CG	5:D:7:ARG:NH1	2.79	0.41
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.48	0.41
7:F:52:THR:N	7:F:70:GLY:O	2.53	0.41
38:F:3066:HOH:O	16:O:15:GLU:HB3	2.21	0.41
11:J:62:GLU:HA	38:J:8373:HOH:O	2.21	0.41
11:J:109:ASP:HB2	38:J:8334:HOH:O	2.20	0.41
12:K:54:VAL:CG1	12:K:138:THR:HG21	2.48	0.41
17:P:59:VAL:CG2	17:P:111:VAL:HG23	2.50	0.41
1:A:123:U:O2'	1:A:124:C:H5'	2.20	0.41
1:A:191:A:N1	1:A:236:A:O2'	2.47	0.41
1:A:266:G:C2	1:A:267:G:C8	3.09	0.41
1:A:295:C:C2'	1:A:296:G:H5'	2.50	0.41
1:A:503:G:H2'	1:A:504:G:H8	1.86	0.41
1:A:906:C:C2	1:A:1300:G:N2	2.88	0.41
1:A:1019:C:O2	19:R:94:GLN:NE2	2.54	0.41
1:A:1268:C:O2'	27:Z:169:ARG:HB2	2.21	0.41
1:A:1285:U:H4'	25:X:74:GLU:OE1	2.21	0.41
1:A:1548:U:H5"	18:Q:59:ARG:CZ	2.50	0.41
1:A:1683:G:N2	1:A:1723:G:H2'	2.36	0.41
1:A:1940:C:H5"	4:C:234:GLY:HA3	2.01	0.41
1:A:2024:A:C2	1:A:2025:G:C8	3.09	0.41
5:D:177:HIS:NE2	5:D:181:ILE:HD11	2.36	0.41
6:E:160:LEU:O	6:E:162:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:135:VAL:HG22	7:F:136:ARG:N	2.35	0.41
9:H:21:GLU:HA	9:H:24:ARG:HE	1.85	0.41
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.83	0.41
11:J:144:GLU:OE1	11:J:144:GLU:HA	2.20	0.41
12:K:42:GLU:O	12:K:131:THR:HG23	2.20	0.41
12:K:81:ARG:HB2	38:K:5750:HOH:O	2.20	0.41
13:L:63:GLU:O	13:L:67:GLN:NE2	2.51	0.41
17:P:59:VAL:HG21	17:P:111:VAL:HG21	2.02	0.41
18:Q:119:TYR:O	18:Q:120:ARG:C	2.57	0.41
18:Q:143:ALA:HA	38:Q:2178:HOH:O	2.19	0.41
20:S:61:GLN:NE2	38:S:8540:HOH:O	2.53	0.41
20:S:76:ASP:N	20:S:76:ASP:OD1	2.53	0.41
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	1.97	0.41
27:Z:122:ARG:NH2	38:Z:8535:HOH:O	2.52	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
1:A:679:G:C6	1:A:680:G:C4	3.09	0.41
1:A:823:U:H2'	1:A:824:G:O4'	2.20	0.41
1:A:949:U:O2'	19:R:40:HIS:HE1	2.04	0.41
1:A:1249:U:H2'	1:A:1250:C:C6	2.55	0.41
1:A:1422:U:H2'	1:A:1423:C:H6	1.83	0.41
1:A:1534:C:O2'	1:A:1656:A:OP1	2.35	0.41
1:A:1643:C:O2'	1:A:1644:C:H5'	2.19	0.41
1:A:2404:G:H4'	19:R:68:GLY:CA	2.51	0.41
1:A:2415:A:O2'	16:O:29:SER:HB3	2.20	0.41
2:B:3061:C:H2'	2:B:3062:A:H8	1.85	0.41
4:C:53:ALA:HB1	4:C:54:PRO:HD2	2.02	0.41
4:C:140:LEU:HB3	4:C:141:PRO:HD2	2.03	0.41
5:D:91:PRO:O	12:K:144:THR:HG21	2.21	0.41
11:J:114:PRO:O	11:J:115:PHE:C	2.59	0.41
11:J:149:ALA:C	11:J:151:MET:N	2.74	0.41
14:M:144:ASP:HA	14:M:147:GLU:HG3	2.02	0.41
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.50	0.41
20:S:56:PRO:HB3	20:S:80:TYR:CE2	2.55	0.41
20:S:98:ASN:N	20:S:98:ASN:ND2	2.69	0.41
22:U:65:VAL:HG22	22:U:72:ILE:HG22	2.02	0.41
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.31	0.41
27:Z:145:LYS:O	27:Z:147:ARG:HG2	2.20	0.41
1:A:189:A:OP1	15:N:171:ARG:NH2	2.53	0.41
1:A:396:U:H3'	38:A:3417:HOH:O	2.21	0.41
1:A:461:C:H2'	38:A:3492:HOH:O	2.20	0.41
1:A:1158:G:O2'	1:A:1159:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2240:U:H5"	38:A:5865:HOH:O	2.21	0.41
1:A:2267:G:H5'	38:A:3022:HOH:O	2.21	0.41
1:A:2631:U:H2'	1:A:2632:G:O4'	2.21	0.41
1:A:2834:G:C4	1:A:2847:G:N2	2.89	0.41
38:A:4185:HOH:O	28:1:54:ILE:HD12	2.20	0.41
4:C:29:HIS:CE1	4:C:107:ASN:HD22	2.39	0.41
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.61	0.41
5:D:14:GLY:HA2	5:D:15:PRO:O	2.21	0.41
5:D:69:VAL:HA	5:D:70:PRO:HD3	1.94	0.41
5:D:88:GLU:O	5:D:88:GLU:HG3	2.21	0.41
5:D:102:THR:CG2	5:D:182:VAL:HG12	2.51	0.41
5:D:146:THR:O	5:D:159:PRO:HB3	2.20	0.41
5:D:280:VAL:HG13	5:D:333:GLU:O	2.21	0.41
5:D:313:PRO:O	5:D:314:ALA:C	2.58	0.41
6:E:233:THR:CG2	6:E:234:VAL:N	2.84	0.41
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.88	0.41
11:J:113:ALA:N	11:J:114:PRO:CD	2.84	0.41
11:J:154:THR:N	11:J:155:PRO:HD2	2.35	0.41
11:J:162:SER:HB3	38:J:8330:HOH:O	2.19	0.41
13:L:90:PHE:HB3	38:L:6115:HOH:O	2.20	0.41
14:M:57:VAL:O	14:M:57:VAL:HG12	2.21	0.41
14:M:61:ALA:HA	38:M:8439:HOH:O	2.20	0.41
15:N:85:ARG:NH1	38:N:8533:HOH:O	2.50	0.41
16:O:47:LEU:CD1	16:O:97:VAL:HG11	2.50	0.41
16:O:74:PRO:CD	16:O:159:TYR:CE2	3.03	0.41
17:P:98:LEU:O	17:P:102:ILE:HG13	2.21	0.41
18:Q:37:ARG:O	18:Q:40:VAL:HB	2.20	0.41
19:R:64:GLU:HG3	19:R:74:ASP:OD2	2.20	0.41
20:S:29:LYS:HB3	38:S:8532:HOH:O	2.20	0.41
20:S:119:VAL:HG11	38:S:8583:HOH:O	2.21	0.41
22:U:3:GLN:HA	22:U:4:PRO:HD3	1.81	0.41
22:U:32:ARG:NH1	22:U:38:ARG:HH12	2.19	0.41
29:2:28:HIS:CD2	29:2:30:LYS:HB2	2.56	0.41
1:A:321:A:O2'	1:A:322:G:H5'	2.21	0.41
1:A:688:A:H62	14:M:111:ALA:HB2	1.85	0.41
1:A:1073:A:H1'	1:A:1088:A:N1	2.36	0.41
1:A:1298:U:H2'	1:A:1299:G:C8	2.56	0.41
1:A:1316:G:H1'	1:A:1340:G:H22	1.81	0.41
1:A:1819:G:O2'	1:A:1820:G:H5'	2.21	0.41
1:A:1883:U:H5"	1:A:2013:G:OP2	2.21	0.41
1:A:1885:A:C2'	1:A:1886:A:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2434:A:O3'	31:4:28:GLY:CA	2.69	0.41
1:A:2442:G:H2'	38:A:8708:HOH:O	2.21	0.41
1:A:2512:U:H2'	38:A:4829:HOH:O	2.21	0.41
1:A:2602:G:H2'	1:A:2603:G:O4'	2.20	0.41
1:A:2715:G:N2	5:D:264:GLU:OE1	2.53	0.41
1:A:2737:C:H3'	1:A:2738:G:C5'	2.51	0.41
1:A:2807:U:OP1	5:D:312:ARG:NH2	2.47	0.41
38:A:3188:HOH:O	8:G:143:GLN:CG	2.68	0.41
38:A:3188:HOH:O	8:G:143:GLN:HG2	2.20	0.41
38:A:5770:HOH:O	27:Z:158:LYS:HD3	2.20	0.41
38:A:7364:HOH:O	16:O:1:ALA:CB	2.69	0.41
4:C:48:ASP:HA	4:C:49:PRO:HD3	1.80	0.41
4:C:130:THR:HG22	4:C:131:HIS:O	2.21	0.41
4:C:165:THR:O	4:C:165:THR:HG22	2.21	0.41
5:D:51:VAL:HG13	5:D:53:LEU:CD1	2.50	0.41
5:D:105:PHE:CD1	5:D:115:VAL:HG11	2.56	0.41
7:F:59:GLY:C	7:F:61:PHE:H	2.20	0.41
7:F:99:ASP:O	7:F:159:PRO:HG3	2.20	0.41
7:F:156:ARG:HG3	7:F:156:ARG:NH1	2.36	0.41
8:G:84:MET:CE	8:G:148:ILE:HG21	2.48	0.41
8:G:93:MET:HE1	8:G:165:GLY:N	2.36	0.41
9:H:17:LEU:O	9:H:21:GLU:HG3	2.20	0.41
9:H:58:GLU:HA	9:H:61:MET:HG3	2.03	0.41
13:L:8:VAL:HG12	13:L:9:THR:N	2.36	0.41
14:M:134:GLU:HG3	38:M:8433:HOH:O	2.21	0.41
14:M:145:LEU:HB2	38:M:8413:HOH:O	2.21	0.41
15:N:28:MET:HA	15:N:31:TRP:HB2	2.03	0.41
15:N:68:ARG:O	15:N:68:ARG:HD3	2.21	0.41
16:O:143:ARG:HA	16:O:172:PHE:CE2	2.55	0.41
16:O:154:LEU:HG	16:O:155:GLU:H	1.85	0.41
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.49	0.41
18:Q:142:ASP:O	18:Q:143:ALA:O	2.38	0.41
20:S:14:ALA:HB3	20:S:147:LEU:HB2	2.03	0.41
22:U:16:LEU:HD23	22:U:16:LEU:HA	1.68	0.41
22:U:49:GLU:HB3	22:U:59:GLU:CG	2.50	0.41
23:V:53:ASP:N	38:V:6796:HOH:O	2.40	0.41
27:Z:100:ARG:HE	27:Z:234:VAL:CG2	2.34	0.41
29:2:1:THR:HA	38:2:435:HOH:O	2.21	0.41
1:A:10:U:HO2'	1:A:11:A:P	2.44	0.41
1:A:1187:U:HO2'	1:A:1188:A:H8	1.66	0.41
1:A:1733:A:C6	1:A:1734:C:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2613:G:H2'	1:A:2614:C:H6	1.86	0.41
1:A:2842:G:C2'	1:A:2843:A:H5'	2.51	0.41
5:D:16:ARG:NH2	38:D:8559:HOH:O	2.48	0.41
6:E:166:ILE:CD1	6:E:207:LEU:HD13	2.51	0.41
11:J:157:ILE:HG22	11:J:158:ASN:N	2.35	0.41
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.21	0.41
