



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 06:54 PM EST

PDB ID : 1VQ7
Title : The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

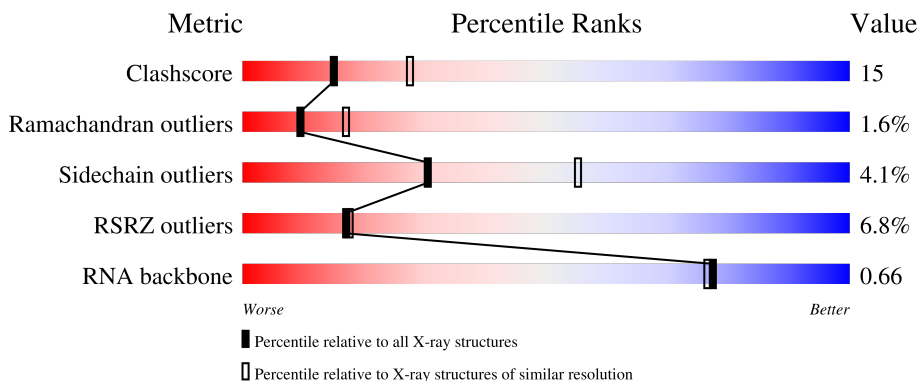
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 60% 29% 5% • 6%</p>
2	9	122	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 58% 32% 8% • .</p>
3	4	8	<div style="display: flex; align-items: center;"> <div style="width: 38%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 62%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">38% 62%</p>
4	A	240	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">7% 64% 30% • •</p>
5	B	338	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">3% 50% 44% 5%</p>

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8092	-	-	-	X
35	NA	S	9112	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99063 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	0	2754	59021	26350	10878	19048	2745	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	130	63	23	39	5	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	A	237	1753	1072	352	324	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	B	337	2625	1616	493	511	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	246	1859	1131	344	383	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	D	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	E	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	F	119	890	551	141	197	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	G	29	240	149	39	51	1	0	0	0

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	H	160	1266	785	237	238	6	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	J	142	1120	696	199	222	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	K	132	992	609	187	192	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	N	186	1445	895	262	286	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	O	115	865	529	161	175	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	P	143	1136	683	229	224	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	Q	95	735	450	141	144	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	R	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	S	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	T	119	950	568	180	202	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	U	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	V	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	W	154	1196	737	209	244	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	X	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	S			
27	Y	142	1130	686	228	216		0	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	11	Total 11	Cl 11	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5809	Total O 5809 5809	0	0
38	9	137	Total O 137 137	0	0
38	4	8	Total O 8 8	0	0
38	A	119	Total O 119 119	0	0
38	B	153	Total O 153 153	0	0
38	C	168	Total O 168 168	0	0
38	D	47	Total O 47 47	0	0
38	E	43	Total O 43 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	23	Total O 23 23	0	0
38	G	18	Total O 18 18	0	0
38	H	65	Total O 65 65	0	0
38	J	51	Total O 51 51	0	0
38	K	58	Total O 58 58	0	0
38	L	82	Total O 82 82	0	0
38	M	116	Total O 116 116	0	0
38	N	63	Total O 63 63	0	0
38	O	42	Total O 42 42	0	0
38	P	64	Total O 64 64	0	0
38	Q	51	Total O 51 51	0	0
38	R	84	Total O 84 84	0	0
38	S	30	Total O 30 30	0	0
38	T	42	Total O 42 42	0	0
38	U	29	Total O 29 29	0	0
38	V	14	Total O 14 14	0	0
38	W	68	Total O 68 68	0	0
38	X	27	Total O 27 27	0	0
38	Y	96	Total O 96 96	0	0
38	Z	32	Total O 32 32	0	0
38	1	53	Total O 53 53	0	0

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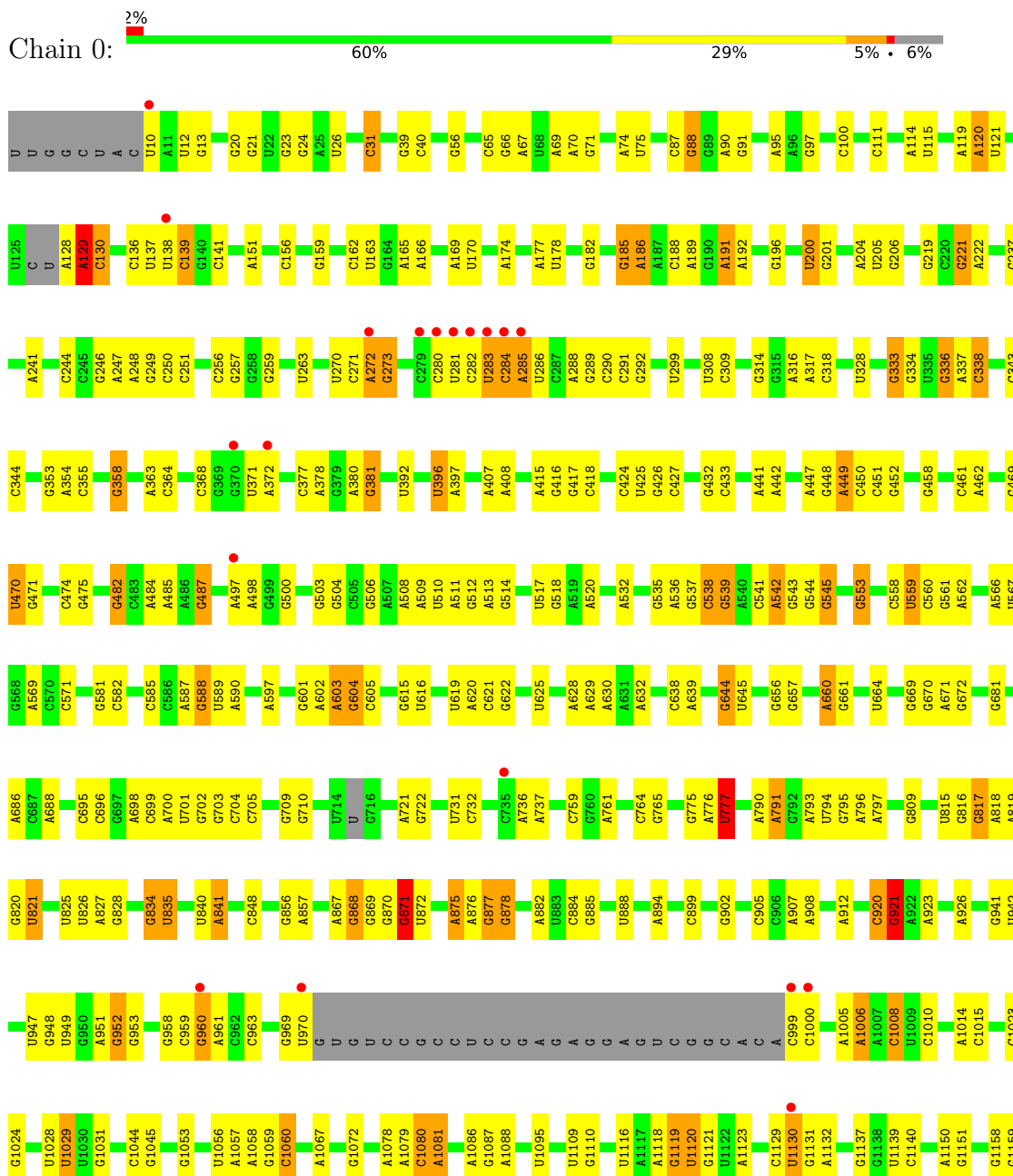
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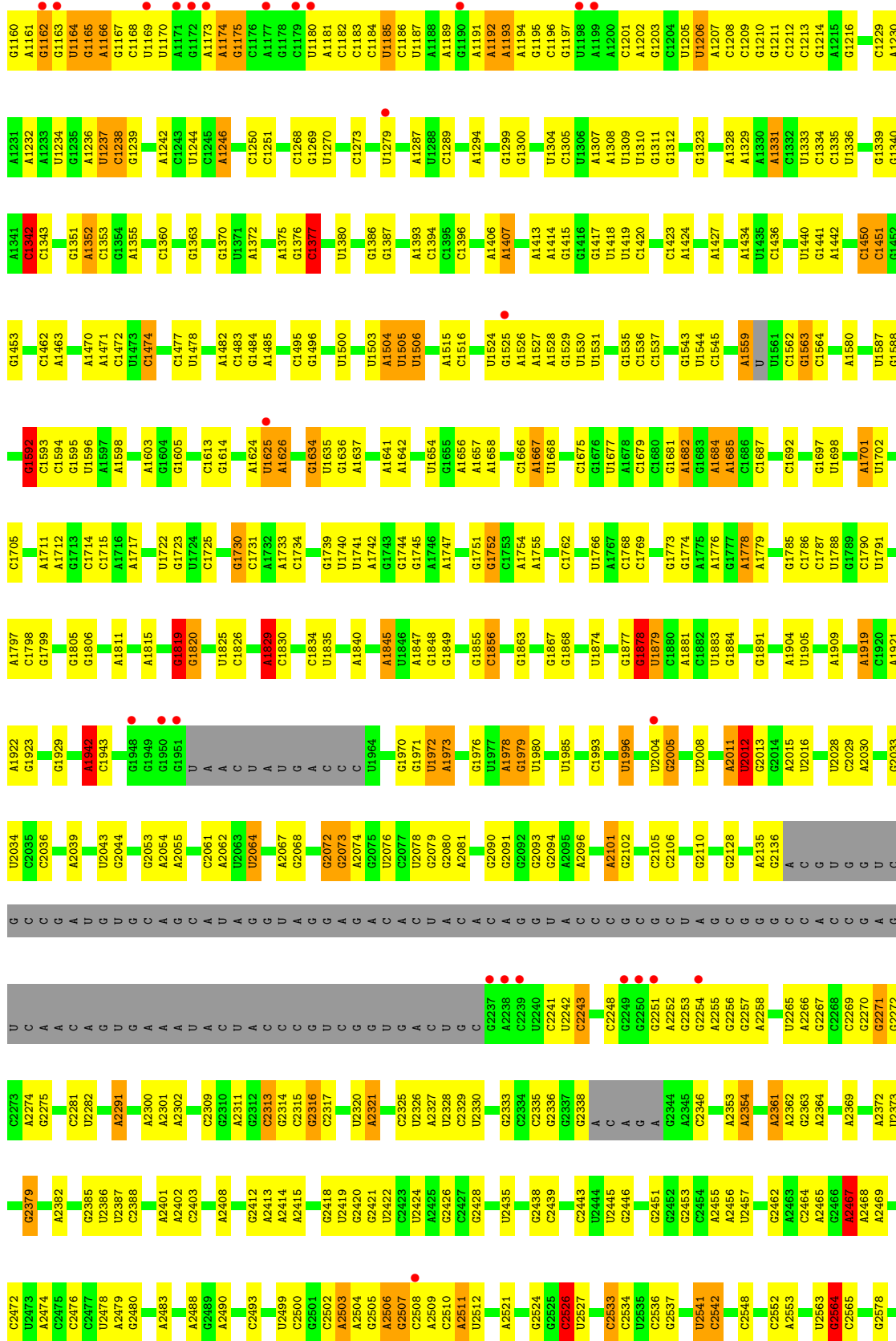
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	2	40	Total O 40 40	0	0
38	3	74	Total O 74 74	0	0
38	I	9	Total O 9 9	0	0