16:O:154:LEU:HG	16:O:155:GLU:N	2.36	0.41
21:T:50:GLU:OE2	21:T:69:SER:HB3	2.21	0.41
25:X:76:ASP:O	25:X:77:ALA:C	2.59	0.41
28:1:45:LYS:HE2	38:1:8409:HOH:O	2.21	0.41
1:A:105:G:O2'	1:A:106:A:H5'	2.21	0.40
1:A:198:A:C2	1:A:2444:U:H1'	2.56	0.40
1:A:244:C:H6	1:A:244:C:O5'	2.03	0.40
1:A:303:C:H2'	1:A:304:G:O4'	2.21	0.40
1:A:1154:A:H2'	1:A:1155:G:H8	1.87	0.40
1:A:1444:G:O2'	1:A:1502:A:N1	2.47	0.40
1:A:1641:A:H2'	1:A:1642:A:C5'	2.49	0.40
1:A:1768:C:H2'	1:A:1769:C:H5'	2.03	0.40
1:A:2345:A:H3'	1:A:2346:C:C5	2.56	0.40
1:A:2438:G:H2'	1:A:2439:C:O4'	2.21	0.40
2:B:3042:C:O2	7:F:76:ARG:HD2	2.21	0.40
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.61	0.40
10:I:12:ILE:HA	38:I:4499:HOH:O	2.19	0.40
13:L:4:LEU:HD22	13:L:116:GLU:HB3	2.02	0.40
15:N:61:ILE:HG22	15:N:62:VAL:N	2.36	0.40
16:O:32:PRO:O	16:O:100:ALA:HA	2.21	0.40
22:U:1:SER:N	38:U:5837:HOH:O	2.55	0.40
25:X:139:GLY:O	25:X:141:HIS:HD2	2.04	0.40
27:Z:196:VAL:HG13	27:Z:201:GLU:OE1	2.20	0.40
31:4:70:ARG:CB	38:4:8571:HOH:O	2.69	0.40
1:A:129:A:O2'	1:A:130:C:OP1	2.33	0.40
1:A:343:C:O2'	1:A:344:C:H5'	2.20	0.40
1:A:711:G:C2	1:A:718:C:C2	3.09	0.40
1:A:837:U:H4'	38:A:9892:HOH:O	2.21	0.40
1:A:1006:A:H4'	38:A:4382:HOH:O	2.21	0.40
1:A:1641:A:C8	1:A:1702:U:O4	2.74	0.40
1:A:1886:A:H1'	38:A:4306:HOH:O	2.21	0.40
1:A:1973:A:O2'	38:A:6330:HOH:O	2.22	0.40
1:A:2004:U:H5"	1:A:2005:G:C8	2.56	0.40
1:A:2040:C:H2'	1:A:2041:G:O4'	2.21	0.40
1:A:2249:G:C2	1:A:2253:G:C6	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:C:C4'	11:J:151:MET:CG	2.99	0.40
2:B:3024:U:H3'	2:B:3025:G:C5'	2.51	0.40
5:D:36:PRO:HA	5:D:168:GLY:HA2	2.01	0.40
12:K:63:ILE:HG22	12:K:64:GLY:N	2.35	0.40
16:O:10:MET:O	16:O:11:ARG:C	2.59	0.40
18:Q:5:ALA:CB	38:Q:1715:HOH:O	2.69	0.40
18:Q:115:SER:C	18:Q:117:SER:N	2.75	0.40
28:1:13:ARG:NH1	28:1:14:PHE:CE2	2.89	0.40
28:1:81:LYS:O	28:1:82:ALA:C	2.60	0.40
30:3:48:ASP:O	30:3:49:GLU:CB	2.69	0.40
1:A:703:G:O2'	1:A:704:C:H5'	2.21	0.40
1:A:710:G:C2'	1:A:711:G:H5'	2.51	0.40
1:A:783:C:O2'	1:A:784:A:H5'	2.21	0.40
1:A:1307:A:H2'	1:A:1308:A:C8	2.56	0.40
1:A:1334:C:O2'	1:A:1335:C:H5'	2.21	0.40
1:A:1540:G:N2	1:A:1646:G:H1'	2.36	0.40
1:A:1691:A:H5"	38:A:9642:HOH:O	2.19	0.40
1:A:1754:A:N7	38:A:7328:HOH:O	2.37	0.40
1:A:1810:C:H2'	1:A:1811:A:O4'	2.22	0.40
1:A:1838:U:C4	1:A:2622:A:N1	2.89	0.40
1:A:2050:G:H5"	20:S:80:TYR:O	2.21	0.40
1:A:2321:A:OP1	31:4:91:GLN:NE2	2.42	0.40
1:A:2563:U:H2'	1:A:2565:C:O5'	2.22	0.40
1:A:2653:A:H2'	1:A:2654:C:O4'	2.21	0.40
2:B:3107:C:O2'	2:B:3108:C:H5'	2.21	0.40
5:D:294:TYR:CD1	5:D:294:TYR:C	2.94	0.40
6:E:29:ASP:OD1	17:P:5:PRO:HD3	2.21	0.40
6:E:133:ARG:NH1	38:E:8409:HOH:O	2.31	0.40
6:E:236:THR:HG23	6:E:238:SER:H	1.86	0.40
8:G:9:GLU:HG3	8:G:10:ASP:N	2.36	0.40
9:H:27:GLY:HA3	38:H:5413:HOH:O	2.21	0.40
16:O:164:ASP:OD1	16:O:167:ASP:HA	2.21	0.40
22:U:45:GLY:HA3	22:U:102:ASP:HB2	2.03	0.40
25:X:38:THR:O	25:X:42:ARG:HB2	2.21	0.40
26:Y:21:PRO:HD3	38:Y:6179:HOH:O	2.21	0.40
26:Y:72:VAL:C	26:Y:88:GLU:OE2	2.60	0.40
1:A:56:G:C5'	24:W:50:ARG:HH12	2.34	0.40
1:A:128:A:H3'	1:A:128:A:C8	2.57	0.40
1:A:293:A:C5	1:A:360:A:C2	3.09	0.40
1:A:423:A:H2'	1:A:424:C:O4'	2.22	0.40
1:A:547:A:H3'	38:A:4429:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:A:OP2	1:A:592:G:N1	2.48	0.40
1:A:814:G:H4'	38:A:9631:HOH:O	2.22	0.40
1:A:1004:C:O2'	1:A:1005:A:H5'	2.21	0.40
1:A:1311:G:O6	6:E:173:LYS:HE3	2.21	0.40
1:A:1992:U:H2'	1:A:1994:A:OP2	2.21	0.40
1:A:2334:C:H6	1:A:2334:C:O5'	2.04	0.40
38:A:4889:HOH:O	14:M:34:GLY:HA2	2.21	0.40
5:D:60:SER:C	5:D:62:ARG:H	2.25	0.40
6:E:11:ASN:O	6:E:12:THR:C	2.60	0.40
6:E:29:ASP:OD1	17:P:5:PRO:CD	2.69	0.40
6:E:164:ALA:O	6:E:167:ASP:HB2	2.21	0.40
11:J:1:LYS:HA	11:J:2:PRO:HD3	1.88	0.40
11:J:28:ILE:HA	11:J:62:GLU:OE1	2.21	0.40
11:J:49:VAL:C	11:J:157:ILE:HG23	2.42	0.40
14:M:66:VAL:HG23	14:M:67:ARG:H	1.83	0.40
14:M:98:GLU:O	14:M:99:GLU:HB2	2.21	0.40
14:M:142:LEU:HG	14:M:146:GLY:HA3	2.04	0.40
16:O:16:ALA:HB2	38:O:8569:HOH:O	2.22	0.40
17:P:115:ARG:HG3	17:P:115:ARG:HH11	1.86	0.40
18:Q:89:ASN:OD1	18:Q:92:GLU:HB2	2.22	0.40
21:T:10:VAL:O	21:T:10:VAL:HG22	2.21	0.40
1:A:282:C:C2'	1:A:283:U:H5'	2.51	0.40
1:A:308:U:H5'	22:U:97:ARG:NH2	2.37	0.40
1:A:907:A:H2'	1:A:908:A:C8	2.57	0.40
1:A:945:U:O2'	1:A:946:C:H5'	2.21	0.40
1:A:1161:A:C6	1:A:1162:G:N7	2.89	0.40
1:A:1162:G:N1	1:A:1163:G:C5	2.90	0.40
1:A:1204:C:H1'	38:A:4228:HOH:O	2.21	0.40
1:A:1270:U:H2'	1:A:1271:A:C8	2.56	0.40
1:A:1882:C:H2'	1:A:1883:U:C6	2.56	0.40
1:A:2344:G:H8	38:A:6133:HOH:O	2.02	0.40
1:A:2432:C:H2'	1:A:2433:A:C8	2.57	0.40
1:A:2778:A:H1'	8:G:153:ARG:NH1	2.36	0.40
4:C:71:PRO:HG2	4:C:91:GLY:HA2	2.03	0.40
5:D:162:MET:HE2	5:D:310:ARG:CD	2.50	0.40
6:E:57:PRO:HG2	6:E:73:LEU:CD1	2.51	0.40
11:J:93:ILE:HG12	11:J:120:GLY:C	2.42	0.40
18:Q:89:ASN:OD1	18:Q:89:ASN:O	2.40	0.40
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.69	0.40
22:U:96:VAL:HG13	22:U:97:ARG:N	2.36	0.40
23:V:37:GLU:O	23:V:40:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:132:VAL:C	25:X:134:GLU:N	2.74	0.40
28:1:56:MET:HA	28:1:62:TYR:O	2.21	0.40
29:2:10:LYS:CG	38:2:2979:HOH:O	2.65	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	
4	C	235/239 (98%)	199 (85%)	27 (12%)	9 (4%)	3	15
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	4	20
6	E	244/246 (99%)	208 (85%)	31 (13%)	5 (2%)	7	30
7	F	134/176 (76%)	98 (73%)	25 (19%)	11 (8%)	1	3
8	G	170/177 (96%)	156 (92%)	13 (8%)	1 (1%)	25	60
9	H	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	2	12
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	14
11	J	152/167 (91%)	128 (84%)	18 (12%)	6 (4%)	3	14
12	K	140/145 (97%)	124 (89%)	11 (8%)	5 (4%)	3	16
13	L	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	10	38
14	M	141/164 (86%)	114 (81%)	23 (16%)	4 (3%)	5	22
15	N	192/194 (99%)	177 (92%)	10 (5%)	5 (3%)	5	24
16	O	184/186 (99%)	153 (83%)	19 (10%)	12 (6%)	1	5
17	P	113/115 (98%)	105 (93%)	7 (6%)	1 (1%)	17	51
18	Q	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	22	56
19	R	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
20	S	148/154 (96%)	130 (88%)	14 (10%)	4 (3%)	5	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12	41
22	U	117/119 (98%)	106 (91%)	8 (7%)	3 (3%)	5	24
23	V	51/66 (77%)	48 (94%)	1 (2%)	2 (4%)	3	14
24	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	19
25	X	152/154 (99%)	142 (93%)	6 (4%)	4 (3%)	5	24
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	3	15
27	Z	140/240 (58%)	134 (96%)	5 (4%)	1 (1%)	22	56
28	1	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	39
29	2	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	6	28
All	All	3633/4235 (86%)	3205 (88%)	327 (9%)	101 (3%)	5	22

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	206	THR
7	F	93	LEU
7	F	95	THR
7	F	173	GLU
9	H	101	ALA
11	J	162	SER
12	K	143	LYS
14	M	80	ASP
16	O	154	LEU
16	O	164	ASP
16	O	183	ASP
26	Y	87	ALA
4	C	10	GLY
4	C	34	ASP
4	C	37	VAL
4	C	119	ALA
5	D	34	GLY
5	D	169	GLY
5	D	184	ASP
6	E	208	ALA
7	F	11	HIS

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Mol	Chain	Res	Type
7	F	171	ASP
9	H	61	MET
11	J	40	PRO
11	J	164	ALA
12	K	5	GLU
13	L	119	GLN
18	Q	116	SER
20	S	106	GLY
22	U	28	SER
22	U	53	GLY
24	W	43	PRO
25	X	14	HIS
25	X	73	LEU
25	X	77	ALA
28	1	81	LYS
31	4	57	GLY
4	C	132	ASP
5	D	323	LEU
6	E	19	PRO
7	F	16	PRO
7	F	170	TYR
11	J	138	PRO
14	M	21	ARG
14	M	147	GLU
15	N	28	MET
15	N	140	ALA
15	N	148	SER
16	O	55	ASP
16	O	160	SER
16	O	162	ASP
16	O	181	ASP
17	P	20	SER
22	U	93	THR
23	V	7	ASP
4	C	165	THR
4	C	229	ALA
5	D	291	ASP
6	E	201	SER
7	F	20	LYS
7	F	85	GLN
12	K	42	GLU
12	K	89	HIS

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Mol	Chain	Res	Type
13	L	126	SER
16	O	65	ASP
20	S	101	HIS
20	S	136	TRP
23	V	46	ALA
24	W	40	PRO
26	Y	77	PHE
5	D	2	GLN
5	D	185	GLY
6	E	69	HIS
6	E	89	ALA
7	F	137	PRO
8	G	66	GLN
9	H	64	PRO
9	H	71	GLY
9	H	104	ALA
10	I	72	ASP
14	M	105	TYR
21	T	58	MET
25	X	49	ASN
31	4	56	PRO
4	C	170	VAL
7	F	61	PHE
15	N	6	SER
16	O	27	LEU
16	O	167	ASP
11	J	72	VAL
16	O	9	PRO
11	J	110	GLY
4	C	162	GLY
12	K	78	ILE
16	O	74	PRO
20	S	56	PRO
26	Y	70	ILE
5	D	225	GLY
15	N	88	VAL
27	Z	167	GLY

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	169 (94%)	10 (6%)	21	53
5	D	282/282 (100%)	265 (94%)	17 (6%)	19	50
6	E	193/193 (100%)	178 (92%)	15 (8%)	12	38
7	F	117/147 (80%)	108 (92%)	9 (8%)	13	39
8	G	152/155 (98%)	149 (98%)	3 (2%)	55	80
9	H	92/92 (100%)	90 (98%)	2 (2%)	52	79
10	I	27/283 (10%)	26 (96%)	1 (4%)	34	66
11	J	122/122 (100%)	111 (91%)	11 (9%)	9	32
12	K	118/121 (98%)	110 (93%)	8 (7%)	16	45
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	74
14	M	112/126 (89%)	108 (96%)	4 (4%)	35	67
15	N	166/166 (100%)	156 (94%)	10 (6%)	19	50
16	O	149/149 (100%)	142 (95%)	7 (5%)	26	59
17	P	93/93 (100%)	89 (96%)	4 (4%)	29	62
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	74
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	56
20	S	117/121 (97%)	114 (97%)	3 (3%)	46	75
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	102 (97%)	3 (3%)	42	73
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	48 (94%)	3 (6%)	19	50
25	X	130/130 (100%)	122 (94%)	8 (6%)	18	48
26	Y	66/73 (90%)	63 (96%)	3 (4%)	27	61
27	Z	120/195 (62%)	113 (94%)	7 (6%)	20	51
28	1	56/56 (100%)	49 (88%)	7 (12%)	4	17
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	66
All	All	3027/3441 (88%)	2878 (95%)	149 (5%)	25	58

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	190	MET
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	264	GLU
5	D	300	SER
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	56	THR
6	E	67	GLN
6	E	76	ARG
6	E	78	ARG
6	E	94	THR
6	E	115	LEU
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU

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Mol	Chain	Res	Type
7	F	24	HIS
7	F	61	PHE
7	F	99	ASP
7	F	100	ASP
7	F	131	THR
7	F	133	ASN
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	12	ASP
8	G	102	VAL
9	H	1	PRO
9	H	100	ASP
10	I	64	ASN
11	J	1	LYS
11	J	30	GLN
11	J	59	ASN
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	83	PHE
11	J	86	ARG
11	J	94	ARG
11	J	142	VAL
11	J	150	LYS
12	K	46	ILE
12	K	52	GLN
12	K	74	ARG
12	K	79	PHE
12	K	107	ASN
12	K	120	SER
12	K	127	ILE
12	K	131	THR
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	30	ARG
14	M	35	ARG
14	M	80	ASP
14	M	117	GLU
15	N	38	VAL

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Mol	Chain	Res	Type
15	N	46	LEU
15	N	48	ARG
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	159	THR
15	N	164	THR
16	O	26	LEU
16	O	47	LEU
16	O	49	THR
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	67	SER
17	P	98	LEU
17	P	109	SER
17	P	115	ARG
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
22	U	39	ASN
22	U	48	VAL
22	U	73	HIS
24	W	1	THR
24	W	22	ASP
24	W	65	ASP
25	X	26	ILE
25	X	32	CYS
25	X	35	VAL
25	X	52	VAL
25	X	122	ARG
25	X	142	ASP