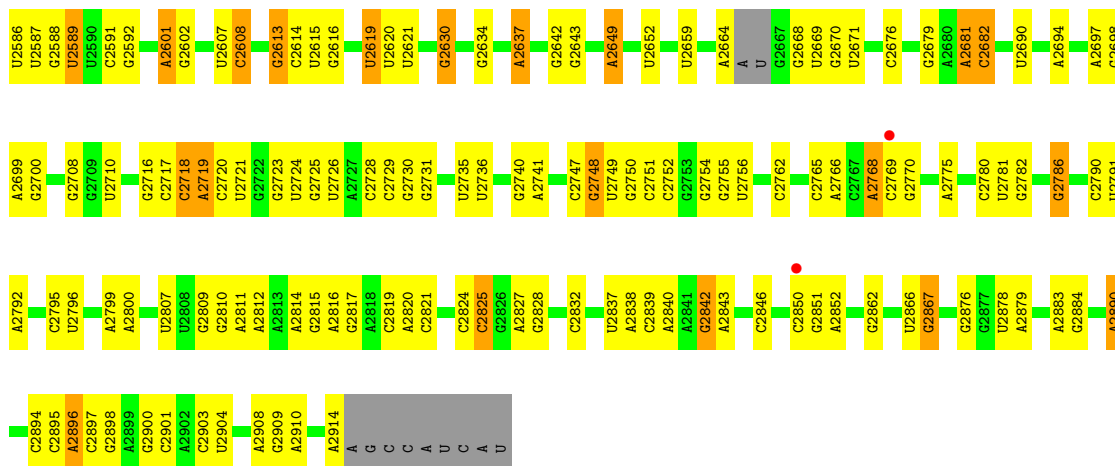
3 Residue-property plots [i](#)

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

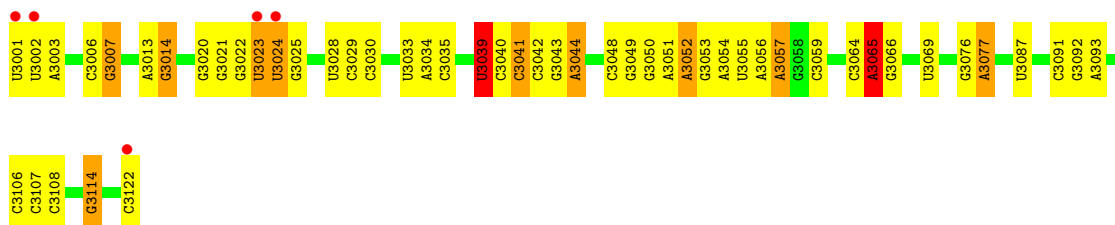
- Molecule 1: 23S ribosomal rna



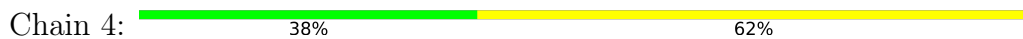




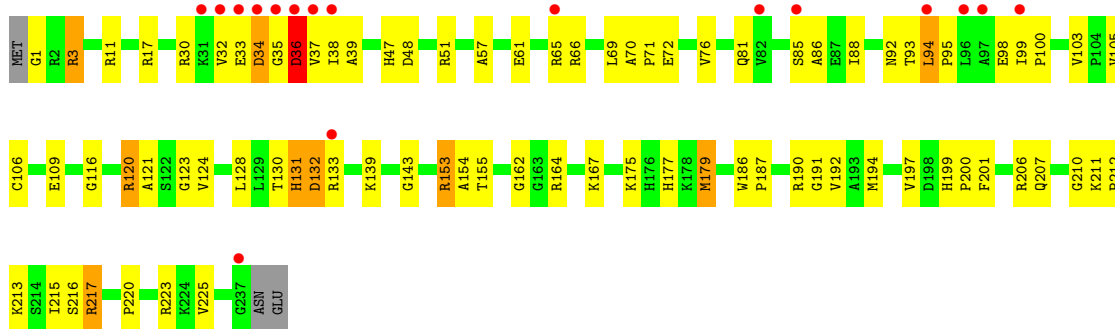
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3'