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Mol	Chain	Res	Type
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	72	VAL
27	Z	154	ARG
27	Z	163	THR
27	Z	172	THR
27	Z	189	ASN
27	Z	203	VAL
27	Z	204	ARG
27	Z	235	GLU
28	1	11	THR
28	1	32	LYS
28	1	42	CYS
28	1	49	ARG
28	1	60	CYS
28	1	64	ILE
28	1	68	CYS
30	3	18	ASN
31	4	42	ARG
31	4	56	PRO
31	4	74	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	29	HIS
4	C	92	ASN
4	C	125	ASN
4	C	188	ASN
4	C	199	HIS
5	D	27	ASN
5	D	94	GLN
5	D	145	HIS
5	D	191	ASN
5	D	221	GLN
5	D	238	ASN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN

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Mol	Chain	Res	Type
6	E	129	HIS
6	E	163	HIS
7	F	47	GLN
7	F	103	ASN
7	F	133	ASN
8	G	71	ASN
8	G	106	ASN
8	G	143	GLN
9	H	80	GLN
10	I	17	GLN
10	I	64	ASN
11	J	35	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	80	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	137	ASN
11	J	166	ASN
12	K	25	GLN
12	K	52	GLN
12	K	107	ASN
13	L	10	GLN
14	M	18	HIS
14	M	41	HIS
14	M	116	HIS
15	N	58	GLN
15	N	176	GLN
16	O	107	ASN
16	O	119	GLN
16	O	153	GLN
17	P	100	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS

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Mol	Chain	Res	Type
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	123	GLN
21	T	53	ASN
21	T	55	GLN
22	U	39	ASN
23	V	38	ASN
23	V	39	ASN
24	W	60	GLN
25	X	2	HIS
25	X	12	ASN
25	X	14	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	18	ASN
30	3	41	HIS
30	3	45	ASN
31	4	18	GLN
31	4	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	246 (8%)	27 (0%)
2	B	121/122 (99%)	17 (14%)	4 (3%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	263 (9%)	31 (1%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	185	G
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	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C

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Mol	Chain	Res	Type
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
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	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	905	C
1	A	920	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	1083	C
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1120	U
1	A	1127	C
1	A	1129	C
1	A	1130	U
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G
1	A	1238	C
1	A	1239	G
1	A	1242	A
1	A	1279	U
1	A	1289	C
1	A	1331	A
1	A	1342	C

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Mol	Chain	Res	Type
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1406	A
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	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	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	1819	G
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1919	A

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Mol	Chain	Res	Type
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1996	U
1	A	2004	U
1	A	2006	C
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	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
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	2465	A
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2509	A

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Mol	Chain	Res	Type
1	A	2511	A
1	A	2533	C
1	A	2537	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	2620	U
1	A	2621	U
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U

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Mol	Chain	Res	Type
2	B	3025	G
2	B	3026	C
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 (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1474	C
1	A	1563	G
1	A	1685	A
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2467	A
1	A	2718	C
1	A	2791	U

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Mol	Chain	Res	Type
2	B	3023	U
2	B	3024	U
2	B	3043	G
2	B	3065	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 233 ligands modelled in this entry, 232 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	$\#\|Z\| > 2$
36	PPU	5	76	3	32,40,41	2.43	6 (18%)	33,57,60	1.15	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PPU	5	76	3	-	4/21/43/44	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	C-N3'	9.69	1.55	1.34
36	5	76	PPU	C10-N6	-4.31	1.35	1.45
36	5	76	PPU	C9-N6	-4.22	1.35	1.45
36	5	76	PPU	CE1-CZ	3.95	1.46	1.38
36	5	76	PPU	CE2-CD2	3.53	1.45	1.38
36	5	76	PPU	CE2-CZ	2.91	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	76	PPU	C3'-N3'-C	-3.76	117.55	123.21
36	5	76	PPU	CM-OC-CZ	2.11	122.08	117.51
36	5	76	PPU	CA-C-N3'	-2.07	113.28	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

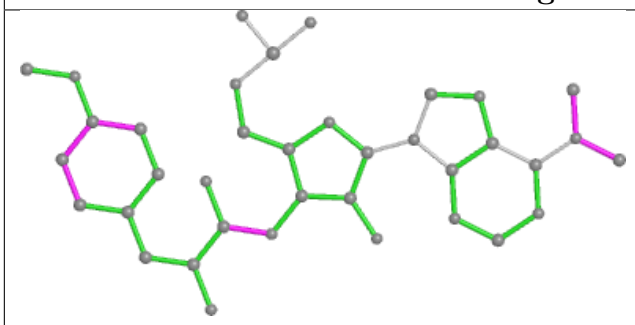
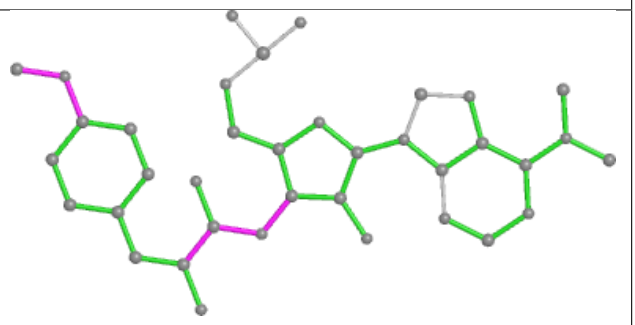
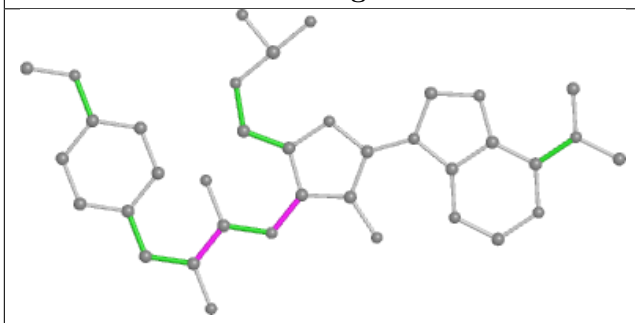
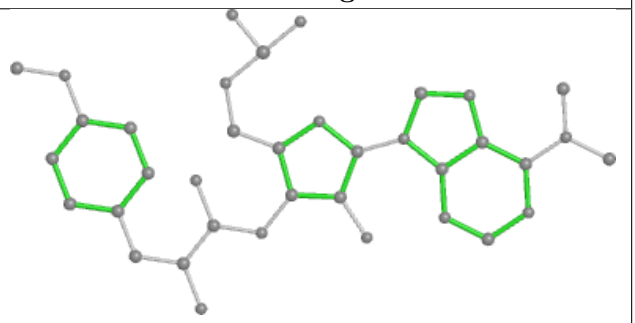
Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB
36	5	76	PPU	C4'-C3'-N3'-C
36	5	76	PPU	C2'-C3'-N3'-C

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PPU 5 76	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.08	70 (2%)	57	40	24, 52, 101, 153	0
2	B	122/122 (100%)	0.27	6 (4%)	29	18	42, 71, 102, 149	0
3	5	2/2 (100%)	2.87	2 (100%)	0	0	96, 96, 96, 111	0
4	C	237/239 (99%)	0.52	23 (9%)	7	4	28, 62, 98, 116	0
5	D	337/337 (100%)	0.26	4 (1%)	79	63	29, 60, 88, 96	0
6	E	246/246 (100%)	0.04	3 (1%)	79	63	27, 53, 76, 87	0
7	F	140/176 (79%)	2.24	70 (50%)	0	0	69, 108, 125, 135	0
8	G	172/177 (97%)	1.03	25 (14%)	2	1	50, 75, 99, 106	0
9	H	119/119 (100%)	0.92	21 (17%)	1	1	59, 82, 106, 110	0
10	I	29/348 (8%)	2.95	19 (65%)	0	0	81, 104, 108, 109	0
11	J	156/167 (93%)	0.50	13 (8%)	11	6	40, 61, 92, 97	0
12	K	142/145 (97%)	0.23	3 (2%)	63	46	40, 55, 75, 83	0
13	L	132/132 (100%)	0.12	3 (2%)	60	43	37, 59, 85, 88	0
14	M	145/164 (88%)	1.10	30 (20%)	1	0	27, 83, 118, 124	0
15	N	194/194 (100%)	0.21	6 (3%)	49	32	34, 54, 73, 81	0
16	O	186/186 (100%)	0.95	33 (17%)	1	1	46, 74, 114, 127	0
17	P	115/115 (100%)	0.34	2 (1%)	70	53	47, 63, 86, 91	0
18	Q	143/148 (96%)	0.59	12 (8%)	11	6	43, 63, 82, 90	0
19	R	95/95 (100%)	0.00	1 (1%)	80	65	40, 52, 61, 75	0
20	S	150/154 (97%)	0.04	1 (0%)	87	76	33, 49, 68, 76	0
21	T	81/84 (96%)	0.36	2 (2%)	57	40	55, 69, 88, 92	0
22	U	119/119 (100%)	0.55	9 (7%)	13	7	45, 61, 82, 91	0
23	V	53/66 (80%)	1.55	15 (28%)	0	0	73, 83, 98, 119	0
24	W	65/70 (92%)	1.52	18 (27%)	0	0	58, 84, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	154/154 (100%)	0.06	0 100 100	43, 55, 73, 83	0
26	Y	82/91 (90%)	0.48	9 (10%) 5 3	43, 64, 88, 102	0
27	Z	142/240 (59%)	0.21	8 (5%) 24 15	33, 51, 74, 92	0
28	1	73/73 (100%)	3.16	40 (54%) 0 0	76, 107, 118, 119	0
29	2	56/56 (100%)	-0.25	0 100 100	29, 37, 45, 48	0
30	3	46/48 (95%)	0.26	3 (6%) 18 11	41, 62, 83, 97	0
31	4	92/92 (100%)	8.53	92 (100%) 0 0	110, 126, 134, 137	0
All	All	6579/7281 (90%)	0.48	543 (8%) 11 6	24, 59, 111, 153	0