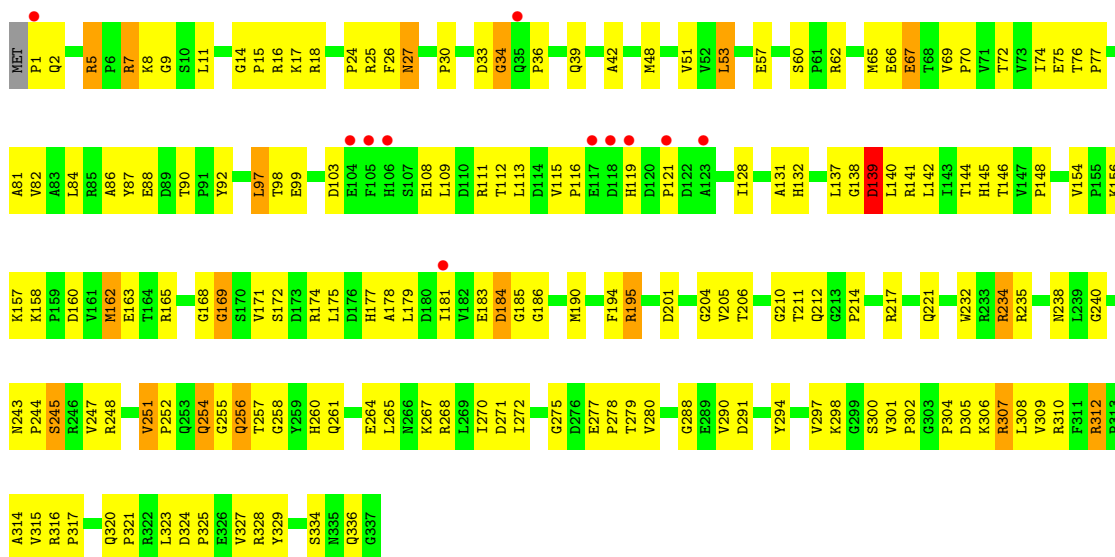


• Molecule 4: 50S ribosomal protein L2P

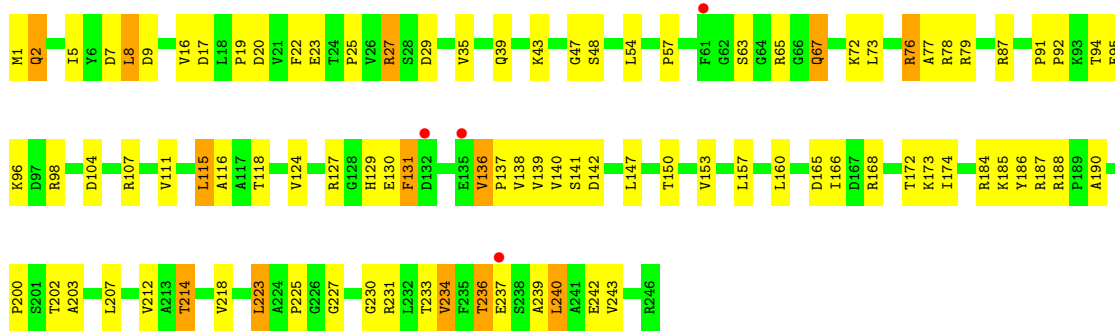


• Molecule 5: 50S ribosomal protein L3P

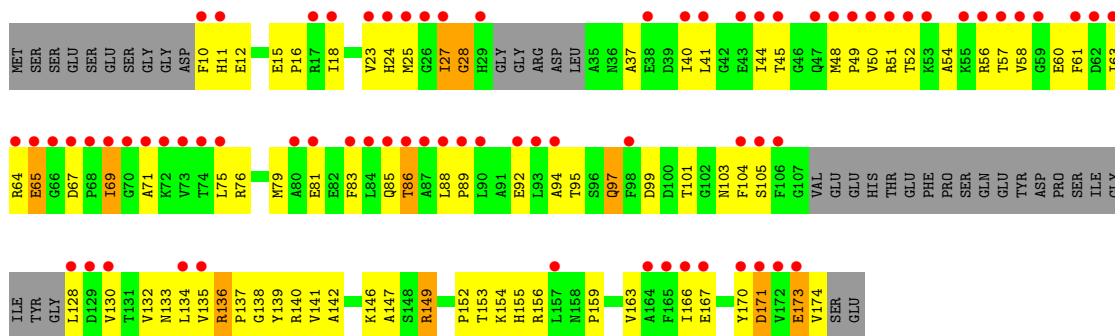




• Molecule 6: 50S ribosomal protein L4E

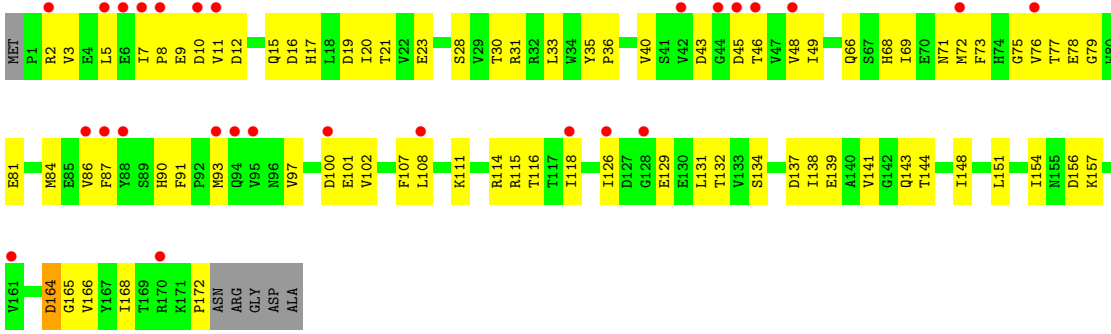


• Molecule 7: 50S ribosomal protein L5P

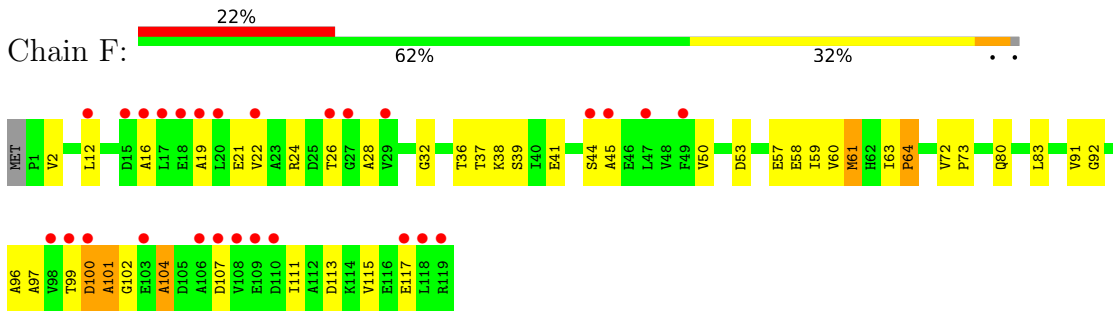


• Molecule 8: 50S ribosomal protein L6P

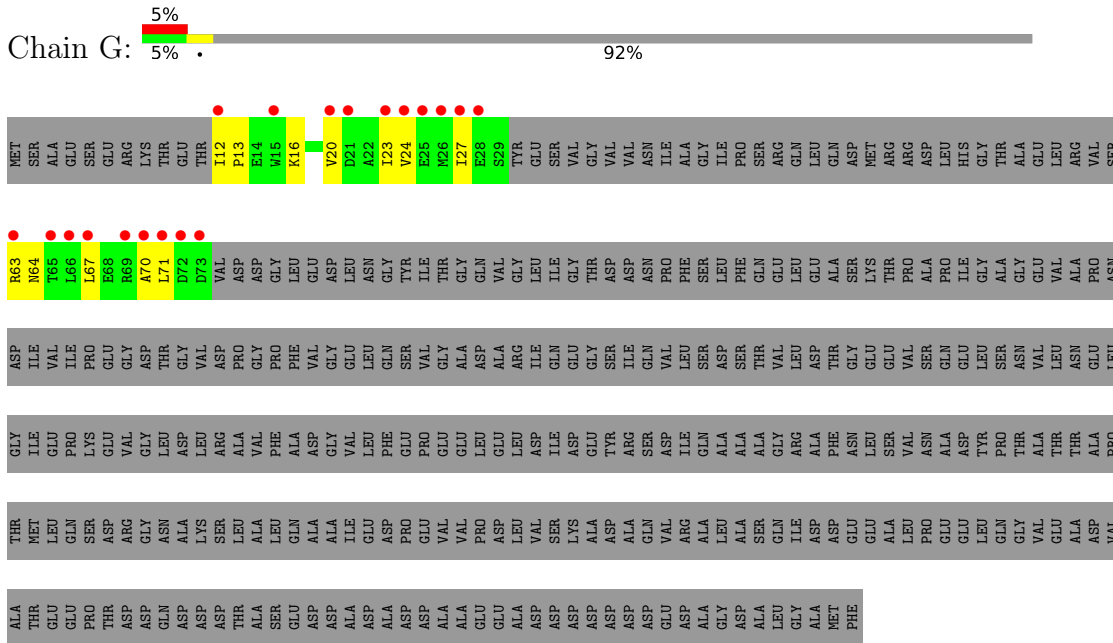




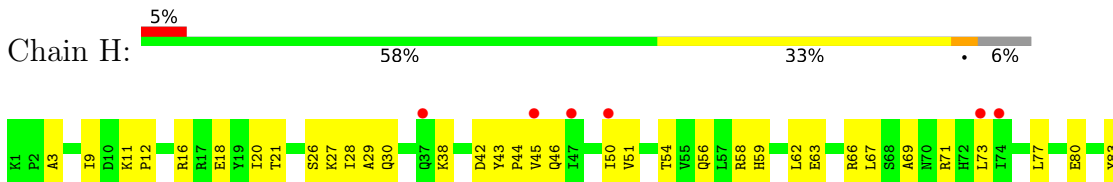
- Molecule 9: 50S ribosomal protein L7AE



- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



- Molecule 11: 50S RIBOSOMAL PROTEIN L10E





- Molecule 12: 50S ribosomal protein L13P

Chain J: 61% 30% 6%



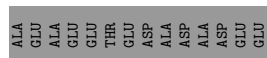
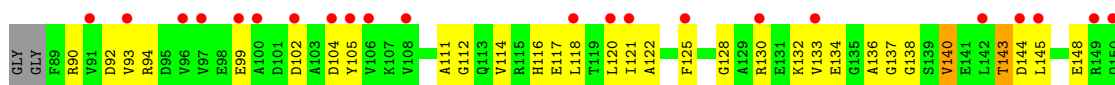
- Molecule 13: 50S ribosomal protein L14P

Chain K: 61% 36% 2%



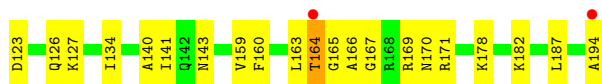
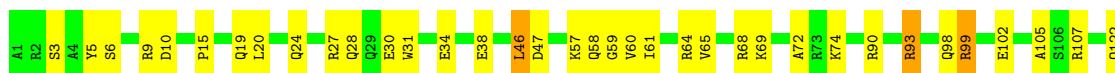
- Molecule 14: 50S ribosomal protein L15P

Chain L: 51% 34% 12%

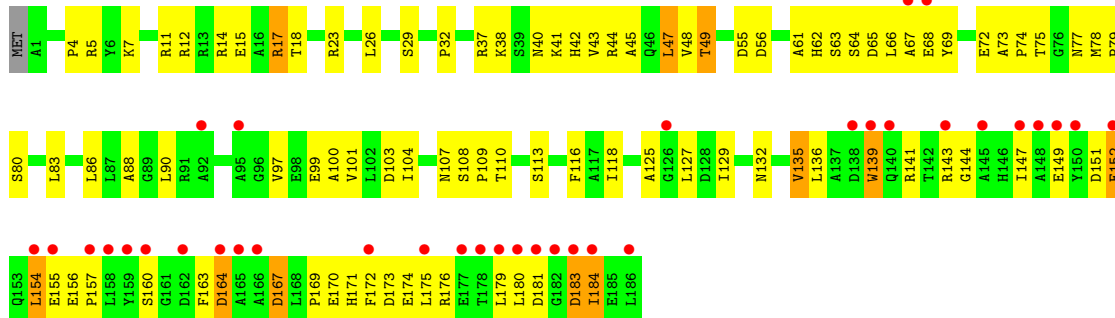


- Molecule 15: 50S Ribosomal Protein L15E

Chain M: 71% 27% 1%



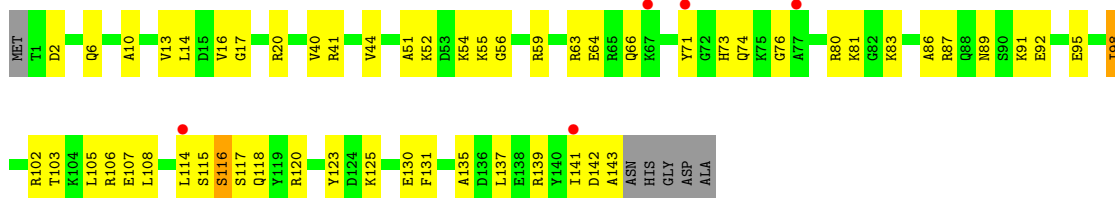
- Molecule 16: 50S ribosomal protein L18P



- Molecule 17: 50S ribosomal protein L18e



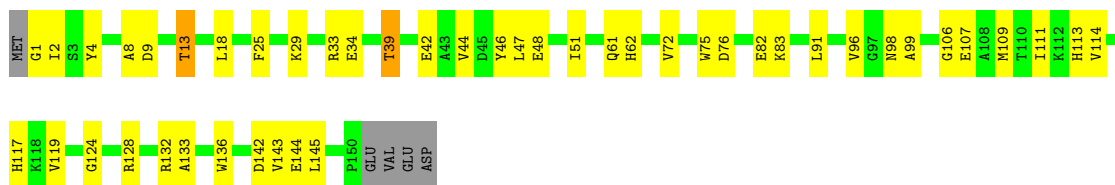
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



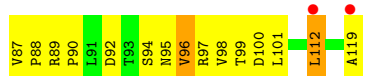
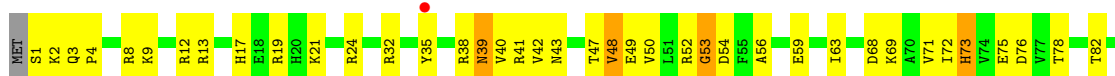
- Molecule 20: 50S ribosomal protein L22P



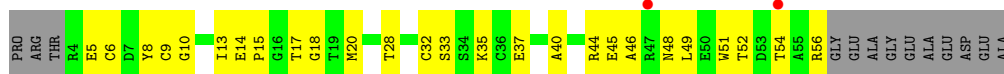
- Molecule 21: 50S ribosomal protein L23P



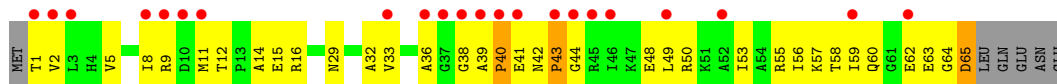
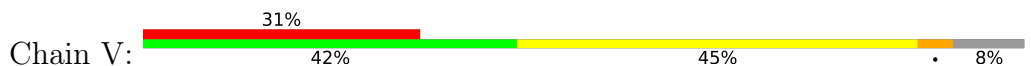
- Molecule 22: 50S ribosomal protein L24P



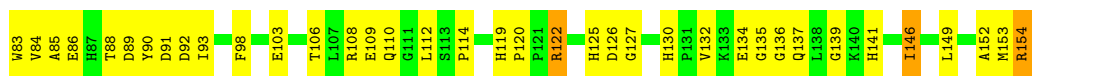
- Molecule 23: 50S ribosomal protein L24E



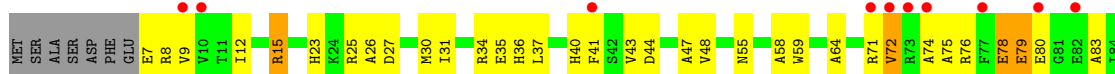
- Molecule 24: 50S ribosomal protein L29P



- Molecule 25: 50S ribosomal protein L30P

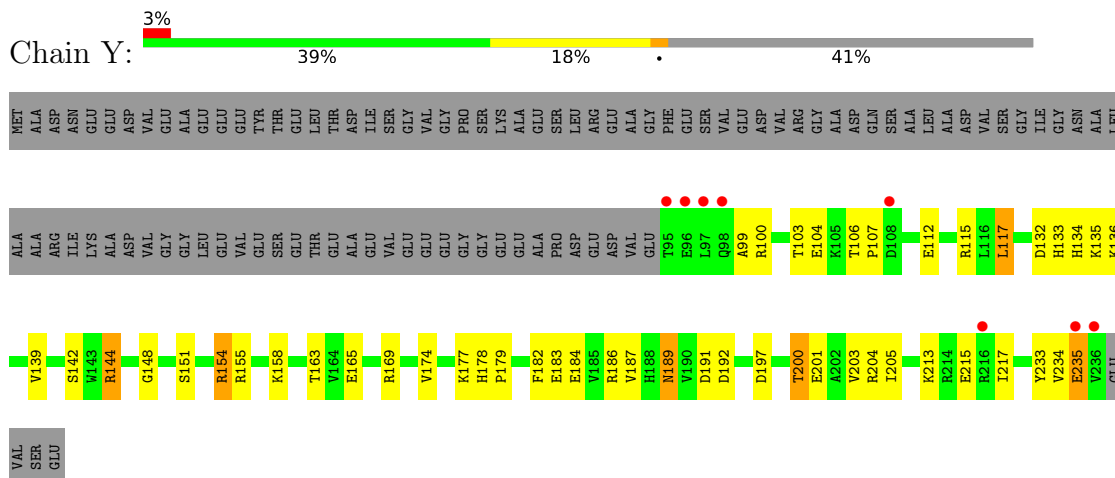


- Molecule 26: 50S ribosomal protein L31e

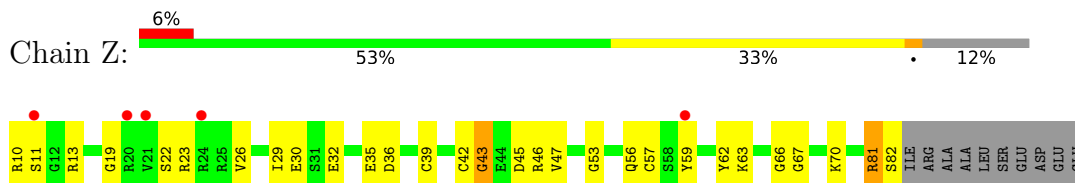




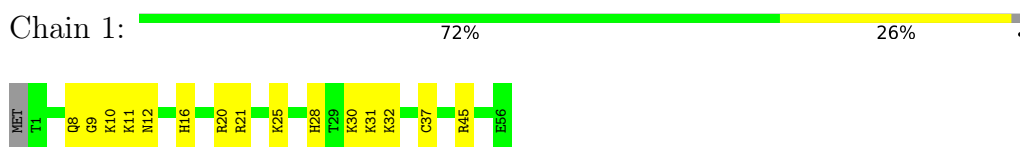
- Molecule 27: 50S ribosomal protein L32E



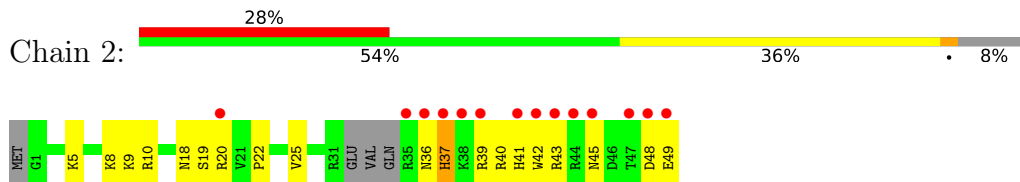
- Molecule 28: 50S ribosomal protein L37Ae



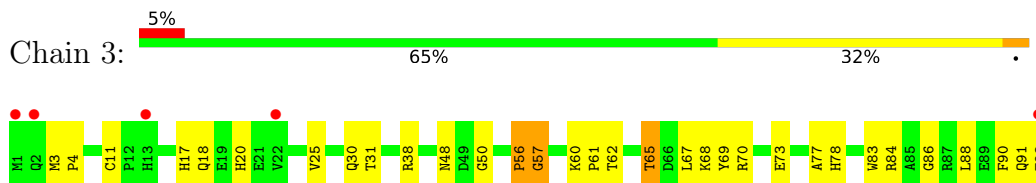
- Molecule 29: 50S ribosomal protein L37e



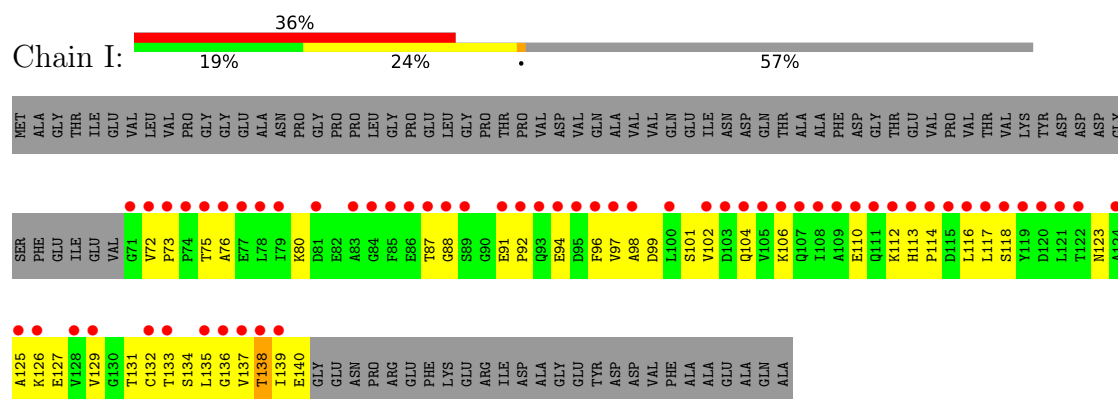
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (49.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.244 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5AA, OMG, OMU, UR3, PSU, NA, CD, 1MA, 2OP, CL, PAE, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.37	0/65959	0.69	23/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.43	0/102	0.65	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.38	0/1884	0.66	0/2551
7	D	0.30	0/1111	0.54	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.45	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.65	0/1509
15	M	0.35	0/1584	0.62	0/2119
16	N	0.29	0/1474	0.63	0/1999
17	O	0.34	0/874	0.60	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.67	0/1005
20	R	0.36	0/1172	0.63	0/1578
21	S	0.33	0/648	0.60	0/875
22	T	0.31	0/958	0.63	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.63	0/1655
26	X	0.33	0/664	0.58	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.36	0/589	0.65	0/787
29	1	0.41	0/438	0.66	0/578
30	2	0.32	0/401	0.52	0/529
31	3	0.39	0/771	0.61	0/1024
32	I	0.31	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	24/147726 (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	0	1	54
2	9	0	3
All	All	1	57

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.68	130.79	109.50
1	0	1942	A	C5'-C4'-C3'	8.39	129.43	116.00
1	0	1979	G	C2'-C3'-O3'	7.72	126.49	109.50
1	0	871	G	C5'-C4'-O4'	-7.18	100.48	109.10
2	9	3039	U	N1-C1'-C2'	7.03	123.14	114.00
1	0	1504	A	N9-C1'-C2'	6.38	122.30	114.00
1	0	1819	G	C5'-C4'-C3'	6.19	125.91	116.00
1	0	1120	U	C5'-C4'-C3'	-6.15	106.17	116.00
1	0	2316	G	C5'-C4'-C3'	-6.09	106.25	116.00
1	0	2313	C	C5'-C4'-O4'	6.06	116.38	109.10
1	0	1504	A	C1'-O4'-C4'	-5.96	105.13	109.90
1	0	2012	U	N1-C1'-C2'	5.87	121.62	114.00
1	0	2467	A	C1'-O4'-C4'	-5.70	105.34	109.90
1	0	129	A	C2'-C3'-O3'	5.63	122.71	113.70
1	0	921	G	N9-C1'-C2'	5.51	121.17	114.00
1	0	206	G	C5'-C4'-C3'	-5.51	107.19	116.00
1	0	1592	G	N9-C1'-C2'	5.51	121.16	114.00
1	0	1942	A	C4'-C3'-C2'	-5.43	97.17	102.60
1	0	1878	G	O4'-C1'-N9	5.32	112.46	108.20
1	0	1942	A	C5'-C4'-O4'	5.24	115.38	109.10
1	0	535	G	N9-C1'-C2'	5.14	120.68	114.00
1	0	777	U	O4'-C1'-N1	5.06	112.25	108.20
1	0	841	A	C1'-O4'-C4'	-5.05	105.86	109.90
1	0	1942	A	C1'-O4'-C4'	-5.02	105.88	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1323	G	Sidechain
1	0	1342	C	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1978	A	Sidechain
1	0	1993	C	Sidechain
1	0	2076	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	246	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	449	A	Sidechain
1	0	458	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	791	A	Sidechain
1	0	795	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	882	A	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
2	9	3087	U	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	0	59021	0	29813	813	0
2	9	2600	0	1326	57	0
3	4	130	0	77	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	167	0
6	C	1859	0	1816	100	0
7	D	1094	0	1085	85	0
8	E	1357	0	1266	84	0
9	F	890	0	843	43	0
10	G	240	0	231	14	0
11	H	1266	0	1268	64	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	1560	0	1568	58	0
16	N	1445	0	1401	104	0
17	O	865	0	873	32	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	21	0
20	R	1149	0	1122	60	0
21	S	641	0	605	21	0
22	T	950	0	923	56	0
23	U	410	0	364	29	0
24	V	499	0	511	35	0
25	W	1196	0	1137	95	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	25	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	27	0
32	I	519	0	500	47	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0
38	G	18	0	0	2	0
38	H	65	0	0	4	0
38	I	9	0	0	2	0
38	J	51	0	0	4	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	3	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2271	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 15.