All (543) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	21.2
31	4	65	THR	20.2
31	4	83	TRP	18.5
31	4	85	ALA	15.1
31	4	62	THR	14.6
28	1	11	THR	14.3
31	4	38	ARG	14.0
31	4	35	TRP	14.0
31	4	3	MET	13.6
31	4	37	ASP	13.5
31	4	84	ARG	13.3
31	4	36	ILE	12.8
31	4	22	VAL	12.3
31	4	71	CYS	12.2
31	4	81	GLU	12.2
31	4	43	ASN	11.9
31	4	88	LEU	11.7
31	4	11	CYS	11.0
31	4	42	ARG	10.6
31	4	64	LYS	10.6
24	W	1	THR	10.6
31	4	4	PRO	10.5
31	4	74	CYS	10.4
31	4	78	HIS	10.4
31	4	72	GLY	10.3
31	4	19	GLU	10.3
31	4	25	VAL	10.1
31	4	9	THR	9.9

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Mol	Chain	Res	Type	RSRZ
31	4	59	ASP	9.8
31	4	63	LYS	9.8
10	I	27	ILE	9.8
31	4	23	GLU	9.8
31	4	40	ARG	9.6
31	4	80	ARG	9.6
31	4	67	LEU	9.5
31	4	33	MET	9.4
28	1	19	GLY	9.2
31	4	53	SER	9.2
31	4	18	GLN	9.0
31	4	17	HIS	9.0
31	4	91	GLN	9.0
31	4	1	MET	9.0
31	4	86	GLY	8.8
16	O	186	LEU	8.8
31	4	32	GLY	8.6
31	4	24	LYS	8.6
31	4	69	TYR	8.6
28	1	20	LEU	8.6
31	4	34	LYS	8.5
31	4	7	PHE	8.4
31	4	8	ASN	8.4
31	4	12	PRO	8.2
28	1	30	GLU	8.1
28	1	12	GLY	8.0
10	I	24	VAL	7.9
31	4	20	HIS	7.9
7	F	26	GLY	7.7
31	4	14	CYS	7.7
31	4	39	GLN	7.7
31	4	44	SER	7.7
28	1	26	VAL	7.6
31	4	47	GLY	7.6
31	4	41	GLU	7.6
31	4	48	ASN	7.5
7	F	88	LEU	7.5
10	I	23	ILE	7.5
31	4	66	ASP	7.5
31	4	13	HIS	7.5
31	4	10	TYR	7.4
31	4	52	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
31	4	2	GLN	7.4
31	4	68	LYS	7.2
31	4	50	GLY	7.1
7	F	44	ILE	7.1
31	4	29	ARG	6.9
31	4	51	LYS	6.9
31	4	61	PRO	6.8
10	I	20	VAL	6.7
31	4	21	GLU	6.7
31	4	60	LYS	6.6
31	4	26	ARG	6.5
31	4	46	ILE	6.5
28	1	35	LYS	6.4
28	1	16	PRO	6.4
31	4	49	ASP	6.3
2	B	3001	U	6.3
31	4	92	GLU	6.2
31	4	58	GLY	6.2
5	D	1	PRO	6.2
31	4	70	ARG	6.2
1	A	1173	A	6.1
28	1	44	PHE	6.1
28	1	18	TYR	6.1
31	4	6	ARG	6.0
28	1	24	VAL	6.0
7	F	18	ILE	5.9
28	1	31	ILE	5.9
28	1	33	HIS	5.8
31	4	76	LYS	5.8
4	C	236	GLY	5.7
4	C	37	VAL	5.7
31	4	87	ARG	5.7
28	1	14	PHE	5.7
31	4	31	THR	5.7
16	O	166	ALA	5.6
28	1	22	ILE	5.6
31	4	75	GLY	5.6
31	4	15	ASN	5.6
7	F	57	THR	5.5
16	O	158	LEU	5.4
28	1	36	LYS	5.4
7	F	80	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
28	1	10	ARG	5.4
23	V	4	ARG	5.3
16	O	147	ILE	5.3
28	1	17	ARG	5.2
28	1	34	LYS	5.2
7	F	63	ILE	5.2
7	F	24	HIS	5.1
16	O	179	LEU	5.1
1	A	735	C	5.1
2	B	3025	G	5.1
10	I	71	LEU	5.1
28	1	45	LYS	5.1
16	O	160	SER	5.1
7	F	69	ILE	5.0
23	V	54	THR	5.0
7	F	58	VAL	5.0
14	M	73	VAL	4.9
14	M	104	ASP	4.9
28	1	40	PRO	4.9
28	1	25	ARG	4.8
31	4	16	GLU	4.8
7	F	87	ALA	4.8
31	4	56	PRO	4.8
31	4	77	ALA	4.7
1	A	1172	G	4.7
28	1	37	HIS	4.7
1	A	1951	G	4.7
7	F	62	ASP	4.7
28	1	13	ARG	4.6
14	M	59	GLU	4.6
28	1	39	CYS	4.6
7	F	10	PHE	4.6
7	F	40	ILE	4.6
7	F	41	LEU	4.5
10	I	65	THR	4.5
1	A	2237	G	4.5
7	F	84	LEU	4.5
1	A	1177	A	4.5
1	A	1175	G	4.5
4	C	36	ASP	4.5
1	A	2344	G	4.4
31	4	79	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
14	M	105	TYR	4.4
16	O	162	ASP	4.4
28	1	28	ASP	4.3
14	M	61	ALA	4.3
16	O	150	TYR	4.3
31	4	57	GLY	4.3
7	F	27	ILE	4.3
28	1	29	VAL	4.3
22	U	119	ALA	4.3
28	1	23	ARG	4.3
7	F	75	LEU	4.3
7	F	25	MET	4.3
7	F	45	THR	4.2
7	F	61	PHE	4.2
31	4	5	ARG	4.2
14	M	97	VAL	4.1
7	F	12	GLU	4.1
14	M	91	VAL	4.1
28	1	15	GLY	4.1
28	1	27	ALA	4.0
16	O	157	PRO	4.0
31	4	28	GLY	3.9
14	M	81	VAL	3.9
9	H	103	ALA	3.9
14	M	76	LEU	3.9
28	1	47	LEU	3.9
23	V	52	THR	3.9
9	H	108	LEU	3.9
1	A	1171	A	3.9
7	F	96	SER	3.9
14	M	80	ASP	3.9
1	A	282	C	3.9
7	F	28	GLY	3.8
10	I	12	ILE	3.8
24	W	8	ILE	3.8
31	4	30	GLN	3.8
9	H	102	GLY	3.8
7	F	17	ARG	3.8
10	I	72	ASP	3.8
23	V	51	TRP	3.8
1	A	1188	A	3.8
9	H	106	THR	3.8

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Mol	Chain	Res	Type	RSRZ
23	V	9	CYS	3.7
10	I	17	GLN	3.7
10	I	16	LYS	3.7
31	4	89	GLU	3.7
16	O	167	ASP	3.7
7	F	56	ARG	3.7
7	F	166	ILE	3.7
14	M	106	VAL	3.6
14	M	118	LEU	3.6
28	1	38	LYS	3.6
28	1	41	VAL	3.6
31	4	55	VAL	3.6
28	1	32	LYS	3.6
4	C	64	ASP	3.6
1	A	1192	A	3.6
1	A	1525	G	3.5
16	O	137	ALA	3.5
2	B	3002	U	3.5
24	W	38	GLY	3.5
24	W	52	ALA	3.5
7	F	73	VAL	3.5
16	O	165	ALA	3.5
4	C	32	VAL	3.5
14	M	60	GLU	3.5
26	Y	80	GLU	3.5
7	F	90	LEU	3.5
2	B	3065	A	3.5
31	4	73	GLU	3.4
14	M	144	ASP	3.4
4	C	38	ILE	3.4
3	5	74	C	3.4
1	A	736	A	3.4
7	F	50	VAL	3.4
28	1	59	HIS	3.4
14	M	89	PHE	3.4
7	F	19	GLU	3.4
31	4	90	PHE	3.3
23	V	6	CYS	3.3
23	V	55	ALA	3.3
14	M	142	LEU	3.3
16	O	159	TYR	3.3
2	B	3023	U	3.3

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Mol	Chain	Res	Type	RSRZ
9	H	16	ALA	3.3
7	F	86	THR	3.3
7	F	49	PRO	3.3
24	W	11	MET	3.3
23	V	47	ARG	3.3
9	H	101	ALA	3.3
16	O	152	GLU	3.3
4	C	237	GLY	3.3
11	J	83	PHE	3.2
8	G	122	THR	3.2
7	F	104	PHE	3.2
10	I	64	ASN	3.2
1	A	970	U	3.2
28	1	79	VAL	3.2
7	F	170	TYR	3.2
14	M	58	GLN	3.2
28	1	21	LYS	3.2
19	R	95	GLU	3.2
1	A	2436	U	3.2
21	T	81	ILE	3.2
7	F	171	ASP	3.2
14	M	120	LEU	3.1
4	C	85	ASP	3.1
16	O	183	ASP	3.1
7	F	72	LYS	3.1
9	H	19	ALA	3.1
7	F	85	GLN	3.1
11	J	163	PRO	3.1
26	Y	88	GLU	3.1
7	F	37	ALA	3.1
10	I	28	GLU	3.1
22	U	82	THR	3.1
1	A	1168	C	3.1
8	G	86	VAL	3.1
1	A	1167	G	3.1
31	4	27	SER	3.0
1	A	2004	U	3.0
9	H	20	LEU	3.0
16	O	184	ILE	3.0
1	A	960	G	3.0
1	A	1950	G	3.0
7	F	83	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
11	J	135	TRP	3.0
14	M	79	ASP	3.0
7	F	106	PHE	3.0
1	A	2345	A	3.0
17	P	111	VAL	3.0
1	A	1169	U	2.9
1	A	2637	A	2.9
9	H	119	ARG	2.9
1	A	1180	U	2.9
1	A	1198	U	2.9
30	3	35	ARG	2.9
7	F	70	GLY	2.9
24	W	10	ASP	2.9
7	F	92	GLU	2.9
1	A	2249	G	2.9
4	C	62	ASP	2.9
14	M	46	LEU	2.9
4	C	94	LEU	2.9
9	H	15	ASP	2.9
10	I	15	TRP	2.8
24	W	43	PRO	2.8
8	G	124	VAL	2.8
1	A	716	G	2.8
1	A	1182	C	2.8
23	V	19	THR	2.8
10	I	26	MET	2.8
18	Q	28	GLN	2.8
7	F	60	GLU	2.8
7	F	89	PRO	2.8
16	O	138	ASP	2.8
31	4	54	LYS	2.8
8	G	131	LEU	2.8
14	M	90	ARG	2.8
11	J	43	PRO	2.8
7	F	128	LEU	2.8
18	Q	127	GLY	2.8
4	C	97	ALA	2.7
8	G	82	TYR	2.7
7	F	16	PRO	2.7
8	G	100	ASP	2.7
4	C	129	LEU	2.7
7	F	22	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	3122	C	2.7
18	Q	105	LEU	2.7
23	V	56	ARG	2.7
1	A	2250	G	2.7
7	F	74	THR	2.7
7	F	165	PHE	2.7
8	G	126	ILE	2.7
1	A	1204	C	2.7
1	A	1166	A	2.7
1	A	1203	G	2.7
26	Y	10	VAL	2.7
8	G	1	PRO	2.7
8	G	170	ARG	2.7
1	A	1181	A	2.6
11	J	36	ASN	2.6
16	O	151	ASP	2.6
1	A	1190	G	2.6
1	A	1948	G	2.6
22	U	80	GLU	2.6
7	F	93	LEU	2.6
16	O	67	ALA	2.6
28	1	42	CYS	2.6
1	A	1162	G	2.6
28	1	68	CYS	2.6
5	D	119	HIS	2.6
17	P	26	TRP	2.6
7	F	59	GLY	2.6
4	C	86	ALA	2.6
24	W	63	GLU	2.6
9	H	90	GLU	2.6
7	F	38	GLU	2.6
10	I	67	LEU	2.6
14	M	150	GLN	2.5
9	H	22	VAL	2.5
18	Q	130	GLU	2.5
24	W	62	GLU	2.5
31	4	45	GLY	2.5
4	C	128	LEU	2.5
18	Q	131	PHE	2.5
1	A	2251	G	2.5
7	F	11	HIS	2.5
1	A	2238	A	2.5

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Mol	Chain	Res	Type	RSRZ
24	W	3	LEU	2.5
22	U	83	ASP	2.5
12	K	7	ASP	2.5
9	H	117	GLU	2.5
16	O	95	ALA	2.5
7	F	47	GLN	2.5
14	M	128	GLY	2.5
7	F	13	MET	2.5
7	F	43	GLU	2.5
8	G	10	ASP	2.5
1	A	272	A	2.5
1	A	1193	A	2.5
8	G	96	ASN	2.5
18	Q	1	THR	2.5
8	G	125	GLU	2.5
26	Y	82	GLU	2.5
27	Z	108	ASP	2.5
7	F	97	GLN	2.5
7	F	137	PRO	2.4
14	M	130	ARG	2.4
22	U	115	GLU	2.4
1	A	1949	G	2.4
23	V	12	ASP	2.4
20	S	8	ALA	2.4
4	C	96	LEU	2.4
16	O	185	GLU	2.4
1	A	713	U	2.4
4	C	83	GLY	2.4
24	W	39	ALA	2.4
14	M	44	GLU	2.4
16	O	136	LEU	2.4
8	G	88	TYR	2.4
21	T	45	TYR	2.4
27	Z	196	VAL	2.4
7	F	161	ASP	2.4
26	Y	7	GLU	2.4
8	G	166	VAL	2.4
14	M	141	GLU	2.4
1	A	1186	C	2.4
16	O	146	HIS	2.4
24	W	40	PRO	2.4
6	E	237	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
7	F	76	ARG	2.4
4	C	84	VAL	2.4
16	O	163	PHE	2.4
5	D	118	ASP	2.4
8	G	42	VAL	2.4
24	W	5	VAL	2.4
8	G	127	ASP	2.4
1	A	1199	A	2.4
8	G	157	LYS	2.4
16	O	153	GLN	2.3
18	Q	101	GLN	2.3
1	A	370	G	2.3
1	A	285	A	2.3
13	L	132	VAL	2.3
1	A	1205	U	2.3
9	H	26	THR	2.3
1	A	514	G	2.3
1	A	1522	A	2.3
1	A	1184	C	2.3
1	A	2508	C	2.3
3	5	75	C	2.3
18	Q	137	LEU	2.3
1	A	1178	G	2.3
4	C	82	VAL	2.3
1	A	281	U	2.3
18	Q	119	TYR	2.3
7	F	71	ALA	2.3
27	Z	103	THR	2.3
1	A	1526	A	2.3
11	J	32	ASP	2.3
1	A	280	C	2.3
8	G	118	ILE	2.3
16	O	127	LEU	2.3
9	H	99	THR	2.3
10	I	13	PRO	2.3
16	O	143	ARG	2.3
7	F	134	LEU	2.3
9	H	118	LEU	2.3
16	O	172	PHE	2.3
1	A	1165	G	2.3
1	A	1279	U	2.2
1	A	368	C	2.2