All (2271) 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)
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
1:0:156:C:H5''	15:M:171:ARG:HD3	1.29	1.14
5:B:62:ARG:HA	5:B:65:MET:HE3	1.29	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.20	1.11
1:0:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09
6:C:236:THR:HG22	6:C:239:ALA:H	1.16	1.08
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.30	1.08
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.34	1.07
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.72	1.04
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.21	1.04
1:0:1751:G:H2'	1:0:1752:G:H5''	1.40	1.01
2:9:3076:G:H3'	2:9:3077:A:H5''	1.38	1.01
20:R:39:THR:HG22	20:R:42:GLU:H	1.26	1.00
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.76	1.00
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.40	1.00
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.40	1.00
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.77	0.99
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.42	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.46	0.98
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.45	0.97
13:K:10:GLN:NE2	13:K:10:GLN:H	1.61	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	1.10	0.97
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.47	0.96
7:D:154:LYS:H	7:D:154:LYS:HD2	1.29	0.96
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.94
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.50	0.94
13:K:10:GLN:HE21	13:K:10:GLN:N	1.65	0.94
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.49	0.93
1:0:1187:U:HO2'	1:0:1189:A:H2	1.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.93
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.51	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.32	0.92
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.35	0.92
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.52	0.92
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.11	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.92
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.52	0.91
12:J:131:THR:HG22	12:J:134:GLU:H	1.34	0.91
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.11	0.91
1:0:541:C:H2'	1:0:542:A:H5''	1.53	0.91
6:C:1:MET:HG2	6:C:2:GLN:H	1.33	0.91
15:M:164:THR:HG22	15:M:167:GLY:H	1.33	0.91
1:0:2717:C:C2'	1:0:2718:C:H5''	2.01	0.90
1:0:1835:U:H5	1:0:1840:A:N7	1.69	0.90
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.90
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.53	0.90
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.54	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
1:0:542:A:H5'	1:0:542:A:H8	1.37	0.89
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.52	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	1.01	0.89
1:0:1701:A:H4'	1:0:1702:U:H5''	1.55	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.88	0.89
1:0:1372:A:H3'	38:0:7406:HOH:O	1.72	0.89
1:0:21:G:H5'	20:R:2:ILE:HA	1.55	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.88
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.74	0.87
16:N:144:GLY:O	16:N:147:ILE:HG22	1.74	0.87
5:B:248:ARG:O	5:B:251:VAL:HG12	1.73	0.87
1:0:1160:G:C5'	1:0:1161:A:H5'	2.05	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.75	0.86
26:X:30:MET:HE1	26:X:55:ASN:HA	1.57	0.86
1:0:870:G:H2'	1:0:871:G:H5''	1.55	0.86
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.24	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.24	0.85
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.34	0.85
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.58	0.85
1:0:1159:G:H21	1:0:1189:A:H8	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.58	0.84
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.59	0.84
1:0:21:G:C5'	20:R:2:ILE:HA	2.07	0.84
5:B:321:PRO:HA	38:B:9463:HOH:O	1.78	0.83
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.60	0.83
1:0:2291:A:C8	1:0:2309:C:H5'	2.13	0.83
5:B:98:THR:HG22	5:B:99:GLU:H	1.44	0.83
1:0:2586:U:H3	1:0:2592:G:H22	1.26	0.83
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.79	0.83
2:9:3051:A:H5'	16:N:160:SER:HB3	1.61	0.83
1:0:1160:G:H5'	1:0:1161:A:C5'	2.08	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.61	0.82
32:I:138:THR:HG22	32:I:139:ILE:H	1.43	0.82
13:K:10:GLN:H	13:K:10:GLN:HE21	0.84	0.82
23:U:52:THR:HG22	23:U:54:THR:H	1.43	0.82
1:0:871:G:H5'	1:0:871:G:H8	1.44	0.82
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.59	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.82	0.82
6:C:139:VAL:HG13	38:C:9246:HOH:O	1.80	0.81
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.43	0.81
1:0:2105:C:H5'	38:4:7924:HOH:O	1.79	0.81
21:S:57:THR:HG22	21:S:59:ASP:H	1.44	0.81
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.44	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.81
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.63	0.81
1:0:2908:A:H2'	1:0:2909:G:O4'	1.80	0.81
11:H:166:SER:HB2	11:H:167:PRO:CD	2.09	0.81
5:B:51:VAL:HG23	5:B:329:TYR:O	1.81	0.81
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.61	0.81
5:B:179:LEU:O	5:B:183:GLU:HG2	1.81	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.82	0.80
7:D:25:MET:HE2	7:D:41:LEU:HG	1.63	0.80
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.12	0.80
25:W:88:THR:HG22	25:W:89:ASP:H	1.44	0.80
1:0:282:C:H1'	1:0:368:C:N4	1.97	0.79
1:0:1593:C:H5'	18:P:116:SER:O	1.82	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.62	0.79
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.65	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.64	0.79
1:0:559:U:H6	1:0:559:U:H5'	1.47	0.79
1:0:289:G:H22	1:0:363:A:H2	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1559:A:H1'	38:0:6127:HOH:O	1.81	0.79
6:C:236:THR:H	6:C:239:ALA:HB3	1.47	0.78
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.82	0.78
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.81	0.78
1:0:1751:G:C2'	1:0:1752:G:H5''	2.13	0.78
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.65	0.78
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.47	0.78
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.49	0.78
1:0:2840:A:OP1	5:B:211:THR:HG23	1.84	0.78
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.14	0.78
4:A:131:HIS:O	4:A:132:ASP:HB2	1.83	0.78
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.48	0.78
2:9:3039:U:H1'	2:9:3044:A:H61	1.48	0.78
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.82	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.77
25:W:65:VAL:HA	25:W:68:THR:HG22	1.66	0.77
1:0:1603:A:H5'	1:0:1605:G:O4'	1.84	0.77
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.66	0.77
1:0:541:C:C2'	1:0:542:A:H5''	2.12	0.77
1:0:2533:C:H5'	1:0:2533:C:H6	1.49	0.77
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.85	0.77
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.66	0.77
11:H:27:LYS:H	11:H:59:HIS:HD2	1.30	0.77
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.14	0.77
27:Y:117:LEU:HD12	27:Y:174:VAL:CG1	2.14	0.77
1:0:159:G:OP1	15:M:74:LYS:HE3	1.84	0.77
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.66	0.77
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.50	0.77
1:0:1209:C:H2'	1:0:1210:G:H8	1.49	0.77
1:0:2608:C:H2'	38:0:8228:HOH:O	1.85	0.77
12:J:107:ASN:ND2	12:J:109:TYR:H	1.83	0.77
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.66	0.76
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.50	0.76
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.67	0.76
24:V:1:THR:HG23	24:V:2:VAL:H	1.49	0.76
7:D:57:THR:HG23	7:D:63:ILE:HA	1.68	0.76
25:W:52:VAL:HG22	25:W:53:ALA:H	1.49	0.76
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.66	0.76
38:0:4965:HOH:O	5:B:300:SER:HB3	1.86	0.76
1:0:111:C:O2'	29:1:20:ARG:HG2	1.85	0.76
11:H:166:SER:CB	11:H:167:PRO:HD3	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:O2'	1:0:1118:A:H2	1.68	0.76
5:B:98:THR:HG22	5:B:99:GLU:N	2.00	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	1.27	0.76
26:X:78:GLU:HG2	26:X:79:GLU:H	1.49	0.76
16:N:113:SER:HB2	38:N:9357:HOH:O	1.85	0.75
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75
1:0:871:G:H8	1:0:871:G:C5'	1.98	0.75
1:0:244:C:OP2	9:F:38:LYS:HE3	1.85	0.75
1:0:2679:G:H2'	1:0:2681:A:OP2	1.86	0.75
2:9:3014:G:H5'	2:9:3014:G:H8	1.51	0.75
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.86	0.75
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.68	0.75
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.68	0.75
1:0:281:U:H2'	1:0:282:C:O4'	1.87	0.75
1:0:447:A:OP2	22:T:1:SER:HB2	1.85	0.75
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.68	0.75
1:0:2094:G:H4'	5:B:245:SER:HB3	1.67	0.74
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.69	0.74
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.69	0.74
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.67	0.74
18:P:115:SER:OG	18:P:118:GLN:HG3	1.87	0.74
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.74
32:I:101:SER:H	32:I:104:GLN:NE2	1.85	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.03	0.74
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.69	0.74
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.70	0.74
24:V:12:THR:HG22	24:V:15:GLU:CG	2.15	0.74
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.53	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.36	0.74
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.68	0.74
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.17	0.74
1:0:793:A:H5''	18:P:83:LYS:HG2	1.70	0.74
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.70	0.74
1:0:545:G:H5'	1:0:545:G:H8	1.52	0.73
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.18	0.73
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
5:B:62:ARG:CA	5:B:65:MET:HE3	2.15	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.73
1:0:2426:G:H1'	38:0:6343:HOH:O	1.87	0.73
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.73
4:A:191:GLY:HA2	4:A:194:MET:CE	2.19	0.73
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.89	0.73
1:0:2256:G:H2'	1:0:2257:G:H5'	1.71	0.72
1:0:381:G:H5''	38:0:4621:HOH:O	1.89	0.72
7:D:99:ASP:HB3	7:D:103:ASN:H	1.54	0.72
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.70	0.72
1:0:182:G:H5'	38:0:5437:HOH:O	1.88	0.72
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.90	0.72
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.89	0.72
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.89	0.72
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.70	0.72
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.71	0.72
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.72	0.72
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.93	0.72
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.20	0.71
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.05	0.71
14:L:133:VAL:HA	38:L:9370:HOH:O	1.89	0.71
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.72	0.71
1:0:2827:A:H2'	1:0:2828:G:O4'	1.89	0.71
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.71
8:E:69:ILE:HA	8:E:72:MET:CE	2.20	0.71
1:0:820:G:H5''	38:0:3359:HOH:O	1.90	0.71
9:F:91:VAL:HG12	9:F:92:GLY:H	1.55	0.71
1:0:2054:A:N3	20:R:128:ARG:NH2	2.38	0.70
5:B:307:ARG:HH11	5:B:307:ARG:HB2	1.56	0.70
1:0:21:G:H5''	20:R:1:GLY:O	1.91	0.70
1:0:450:C:OP1	6:C:184:ARG:NH2	2.24	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.90	0.70