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Mol	Chain	Res	Type	RSRZ
7	F	64	ARG	2.2
18	Q	116	SER	2.2
22	U	103	LEU	2.2
18	Q	98	ILE	2.2
6	E	135	GLU	2.2
10	I	68	GLU	2.2
27	Z	235	GLU	2.2
11	J	72	VAL	2.2
24	W	2	VAL	2.2
8	G	98	GLU	2.2
14	M	74	THR	2.2
23	V	10	GLY	2.2
16	O	149	GLU	2.2
16	O	74	PRO	2.2
23	V	15	PRO	2.2
1	A	2664	A	2.2
15	N	152	ARG	2.2
9	H	115	VAL	2.2
23	V	53	ASP	2.2
30	3	44	ARG	2.2
14	M	121	ILE	2.2
11	J	84	ARG	2.2
24	W	49	LEU	2.2
8	G	91	PHE	2.2
15	N	140	ALA	2.2
11	J	140	PRO	2.2
8	G	81	GLU	2.2
8	G	108	LEU	2.2
9	H	100	ASP	2.2
9	H	23	ALA	2.2
9	H	28	ALA	2.2
14	M	62	ALA	2.2
11	J	139	ASP	2.1
11	J	35	ASN	2.1
4	C	87	GLU	2.1
7	F	51	ARG	2.1
8	G	117	THR	2.1
4	C	35	GLY	2.1
1	A	138	U	2.1
7	F	91	ALA	2.1
15	N	156	ARG	2.1
1	A	1527	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2914	A	2.1
7	F	77	ASP	2.1
4	C	133	ARG	2.1
13	L	119	GLN	2.1
16	O	81	ALA	2.1
11	J	80	ASN	2.1
8	G	76	VAL	2.1
15	N	194	ALA	2.1
15	N	78	ASN	2.1
28	1	61	GLY	2.1
26	Y	73	ARG	2.1
16	O	140	GLN	2.1
1	A	734	U	2.1
15	N	87	MET	2.1
1	A	284	C	2.1
1	A	2825	C	2.1
22	U	112	LEU	2.1
24	W	58	THR	2.1
7	F	129	ASP	2.1
4	C	154	ALA	2.1
1	A	1626	A	2.1
24	W	16	ARG	2.1
16	O	64	SER	2.1
27	Z	98	GLN	2.1
5	D	86	ALA	2.1
8	G	148	ILE	2.1
11	J	114	PRO	2.1
1	A	2248	C	2.1
18	Q	114	LEU	2.1
26	Y	77	PHE	2.1
24	W	37	GLY	2.1
13	L	98	VAL	2.1
23	V	49	LEU	2.0
22	U	108	ARG	2.0
27	Z	221	ALA	2.0
14	M	140	VAL	2.0
9	H	49	PHE	2.0
10	I	21	ASP	2.0
12	K	27	ALA	2.0
7	F	81	GLU	2.0
10	I	19	GLU	2.0
12	K	109	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
26	Y	74	ALA	2.0
6	E	139	VAL	2.0
22	U	37	GLN	2.0
27	Z	97	LEU	2.0
30	3	27	LEU	2.0
7	F	154	LYS	2.0
1	A	1176	C	2.0
1	A	1197	G	2.0
4	C	105	VAL	2.0
27	Z	234	VAL	2.0
26	Y	41	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	T	8312	1/1	-0.44	0.49	163,163,163,163	0
35	CL	4	8504	1/1	0.34	0.54	114,114,114,114	0
34	NA	B	8351	1/1	0.46	0.43	90,90,90,90	0
34	NA	S	8386	1/1	0.51	0.52	77,77,77,77	0
32	MG	A	8076	1/1	0.53	0.37	123,123,123,123	0
32	MG	A	8070	1/1	0.55	1.20	98,98,98,98	0
32	MG	4	8078	1/1	0.55	0.62	117,117,117,117	0
32	MG	A	8024	1/1	0.59	1.06	84,84,84,84	0
35	CL	A	8510	1/1	0.64	0.30	83,83,83,83	0
32	MG	A	8046	1/1	0.64	0.12	74,74,74,74	0
34	NA	A	8384	1/1	0.65	0.74	105,105,105,105	0
35	CL	A	8515	1/1	0.66	0.51	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	4	8114	1/1	0.68	0.74	111,111,111,111	0
34	NA	A	8363	1/1	0.69	0.36	56,56,56,56	0
32	MG	A	8097	1/1	0.70	0.45	80,80,80,80	0
34	NA	A	8359	1/1	0.71	0.41	53,53,53,53	0
34	NA	A	8382	1/1	0.72	0.24	44,44,44,44	0
32	MG	A	8089	1/1	0.74	0.26	89,89,89,89	0
34	NA	A	8355	1/1	0.74	0.41	88,88,88,88	0
37	CD	P	8405	1/1	0.77	0.45	202,202,202,202	0
37	CD	4	8404	1/1	0.78	0.46	202,202,202,202	0
34	NA	A	8357	1/1	0.79	0.13	43,43,43,43	0
34	NA	A	8377	1/1	0.79	0.55	72,72,72,72	0
34	NA	A	8322	1/1	0.79	0.26	76,76,76,76	0
34	NA	A	8371	1/1	0.80	0.18	35,35,35,35	0
34	NA	A	8370	1/1	0.80	0.39	82,82,82,82	0
32	MG	A	8106	1/1	0.81	0.09	101,101,101,101	0
34	NA	S	8338	1/1	0.83	0.19	84,84,84,84	0
32	MG	A	8044	1/1	0.83	0.21	64,64,64,64	0
32	MG	1	8105	1/1	0.83	0.46	80,80,80,80	0
32	MG	A	8068	1/1	0.83	0.08	59,59,59,59	0
32	MG	A	8092	1/1	0.84	0.28	105,105,105,105	0
35	CL	O	8507	1/1	0.84	0.18	72,72,72,72	0
37	CD	V	8401	1/1	0.84	0.37	202,202,202,202	0
35	CL	P	8508	1/1	0.84	0.16	99,99,99,99	0
36	PPU	5	76	37/38	0.85	0.36	90,95,100,100	0
32	MG	A	8099	1/1	0.85	0.19	55,55,55,55	0
32	MG	A	8116	1/1	0.85	0.32	117,117,117,117	0
34	NA	A	8350	1/1	0.85	0.23	21,21,21,21	0
34	NA	A	8375	1/1	0.86	0.34	44,44,44,44	0
34	NA	E	8304	1/1	0.86	0.12	23,23,23,23	0
32	MG	A	8052	1/1	0.87	0.14	42,42,42,42	0
32	MG	A	8043	1/1	0.87	0.13	67,67,67,67	0
34	NA	A	8344	1/1	0.87	0.09	20,20,20,20	0
32	MG	A	8051	1/1	0.87	0.16	97,97,97,97	0
35	CL	A	8514	1/1	0.88	0.19	62,62,62,62	0
34	NA	A	8366	1/1	0.88	0.16	38,38,38,38	0
35	CL	C	8509	1/1	0.88	0.26	92,92,92,92	0
34	NA	A	8369	1/1	0.88	0.15	41,41,41,41	0
32	MG	U	8073	1/1	0.88	0.13	34,34,34,34	0
32	MG	A	8111	1/1	0.88	0.25	69,69,69,69	0
34	NA	A	8333	1/1	0.88	0.09	25,25,25,25	0
34	NA	A	8341	1/1	0.88	0.10	28,28,28,28	0
32	MG	A	8066	1/1	0.88	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CL	A	8511	1/1	0.88	0.21	73,73,73,73	0
34	NA	A	8361	1/1	0.89	0.27	48,48,48,48	0
34	NA	B	8383	1/1	0.89	0.20	52,52,52,52	0
34	NA	A	8319	1/1	0.89	0.11	41,41,41,41	0
35	CL	A	8505	1/1	0.89	0.14	68,68,68,68	0
34	NA	A	8339	1/1	0.90	0.13	15,15,15,15	0
34	NA	A	8356	1/1	0.90	0.37	46,46,46,46	0
32	MG	A	8008	1/1	0.90	0.08	50,50,50,50	0
34	NA	A	8381	1/1	0.90	0.08	35,35,35,35	0
35	CL	S	8506	1/1	0.90	0.16	60,60,60,60	0
34	NA	A	8314	1/1	0.91	0.26	35,35,35,35	0
35	CL	K	8502	1/1	0.91	0.21	83,83,83,83	0
32	MG	A	8040	1/1	0.91	0.17	86,86,86,86	0
32	MG	A	8102	1/1	0.91	0.74	106,106,106,106	0
34	NA	A	8323	1/1	0.91	0.29	55,55,55,55	0
34	NA	A	8331	1/1	0.91	0.19	37,37,37,37	0
32	MG	A	8071	1/1	0.91	0.07	65,65,65,65	0
32	MG	A	8039	1/1	0.91	0.09	66,66,66,66	0
32	MG	A	8112	1/1	0.91	0.26	70,70,70,70	0
34	NA	A	8306	1/1	0.91	0.40	38,38,38,38	0
32	MG	A	8047	1/1	0.92	0.21	76,76,76,76	0
32	MG	A	8062	1/1	0.92	0.08	32,32,32,32	0
34	NA	A	8367	1/1	0.92	0.14	40,40,40,40	0
34	NA	A	8368	1/1	0.92	0.08	22,22,22,22	0
37	CD	2	8402	1/1	0.92	0.11	67,67,67,67	0
35	CL	Z	8520	1/1	0.92	0.15	49,49,49,49	0
34	NA	A	8372	1/1	0.93	0.15	30,30,30,30	0
35	CL	A	8512	1/1	0.93	0.11	43,43,43,43	0
34	NA	A	8317	1/1	0.93	0.12	25,25,25,25	0
32	MG	A	8085	1/1	0.93	0.18	60,60,60,60	0
35	CL	A	8522	1/1	0.93	0.48	72,72,72,72	0
32	MG	A	8049	1/1	0.93	0.17	61,61,61,61	0
32	MG	A	8091	1/1	0.93	0.07	53,53,53,53	0
32	MG	A	8045	1/1	0.93	0.12	69,69,69,69	0
32	MG	A	8096	1/1	0.93	0.14	55,55,55,55	0
34	NA	A	8365	1/1	0.93	0.12	21,21,21,21	0
32	MG	A	8027	1/1	0.93	0.09	56,56,56,56	0
34	NA	J	8309	1/1	0.93	0.10	23,23,23,23	0
34	NA	A	8340	1/1	0.93	0.38	37,37,37,37	0
32	MG	A	8041	1/1	0.93	0.30	72,72,72,72	0
34	NA	A	8342	1/1	0.93	0.15	31,31,31,31	0
32	MG	A	8063	1/1	0.93	0.09	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8082	1/1	0.93	0.10	35,35,35,35	0
32	MG	A	8087	1/1	0.94	0.29	42,42,42,42	0
32	MG	A	8101	1/1	0.94	0.09	42,42,42,42	0
32	MG	A	8018	1/1	0.94	0.12	26,26,26,26	0
34	NA	A	8302	1/1	0.94	0.10	36,36,36,36	0
34	NA	A	8305	1/1	0.94	0.14	22,22,22,22	0
32	MG	A	8075	1/1	0.94	0.08	44,44,44,44	0
34	NA	A	8308	1/1	0.94	0.23	61,61,61,61	0
35	CL	D	8519	1/1	0.94	0.32	68,68,68,68	0
32	MG	A	8001	1/1	0.94	0.12	33,33,33,33	0
35	CL	K	8521	1/1	0.94	0.15	49,49,49,49	0
32	MG	A	8058	1/1	0.94	0.12	47,47,47,47	0
32	MG	A	8050	1/1	0.94	0.12	62,62,62,62	0
32	MG	B	8095	1/1	0.94	0.15	90,90,90,90	0
32	MG	D	8055	1/1	0.94	0.08	50,50,50,50	0
34	NA	A	8364	1/1	0.94	0.16	32,32,32,32	0
34	NA	S	8337	1/1	0.94	0.12	57,57,57,57	0
34	NA	A	8325	1/1	0.94	0.17	56,56,56,56	0
32	MG	A	8098	1/1	0.94	0.26	53,53,53,53	0
32	MG	Z	8109	1/1	0.94	0.08	31,31,31,31	0
34	NA	A	8336	1/1	0.94	0.15	72,72,72,72	0
34	NA	A	8329	1/1	0.95	0.08	47,47,47,47	0
32	MG	A	8090	1/1	0.95	0.20	81,81,81,81	0
32	MG	A	8103	1/1	0.95	0.11	45,45,45,45	0
34	NA	A	8335	1/1	0.95	0.15	50,50,50,50	0
32	MG	A	8029	1/1	0.95	0.10	58,58,58,58	0
32	MG	A	8107	1/1	0.95	0.05	64,64,64,64	0
32	MG	A	8059	1/1	0.95	0.12	70,70,70,70	0
32	MG	A	8094	1/1	0.95	0.12	77,77,77,77	0
35	CL	A	8516	1/1	0.95	0.23	57,57,57,57	0
35	CL	A	8517	1/1	0.95	0.29	75,75,75,75	0
34	NA	A	8310	1/1	0.95	0.17	35,35,35,35	0
34	NA	A	8374	1/1	0.95	0.12	36,36,36,36	0
34	NA	A	8313	1/1	0.95	0.45	76,76,76,76	0
34	NA	A	8349	1/1	0.95	0.18	27,27,27,27	0
34	NA	A	8379	1/1	0.95	0.13	30,30,30,30	0
32	MG	A	8048	1/1	0.95	0.10	51,51,51,51	0
34	NA	A	8354	1/1	0.95	0.13	20,20,20,20	0
32	MG	A	8032	1/1	0.95	0.11	24,24,24,24	0
34	NA	A	8385	1/1	0.95	0.40	29,29,29,29	0
32	MG	A	8037	1/1	0.95	0.07	40,40,40,40	0
34	NA	A	8320	1/1	0.95	0.10	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8358	1/1	0.95	0.57	75,75,75,75	0
32	MG	A	8013	1/1	0.95	0.15	27,27,27,27	0
32	MG	A	8100	1/1	0.95	0.11	45,45,45,45	0
32	MG	A	8020	1/1	0.95	0.09	38,38,38,38	0
34	NA	A	8328	1/1	0.96	0.13	39,39,39,39	0
32	MG	A	8036	1/1	0.96	0.06	36,36,36,36	0
35	CL	A	8503	1/1	0.96	0.12	65,65,65,65	0
32	MG	A	8056	1/1	0.96	0.12	53,53,53,53	0
34	NA	A	8332	1/1	0.96	0.17	38,38,38,38	0
33	K	A	8201	1/1	0.96	0.09	53,53,53,53	0
33	K	A	8202	1/1	0.96	0.07	43,43,43,43	0
32	MG	A	8072	1/1	0.96	0.22	64,64,64,64	0
34	NA	A	8303	1/1	0.96	0.18	33,33,33,33	0
32	MG	A	8108	1/1	0.96	0.10	44,44,44,44	0
34	NA	A	8373	1/1	0.96	0.07	40,40,40,40	0
32	MG	A	8011	1/1	0.96	0.09	36,36,36,36	0
32	MG	A	8026	1/1	0.96	0.09	19,19,19,19	0
32	MG	A	8115	1/1	0.96	0.09	41,41,41,41	0
34	NA	A	8378	1/1	0.96	0.12	28,28,28,28	0
32	MG	A	8077	1/1	0.96	0.16	37,37,37,37	0
32	MG	A	8006	1/1	0.96	0.09	33,33,33,33	0
34	NA	A	8352	1/1	0.96	0.20	36,36,36,36	0
32	MG	C	8065	1/1	0.96	0.13	62,62,62,62	0
34	NA	A	8318	1/1	0.96	0.22	62,62,62,62	0
32	MG	A	8028	1/1	0.96	0.06	60,60,60,60	0
32	MG	L	8069	1/1	0.96	0.08	65,65,65,65	0
32	MG	A	8005	1/1	0.96	0.12	39,39,39,39	0
32	MG	A	8088	1/1	0.96	0.07	11,11,11,11	0
32	MG	A	8010	1/1	0.96	0.06	37,37,37,37	0
34	NA	A	8326	1/1	0.96	0.10	31,31,31,31	0
32	MG	A	8033	1/1	0.97	0.09	26,26,26,26	0
32	MG	A	8084	1/1	0.97	0.09	65,65,65,65	0
34	NA	A	8343	1/1	0.97	0.09	17,17,17,17	0
32	MG	A	8113	1/1	0.97	0.10	40,40,40,40	0
35	CL	A	8513	1/1	0.97	0.13	74,74,74,74	0
32	MG	A	8034	1/1	0.97	0.06	32,32,32,32	0
34	NA	A	8301	1/1	0.97	0.26	27,27,27,27	0
32	MG	A	8004	1/1	0.97	0.08	18,18,18,18	0
34	NA	A	8324	1/1	0.97	0.06	26,26,26,26	0
32	MG	A	8053	1/1	0.97	0.16	86,86,86,86	0
32	MG	A	8023	1/1	0.97	0.07	47,47,47,47	0
34	NA	A	8327	1/1	0.97	0.25	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8009	1/1	0.97	0.08	15,15,15,15	0
34	NA	A	8307	1/1	0.97	0.11	28,28,28,28	0
34	NA	A	8360	1/1	0.97	0.15	42,42,42,42	0
32	MG	A	8031	1/1	0.97	0.07	14,14,14,14	0
32	MG	A	8061	1/1	0.97	0.07	40,40,40,40	0
34	NA	A	8311	1/1	0.97	0.12	68,68,68,68	0
34	NA	R	8348	1/1	0.97	0.11	20,20,20,20	0
34	NA	A	8334	1/1	0.97	0.05	36,36,36,36	0
32	MG	A	8093	1/1	0.97	0.19	91,91,91,91	0
32	MG	A	8019	1/1	0.97	0.06	27,27,27,27	0
37	CD	1	8403	1/1	0.97	0.14	187,187,187,187	0
34	NA	A	8315	1/1	0.97	0.11	15,15,15,15	0
34	NA	A	8316	1/1	0.97	0.11	31,31,31,31	0
32	MG	A	8083	1/1	0.98	0.07	40,40,40,40	0
32	MG	A	8003	1/1	0.98	0.19	36,36,36,36	0
32	MG	A	8012	1/1	0.98	0.14	41,41,41,41	0
34	NA	A	8321	1/1	0.98	0.23	53,53,53,53	0
32	MG	A	8104	1/1	0.98	0.09	40,40,40,40	0
32	MG	A	8086	1/1	0.98	0.14	49,49,49,49	0
32	MG	A	8030	1/1	0.98	0.13	31,31,31,31	0
34	NA	A	8376	1/1	0.98	0.12	35,35,35,35	0
34	NA	A	8353	1/1	0.98	0.07	15,15,15,15	0
32	MG	A	8022	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8110	1/1	0.98	0.06	26,26,26,26	0
32	MG	A	8067	1/1	0.98	0.15	41,41,41,41	0
32	MG	A	8002	1/1	0.98	0.11	26,26,26,26	0
32	MG	A	8014	1/1	0.98	0.13	20,20,20,20	0
34	NA	A	8330	1/1	0.98	0.10	37,37,37,37	0
35	CL	N	8518	1/1	0.98	0.08	36,36,36,36	0
32	MG	A	8054	1/1	0.98	0.09	43,43,43,43	0
32	MG	A	8015	1/1	0.98	0.08	35,35,35,35	0
34	NA	C	8345	1/1	0.98	0.15	30,30,30,30	0
34	NA	A	8362	1/1	0.98	0.13	45,45,45,45	0
32	MG	A	8057	1/1	0.98	0.10	16,16,16,16	0
34	NA	M	8380	1/1	0.98	0.15	43,43,43,43	0
32	MG	A	8035	1/1	0.98	0.04	64,64,64,64	0
32	MG	A	8007	1/1	0.98	0.09	22,22,22,22	0
32	MG	A	8079	1/1	0.98	0.07	19,19,19,19	0
32	MG	A	8080	1/1	0.98	0.09	35,35,35,35	0
32	MG	A	8060	1/1	0.98	0.12	39,39,39,39	0
32	MG	A	8117	1/1	0.99	0.06	8,8,8,8	0
34	NA	N	8347	1/1	0.99	0.05	21,21,21,21	0