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.73	0.70
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.09	0.70
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.89	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
5:B:145:HIS:HD2	5:B:146:THR:O	1.72	0.70
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.03	0.70
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.73	0.70
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.74	0.70
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2468:A:H61	31:3:48:ASN:HD21	1.37	0.70
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.22	0.70
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.74	0.70
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.74	0.70
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.07	0.70
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.56	0.69
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.72	0.69
1:0:1667:A:H5'	1:0:1667:A:C8	2.24	0.69
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.72	0.69
20:R:44:VAL:O	20:R:48:GLU:HG3	1.92	0.69
25:W:38:THR:HG22	25:W:39:ASP:H	1.58	0.69
38:0:7097:HOH:O	15:M:178:LYS:HB2	1.91	0.69
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.58	0.69
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.27	0.69
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.40	0.69
4:A:223:ARG:HG3	38:A:9398:HOH:O	1.91	0.69
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.73	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.91	0.69
1:0:338:C:H4'	6:C:174:ILE:CD1	2.23	0.69
20:R:9:ASP:O	20:R:13:THR:HB	1.92	0.69
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.58	0.69
1:0:1184:C:H1'	38:0:7669:HOH:O	1.92	0.69
9:F:38:LYS:NZ	15:M:3:SER:HA	2.08	0.69
21:S:57:THR:HG22	21:S:59:ASP:N	2.07	0.69
27:Y:117:LEU:HD12	27:Y:174:VAL:HG13	1.75	0.69
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.68
1:0:1206:U:H5'	1:0:1206:U:H6	1.58	0.68
1:0:870:G:C2'	1:0:871:G:H5''	2.23	0.68
1:0:1116:U:H3	1:0:1246:A:H62	1.39	0.68
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.74	0.68
9:F:91:VAL:HG12	9:F:92:GLY:N	2.08	0.68
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.08	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.38	0.68
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.76	0.68
30:2:41:HIS:N	30:2:45:ASN:HD22	1.88	0.68
1:0:1666:C:O2'	1:0:1667:A:H5''	1.93	0.68
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.24	0.68
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.19	0.68
1:0:2502:C:H2'	1:0:2503:A:H5'	1.75	0.68
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.59	0.68
1:0:1236:A:C8	12:J:63:ILE:HD11	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.76	0.67
1:0:1474:C:H5'	1:0:1474:C:C6	2.22	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.28	0.67
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.74	0.67
4:A:121:ALA:O	4:A:124:VAL:HG22	1.93	0.67
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.77	0.67
18:P:103:THR:HA	18:P:106:ARG:NH1	2.09	0.67
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.67
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.77	0.67
17:O:32:ARG:O	17:O:32:ARG:HD3	1.94	0.67
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.24	0.67
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.95	0.67
1:0:317:A:H5''	22:T:52:ARG:HD2	1.76	0.67
4:A:179:MET:HA	4:A:179:MET:CE	2.25	0.67
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.09	0.67
1:0:558:C:C2'	1:0:559:U:H5''	2.25	0.67
1:0:2768:A:H2'	1:0:2769:C:O4'	1.94	0.67
20:R:39:THR:HG22	20:R:42:GLU:N	2.05	0.67
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.59	0.67
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.77	0.66
1:0:542:A:H5'	1:0:542:A:C8	2.26	0.66
1:0:1634:G:H3'	38:0:4200:HOH:O	1.94	0.66
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.60	0.66
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.28	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	2.00	0.66
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.66
16:N:169:PRO:O	16:N:172:PHE:HB3	1.96	0.66
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.56	0.66
1:0:560:C:H42	1:0:597:A:H61	1.42	0.66
1:0:1118:A:H8	1:0:1118:A:H3'	1.61	0.66
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.77	0.66
1:0:1377:C:H5'	1:0:1377:C:H6	1.61	0.66
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.78	0.66
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.66
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.11	0.66
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.77	0.66
1:0:506:G:H22	1:0:509:A:H5''	1.61	0.66
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.96	0.66
19:Q:26:PRO:O	19:Q:30:VAL:HG23	1.95	0.66
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.10	0.65
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:H1'	1:0:1209:C:O4'	1.96	0.65
6:C:7:ASP:OD2	6:C:9:ASP:HB2	1.96	0.65
12:J:52:GLN:HG3	12:J:53:ILE:N	2.10	0.65
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.65
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.79	0.65
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.26	0.65
1:0:2502:C:C2'	1:0:2503:A:H5'	2.27	0.65
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.61	0.65
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.78	0.65
1:0:2769:C:C2'	1:0:2770:G:H5'	2.27	0.65
5:B:297:VAL:HB	38:B:9412:HOH:O	1.95	0.65
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.61	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
25:W:149:LEU:HG	25:W:153:MET:HE2	1.79	0.65
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.96	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.65
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.65
7:D:23:VAL:HG12	7:D:130:VAL:HG22	1.79	0.65
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.78	0.65
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.65
1:0:95:A:H5''	1:0:97:G:O4'	1.96	0.65
2:9:3092:G:H2'	2:9:3093:A:C8	2.31	0.65
22:T:47:THR:HB	22:T:100:ASP:HB3	1.79	0.65
2:9:3013:A:O2'	2:9:3014:G:H5''	1.96	0.65
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.77	0.65
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.00	0.65
1:0:1118:A:H3'	1:0:1118:A:C8	2.32	0.64
1:0:2578:G:H5'	1:0:2578:G:H8	1.62	0.64
15:M:9:ARG:HB2	15:M:47:ASP:OD2	1.96	0.64
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.79	0.64
24:V:38:GLY:C	24:V:40:PRO:HD2	2.17	0.64
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.96	0.64
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.78	0.64
1:0:657:G:OP1	6:C:27:ARG:NH2	2.29	0.64
17:O:21:SER:OG	17:O:106:PRO:HB2	1.97	0.64
1:0:603:A:H5''	1:0:604:G:OP1	1.96	0.64
1:0:2878:U:H2'	1:0:2879:A:O4'	1.96	0.64
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.79	0.64
6:C:242:GLU:HG3	38:C:9177:HOH:O	1.96	0.64
12:J:39:VAL:HG13	12:J:106:GLY:O	1.97	0.64
1:0:1116:U:O2'	1:0:1118:A:C2	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3039:U:H1'	2:9:3044:A:N6	2.12	0.64
6:C:218:VAL:HG12	38:C:9222:HOH:O	1.96	0.64
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.37	0.64
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.79	0.64
18:P:64:GLU:HG2	38:P:168:HOH:O	1.97	0.64
1:0:447:A:P	22:T:1:SER:HB2	2.38	0.64
10:G:12:ILE:N	10:G:13:PRO:HD3	2.13	0.64
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.12	0.64
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.10	0.64
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.78	0.64
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.78	0.64
32:I:76:ALA:O	32:I:80:LYS:HG3	1.98	0.64
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.63	0.64
24:V:12:THR:HG23	24:V:14:ALA:H	1.62	0.64
1:0:1299:G:O6	14:L:6:ARG:HD3	1.97	0.63
3:4:176:A:O4'	3:4:175:C:H2'	1.99	0.63
5:B:36:PRO:HA	5:B:168:GLY:CA	2.25	0.63
1:0:31:C:H4'	38:0:7630:HOH:O	1.98	0.63
8:E:69:ILE:HA	8:E:72:MET:HE2	1.81	0.63
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.78	0.63
23:U:52:THR:HG22	23:U:54:THR:N	2.11	0.63
4:A:36:ASP:O	4:A:38:ILE:N	2.32	0.63
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.79	0.63
7:D:25:MET:CE	7:D:37:ALA:HB1	2.29	0.63
8:E:144:THR:O	8:E:148:ILE:HG13	1.98	0.63
9:F:96:ALA:HA	38:F:3111:HOH:O	1.98	0.63
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.19	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.98	0.63
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.78	0.63
1:0:2524:G:H21	1:0:2526:C:N4	1.97	0.63
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.28	0.63
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.28	0.63
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.81	0.63
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.63
38:0:4293:HOH:O	22:T:82:THR:HA	1.99	0.63
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	1.99	0.63
30:2:20:ARG:HB3	38:2:5444:HOH:O	1.97	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63
5:B:138:GLY:O	5:B:139:ASP:O	2.17	0.63
20:R:39:THR:HG23	20:R:107:GLU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.63
2:9:3029:C:C2'	2:9:3030:C:H5'	2.29	0.63
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.79	0.63
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.29	0.63
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.47	0.63
1:0:1641:A:H2'	1:0:1642:A:H5'	1.80	0.62
12:J:107:ASN:HD22	12:J:108:PRO:N	1.97	0.62
26:X:25:ARG:HD3	26:X:64:ALA:O	1.99	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.30	0.62
8:E:15:GLN:HG2	8:E:19:ASP:O	1.99	0.62
10:G:64:ASN:HD22	10:G:64:ASN:N	1.95	0.62
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.00	0.62
2:9:3014:G:H5'	2:9:3014:G:C8	2.33	0.62
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.80	0.62
11:H:170:ASN:HD22	11:H:170:ASN:N	1.96	0.62
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.81	0.62
1:0:88:G:H8	1:0:88:G:H5'	1.65	0.62
7:D:136:ARG:HD2	7:D:155:HIS:O	1.99	0.62
9:F:19:ALA:O	9:F:22:VAL:HG22	1.98	0.62
16:N:32:PRO:HD2	16:N:99:GLU:O	1.99	0.62
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.29	0.62
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.81	0.62
1:0:544:G:H2'	1:0:545:G:H5''	1.82	0.62
1:0:1053:G:OP1	11:H:12:PRO:HG3	1.99	0.62
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.99	0.62
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.12	0.62
1:0:2534:C:H1'	38:O:3802:HOH:O	1.99	0.62
1:0:2824:C:H5''	1:0:2825:C:H5'	1.81	0.62
7:D:50:VAL:O	7:D:71:ALA:HA	2.00	0.62
10:G:16:LYS:O	10:G:20:VAL:HG23	1.99	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.99	0.62
1:0:2896:A:H5''	38:O:6350:HOH:O	2.00	0.62
38:O:7630:HOH:O	22:T:9:LYS:HB2	1.99	0.62
1:0:138:U:H5''	1:0:139:C:OP2	2.00	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.62
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.30	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.15	0.62
1:0:447:A:O2'	1:0:448:G:H5'	2.00	0.61
1:0:558:C:O2'	1:0:559:U:H5''	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:C5'	2.29	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.65	0.61
1:0:2717:C:H2'	1:0:2718:C:C5'	2.27	0.61
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.81	0.61
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.98	0.61
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.61
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.61
1:0:1120:U:H5''	1:0:1120:U:C6	2.35	0.61
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.30	0.61
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.15	0.61
27:Y:144:ARG:CZ	38:Y:8201:HOH:O	2.48	0.61
32:I:138:THR:HG22	32:I:139:ILE:N	2.15	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
6:C:1:MET:HG2	6:C:2:GLN:N	2.10	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.30	0.61
7:D:163:VAL:HA	38:D:6326:HOH:O	2.01	0.61
32:I:99:ASP:OD1	32:I:138:THR:HB	2.00	0.61
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.98	0.61
7:D:23:VAL:HG23	7:D:23:VAL:O	2.01	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.97	0.61
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.66	0.61
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.99	0.61
1:0:2248:C:H3'	38:0:5712:HOH:O	2.01	0.61
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.01	0.61
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.82	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.61
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.83	0.61
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.00	0.61
1:0:316:A:H5'	22:T:54:ASP:OD2	2.01	0.61
1:0:1943:C:H4'	4:A:211:LYS:O	2.01	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.31	0.61
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.82	0.61
8:E:9:GLU:HG3	8:E:10:ASP:N	2.16	0.61
8:E:93:MET:HE1	8:E:165:GLY:N	2.15	0.61
11:H:63:GLU:HA	38:H:9178:HOH:O	2.00	0.61
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.15	0.61
1:0:1741:U:O2'	1:0:2723:G:H4'	2.01	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.61
8:E:7:ILE:HG22	8:E:45:ASP:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:9:ILE:O	11:H:9:ILE:HG22	2.01	0.61
4:A:192:VAL:HG13	38:A:9356:HOH:O	2.00	0.61
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.31	0.61
12:J:133:GLY:O	12:J:137:GLU:HG3	2.01	0.61
19:Q:53:HIS:CE1	19:Q:55:ARG:HG3	2.35	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.32	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.82	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.30	0.60
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.34	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.83	0.60
16:N:110:THR:HB	16:N:113:SER:OG	2.02	0.60
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.60
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.83	0.60
1:O:2716:G:H5''	5:B:206:THR:HG21	1.84	0.60
38:O:3594:HOH:O	13:K:9:THR:HA	2.01	0.60
16:N:37:ARG:NE	38:N:9331:HOH:O	2.34	0.60
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.33	0.60
1:O:2346:C:H6	1:O:2346:C:O5'	1.85	0.60
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.16	0.60
1:O:121:U:OP2	30:2:10:ARG:NH2	2.28	0.60
7:D:153:THR:O	7:D:156:ARG:HB2	2.01	0.60
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.01	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
29:1:10:LYS:HG3	38:1:2979:HOH:O	2.01	0.60
1:O:475:G:H5'	6:C:73:LEU:HD23	1.84	0.60
1:O:1667:A:H2'	1:O:1668:U:C6	2.37	0.60
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.84	0.60
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.84	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.02	0.60
14:L:143:THR:HG22	14:L:144:ASP:N	2.17	0.60
1:O:541:C:H2'	1:O:542:A:C5'	2.28	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
1:O:1878:G:H1'	38:O:6371:HOH:O	2.02	0.60
8:E:23:GLU:HG2	8:E:28:SER:CB	2.31	0.60
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.31	0.60
23:U:52:THR:CG2	23:U:54:THR:HB	2.32	0.60
25:W:88:THR:HG22	25:W:89:ASP:N	2.16	0.60
1:O:474:C:O3'	6:C:73:LEU:HD21	2.01	0.60
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.84	0.60
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.84	0.60
16:N:151:ASP:O	16:N:154:LEU:HB2	2.01	0.60
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.37	0.59
13:K:115:ARG:HB3	13:K:132:VAL:OXT	2.02	0.59
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.59
21:S:56:ASN:O	30:2:8:LYS:NZ	2.34	0.59
1:0:1080:C:H4'	1:0:1081:A:OP1	2.01	0.59
1:0:1119:G:OP2	12:J:49:ARG:HD3	2.02	0.59
1:0:2241:C:O2'	1:0:2242:U:H5'	2.01	0.59
7:D:154:LYS:H	7:D:154:LYS:CD	2.06	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.82	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
1:0:20:G:H21	20:R:117:HIS:HD2	1.49	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.84	0.59
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.85	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.31	0.59
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.03	0.59
6:C:115:LEU:O	6:C:118:THR:HB	2.03	0.59
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.01	0.59
5:B:140:LEU:HD23	38:B:9384:HOH:O	2.02	0.59
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.85	0.59
18:P:103:THR:O	18:P:107:GLU:HG3	2.02	0.59
1:0:247:A:H2'	38:0:4229:HOH:O	2.03	0.59
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.68	0.59
38:0:7658:HOH:O	5:B:211:THR:HG21	2.01	0.59
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.83	0.59
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.35	0.59
13:K:55:VAL:HG12	13:K:56:SER:N	2.18	0.59
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.84	0.59
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.33	0.59
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.32	0.59
1:0:1462:C:H2'	1:0:1463:A:C8	2.38	0.59
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.84	0.59
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.38	0.59
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.02	0.59
12:J:130:VAL:HG12	12:J:131:THR:N	2.17	0.59
16:N:154:LEU:HD12	16:N:156:GLU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.67	0.59
1:0:775:G:OP1	29:1:16:HIS:HE1	1.85	0.59
1:0:1666:C:C2'	1:0:1667:A:H5''	2.33	0.59
1:0:1834:C:H2'	1:0:1840:A:N6	2.17	0.59
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.59
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.02	0.59
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.59
6:C:16:VAL:HG12	6:C:17:ASP:H	1.66	0.59
1:0:289:G:N2	1:0:363:A:H2	1.99	0.59
5:B:177:HIS:O	5:B:181:ILE:HG13	2.02	0.59
5:B:238:ASN:HD22	5:B:240:GLY:N	1.94	0.59
12:J:99:GLU:HA	38:J:9370:HOH:O	2.02	0.59
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
38:0:5498:HOH:O	13:K:39:GLY:HA2	2.02	0.58
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.84	0.58
9:F:58:GLU:HA	9:F:61:MET:HE2	1.85	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
1:0:1189:A:H1'	1:0:1209:C:C1'	2.34	0.58
8:E:69:ILE:HA	8:E:72:MET:HE3	1.84	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
1:0:1118:A:H8	1:0:1119:G:H5''	1.68	0.58
1:0:1527:A:H1'	1:0:1528:A:C8	2.39	0.58
1:0:2541:U:H5'	38:0:9722:HOH:O	2.04	0.58
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.18	0.58
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.19	0.58
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.58
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.58
1:0:2601:A:N1	13:K:38:SER:HB2	2.19	0.58
1:0:2710:U:H1'	38:0:7817:HOH:O	2.03	0.58
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.04	0.58
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.03	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.85	0.58
1:0:553:G:P	27:Y:204:ARG:HH22	2.26	0.58
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.84	0.58
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.03	0.58
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.39	0.58
29:1:25:LYS:HG3	30:2:49:GLU:H	1.69	0.58
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.06	0.58
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.58
5:B:81:ALA:O	5:B:186:GLY:HA3	2.04	0.58
5:B:98:THR:CG2	5:B:99:GLU:H	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:105:ASN:HD21	17:O:109:SER:H	1.48	0.58
25:W:108:ARG:HE	25:W:114:PRO:CG	2.15	0.58
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
1:O:1741:U:H5'	1:O:1742:A:OP1	2.04	0.58
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.17	0.58
1:O:1182:C:H1'	1:O:1192:A:H8	1.68	0.58
16:N:47:LEU:HD12	16:N:97:VAL:HG11	1.86	0.58
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.03	0.58
1:O:1086:A:C6	25:W:11:VAL:HG11	2.38	0.58
1:O:1120:U:H5''	1:O:1120:U:H6	1.69	0.57
1:O:2488:A:H2	38:O:7489:HOH:O	1.87	0.57
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.68	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.86	0.57
1:O:2361:A:H5'	1:O:2361:A:H8	1.69	0.57
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.04	0.57
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.04	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.30	0.57
1:O:1189:A:H3'	38:O:7875:HOH:O	2.03	0.57
4:A:36:ASP:C	4:A:38:ILE:H	2.06	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.85	0.57
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.34	0.57
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.69	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.05	0.57
3:4:77:2OP:HA	3:4:177:PAE:O2	2.04	0.57
6:C:95:GLU:OE1	6:C:95:GLU:N	2.34	0.57
8:E:81:GLU:HG2	8:E:134:SER:CB	2.31	0.57
11:H:97:GLU:HB3	11:H:121:VAL:HG11	1.87	0.57
12:J:8:ALA:HA	12:J:35:THR:HG22	1.84	0.57
16:N:80:SER:HB2	38:N:9333:HOH:O	2.05	0.57
1:O:656:G:OP2	17:O:37:ARG:HD2	2.05	0.57
1:O:1625:U:H4'	38:O:4961:HOH:O	2.03	0.57
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.03	0.57
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.29	0.57
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.57
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.34	0.57
1:O:1441:G:O2'	1:O:1442:A:H5'	2.04	0.57
1:O:2505:G:O2'	1:O:2506:A:H5'	2.04	0.57
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.85	0.57
16:N:155:GLU:O	16:N:156:GLU:HG3	2.04	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.34	0.57
5:B:62:ARG:HA	5:B:65:MET:CE	2.19	0.57
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.87	0.57
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.04	0.57
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.87	0.57
1:O:1500:U:P	18:P:41:ARG:HH22	2.28	0.57
1:O:1596:U:H2'	1:O:1598:A:OP2	2.05	0.57
6:C:16:VAL:HG12	6:C:17:ASP:N	2.20	0.57
6:C:25:PRO:HG2	38:C:9122:HOH:O	2.04	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.38	0.57
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.86	0.57
32:I:92:PRO:O	32:I:94:GLU:HG3	2.05	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.20	0.57
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.70	0.57
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.39	0.57
25:W:13:MET:CE	25:W:17:ILE:HG22	2.34	0.57
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.86	0.57
1:O:503:G:H2'	1:O:504:G:H8	1.69	0.57
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.38	0.57
13:K:74:VAL:HG21	13:K:96:VAL:HG23	1.85	0.57
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.35	0.57
1:O:848:C:H5'	38:O:7487:HOH:O	2.04	0.56
1:O:1010:C:H4'	16:N:4:PRO:HB2	1.86	0.56
23:U:9:CYS:CA	23:U:52:THR:HG23	2.32	0.56
1:O:902:G:N7	14:L:18:HIS:HD2	2.03	0.56
1:O:2649:A:H5'	1:O:2649:A:C8	2.40	0.56
26:X:31:ILE:O	26:X:35:GLU:HG3	2.04	0.56
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.06	0.56
8:E:15:GLN:NE2	8:E:40:VAL:O	2.37	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.53	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
26:X:30:MET:CE	26:X:55:ASN:HA	2.32	0.56
31:3:3:MET:O	31:3:90:PHE:HA	2.05	0.56
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.05	0.56
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.70	0.56
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:27:LYS:N	11:H:59:HIS:HD2	2.01	0.56
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.34	0.56