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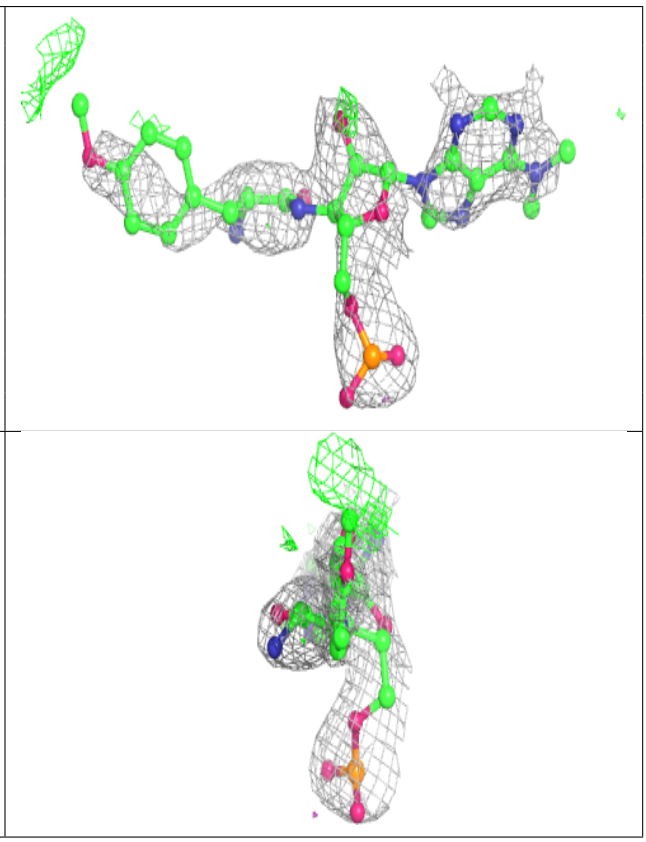
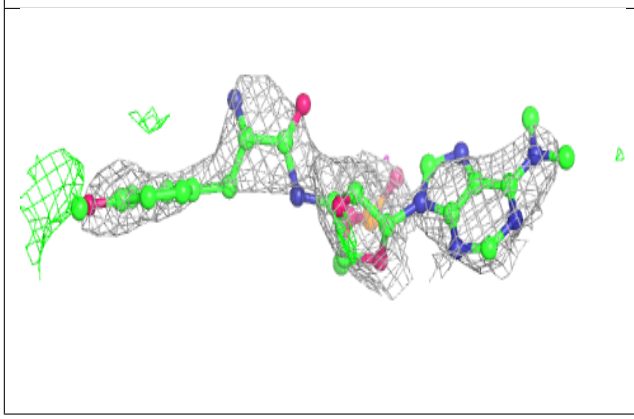
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8017	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8016	1/1	0.99	0.10	26,26,26,26	0
32	MG	A	8021	1/1	0.99	0.10	45,45,45,45	0
32	MG	A	8042	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8081	1/1	0.99	0.13	30,30,30,30	0
32	MG	A	8025	1/1	0.99	0.04	57,57,57,57	0
32	MG	A	8038	1/1	0.99	0.10	30,30,30,30	0
35	CL	K	8501	1/1	0.99	0.10	61,61,61,61	0
32	MG	A	8074	1/1	0.99	0.08	24,24,24,24	0
32	MG	A	8064	1/1	0.99	0.11	18,18,18,18	0
34	NA	K	8346	1/1	1.00	0.06	19,19,19,19	0

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

Electron density around PPU 5 76:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.