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.35	0.56
1:0:2420:G:O2'	1:0:2421:G:H5'	2.06	0.56
2:9:3051:A:H5'	16:N:160:SER:CB	2.32	0.56
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.20	0.56
12:J:76:ASP:HA	38:J:9365:HOH:O	2.05	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
1:0:449:A:N7	6:C:43:LYS:HG2	2.21	0.56
16:N:72:GLU:O	16:N:72:GLU:HG2	2.06	0.56
18:P:115:SER:H	18:P:118:GLN:NE2	1.86	0.56
1:0:2301:A:H5''	1:0:2302:A:H5'	1.87	0.56
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.36	0.56
25:W:52:VAL:HG22	25:W:53:ALA:N	2.20	0.56
25:W:59:GLN:HE22	25:W:98:PHE:HB2	1.69	0.56
1:0:1677:U:OP2	30:2:8:LYS:NZ	2.37	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.88	0.56
7:D:86:THR:C	7:D:89:PRO:HD2	2.26	0.56
1:0:2748:G:H2'	38:0:7739:HOH:O	2.05	0.56
5:B:16:ARG:NH1	38:B:9422:HOH:O	2.38	0.56
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.36	0.56
8:E:137:ASP:O	8:E:141:VAL:HG23	2.06	0.56
11:H:170:ASN:N	11:H:170:ASN:ND2	2.53	0.56
22:T:41:ARG:NH1	22:T:42:VAL:O	2.38	0.56
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.68	0.56
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.70	0.56
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.20	0.56
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.69	0.56
1:0:475:G:C5'	6:C:73:LEU:HD23	2.37	0.55
1:0:709:G:O2'	17:O:25:VAL:HG12	2.07	0.55
1:0:1211:G:O2'	1:0:1212:C:H5'	2.05	0.55
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.05	0.55
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.36	0.55
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.35	0.55
1:0:2036:C:O4'	13:K:44:LEU:HG	2.06	0.55
38:0:6997:HOH:O	16:N:4:PRO:HD2	2.06	0.55
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.30	0.55
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.36	0.55
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.52	0.55
15:M:60:VAL:C	15:M:61:ILE:HD12	2.26	0.55
21:S:77:VAL:O	21:S:80:ARG:HG2	2.06	0.55
24:V:39:ALA:O	24:V:41:GLU:N	2.33	0.55
26:X:78:GLU:HG2	26:X:79:GLU:N	2.21	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.04	0.55
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.05	0.55
5:B:98:THR:CG2	5:B:99:GLU:N	2.70	0.55
9:F:22:VAL:HG21	9:F:104:ALA:HB2	1.89	0.55
38:0:5127:HOH:O	12:J:47:THR:HB	2.06	0.55
2:9:3054:A:O2'	2:9:3055:U:H5'	2.07	0.55
7:D:138:GLY:N	38:D:7597:HOH:O	2.39	0.55
8:E:132:THR:HG23	8:E:132:THR:O	2.05	0.55
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.42	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.06	0.55
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.55
1:0:704:C:H2'	1:0:705:C:H6	1.71	0.55
1:0:1058:A:H2'	1:0:1060:C:H5''	1.89	0.55
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.06	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.87	0.55
6:C:138:VAL:O	6:C:234:VAL:HA	2.07	0.55
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.36	0.55
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.88	0.55
9:F:37:THR:O	9:F:41:GLU:HG3	2.07	0.55
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.87	0.55
1:0:1123:A:C6	1:0:1238:C:H5'	2.41	0.55
38:0:5728:HOH:O	10:G:12:ILE:HA	2.05	0.55
6:C:236:THR:HA	38:C:9249:HOH:O	2.06	0.55
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.63	0.55
25:W:46:ALA:O	25:W:49:ASN:HB2	2.06	0.55
25:W:65:VAL:CA	25:W:68:THR:HG22	2.35	0.55
1:0:644:G:H5'	1:0:644:G:N3	2.21	0.55
1:0:1185:U:H2'	1:0:1186:C:C6	2.41	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.72	0.55
5:B:103:ASP:HB2	38:B:9399:HOH:O	2.06	0.55
16:N:86:LEU:O	16:N:90:LEU:HG	2.07	0.55
27:Y:155:ARG:NH1	38:Y:8144:HOH:O	2.40	0.55
1:0:263:U:O4'	9:F:59:ILE:HD13	2.07	0.55
1:0:1441:G:H1'	38:0:7960:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:135:VAL:HG22	7:D:136:ARG:H	1.71	0.55
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.88	0.55
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.42	0.55
1:0:1333:U:H2'	1:0:1334:C:C6	2.42	0.54
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.42	0.54
2:9:3028:U:H5''	16:N:40:ASN:HD21	1.72	0.54
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.89	0.54
20:R:29:LYS:NZ	38:R:9338:HOH:O	2.40	0.54
20:R:39:THR:HB	20:R:42:GLU:CD	2.27	0.54
1:0:56:G:H5''	24:V:50:ARG:NH1	2.22	0.54
1:0:299:U:H5'	38:0:7544:HOH:O	2.08	0.54
1:0:1406:A:H4'	1:0:1407:A:H5''	1.89	0.54
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.90	0.54
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.42	0.54
20:R:39:THR:HB	20:R:42:GLU:CG	2.37	0.54
25:W:125:HIS:CD2	25:W:127:GLY:H	2.25	0.54
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.20	0.54
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.22	0.54
8:E:9:GLU:HG3	8:E:10:ASP:H	1.73	0.54
12:J:135:ILE:O	12:J:139:LEU:HG	2.07	0.54
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.23	0.54
14:L:148:GLU:HA	38:L:9369:HOH:O	2.07	0.54
1:0:870:G:OP2	4:A:3:ARG:HD3	2.08	0.54
5:B:14:GLY:HA3	38:B:9415:HOH:O	2.08	0.54
5:B:86:ALA:HA	38:B:9384:HOH:O	2.07	0.54
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.72	0.54
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.10	0.54
1:0:380:A:H2'	38:0:7443:HOH:O	2.07	0.54
1:0:1352:A:N1	6:C:48:SER:HB3	2.23	0.54
15:M:24:GLN:O	15:M:28:GLN:HG3	2.07	0.54
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.38	0.54
1:0:2055:A:H4'	20:R:132:ARG:NH2	2.23	0.54
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.54
1:0:2815:G:N7	12:J:80:LYS:NZ	2.55	0.54
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.54
1:0:797:A:H4'	28:Z:10:ARG:N	2.23	0.54
1:0:1451:C:H5'	1:0:1505:U:H3	1.73	0.54
5:B:144:THR:HG22	5:B:145:HIS:N	2.23	0.54
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.07	0.54
1:0:462:A:C2	30:2:37:HIS:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.54
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.54
1:0:2054:A:C2	20:R:128:ARG:NH2	2.72	0.54
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.90	0.54
5:B:82:VAL:O	5:B:82:VAL:HG12	2.08	0.54
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.89	0.54
25:W:11:VAL:O	25:W:12:ASN:HB2	2.08	0.54
1:0:625:U:H5''	1:0:1044:C:N4	2.23	0.53
1:0:1667:A:H2'	1:0:1668:U:H6	1.72	0.53
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.53
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.53
2:9:3107:C:H2'	2:9:3108:C:C6	2.43	0.53
7:D:159:PRO:O	7:D:163:VAL:HG23	2.08	0.53
12:J:45:VAL:HG22	12:J:46:ILE:N	2.23	0.53
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.08	0.53
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.53
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.41	0.53
1:0:1679:C:H5'	38:0:9641:HOH:O	2.07	0.53
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.90	0.53
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.72	0.53
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.43	0.53
5:B:84:LEU:HD23	5:B:178:ALA:HB1	1.90	0.53
7:D:170:TYR:O	7:D:171:ASP:HB3	2.08	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.09	0.53
1:0:396:U:OP2	31:3:38:ARG:HD2	2.08	0.53
1:0:2467:A:O2'	1:0:2468:A:H2'	2.09	0.53
38:0:7567:HOH:O	4:A:177:HIS:HE1	1.91	0.53
5:B:27:ASN:HD22	5:B:27:ASN:H	1.57	0.53
6:C:140:VAL:HB	38:C:9249:HOH:O	2.08	0.53
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.89	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.89	0.53
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.90	0.53
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.53
1:0:2565:C:H4'	38:0:5126:HOH:O	2.08	0.53
1:0:2769:C:H2'	1:0:2770:G:O4'	2.08	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.90	0.53
7:D:154:LYS:HD2	7:D:154:LYS:N	2.12	0.53
8:E:81:GLU:O	8:E:172:PRO:HD3	2.08	0.53
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.91	0.53
1:0:475:G:OP1	6:C:73:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:H2'	1:0:559:U:H5''	1.90	0.53
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
38:0:9935:HOH:O	9:F:38:LYS:HE2	2.08	0.53
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.07	0.53
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.90	0.53
25:W:1:MET:HB2	25:W:103:GLU:HG2	1.89	0.53
32:I:96:PHE:HA	32:I:136:GLY:CA	2.39	0.53
1:0:1250:C:O2'	1:0:1251:C:H5'	2.08	0.53
1:0:2748:G:H1'	38:0:8202:HOH:O	2.09	0.53
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.91	0.53
1:0:517:U:H1'	38:0:7774:HOH:O	2.09	0.53
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.53
38:0:7754:HOH:O	31:3:60:LYS:HG3	2.08	0.53
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.91	0.53
14:L:92:ASP:HA	14:L:121:ILE:HB	1.91	0.53
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.37	0.53
1:0:1636:G:O2'	1:0:1637:A:H5'	2.08	0.53
1:0:2241:C:H2'	1:0:2242:U:C6	2.44	0.53
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.42	0.53
1:0:441:A:H1'	1:0:442:A:N7	2.24	0.53
1:0:947:U:H2'	1:0:948:G:H8	1.73	0.53
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.91	0.53
6:C:150:THR:HA	6:C:203:ALA:O	2.09	0.53
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.09	0.53
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.24	0.53
15:M:6:SER:O	15:M:10:ASP:HB2	2.09	0.53
24:V:56:ILE:O	24:V:60:GLN:HG3	2.09	0.53
27:Y:136:LYS:HB3	27:Y:139:VAL:HG23	1.91	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.52
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.08	0.52
5:B:162:MET:CE	5:B:310:ARG:HD3	2.37	0.52
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.39	0.52
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.43	0.52
12:J:130:VAL:HG12	12:J:131:THR:H	1.72	0.52
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.91	0.52
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.38	0.52
18:P:103:THR:HB	38:P:180:HOH:O	2.09	0.52
23:U:33:SER:O	23:U:37:GLU:HG3	2.09	0.52
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
25:W:82:GLU:O	25:W:86:GLU:HG3	2.09	0.52
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.74	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.52
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.90	0.52
5:B:128:ILE:O	5:B:131:ALA:HB3	2.09	0.52
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.52
6:C:118:THR:O	6:C:136:VAL:HG13	2.08	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.24	0.52
17:O:39:THR:O	17:O:115:ARG:NH2	2.39	0.52
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.52
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.09	0.52
23:U:17:THR:HG22	23:U:18:GLY:N	2.24	0.52
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.10	0.52
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.73	0.52
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.09	0.52
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.09	0.52
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.52
6:C:79:ARG:O	6:C:87:ARG:HG2	2.09	0.52
11:H:21:THR:O	11:H:120:ILE:HD12	2.09	0.52
14:L:143:THR:CG2	14:L:144:ASP:N	2.72	0.52
1:0:137:U:H2'	1:0:139:C:C5	2.44	0.52
1:0:1484:G:H2'	38:0:9420:HOH:O	2.08	0.52
1:0:2694:A:H5''	8:E:90:HIS:CE1	2.44	0.52
4:A:105:VAL:HG12	4:A:106:CYS:N	2.24	0.52
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.08	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.52
16:N:132:ASN:O	16:N:135:VAL:HG12	2.10	0.52
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.43	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.91	0.52
24:V:12:THR:HG23	24:V:14:ALA:N	2.25	0.52
32:I:113:HIS:N	32:I:114:PRO:HD2	2.24	0.52
1:0:328:U:O4'	6:C:202:THR:HG22	2.10	0.52
1:0:703:G:O2'	1:0:704:C:H5'	2.10	0.52
1:0:1923:G:H4'	31:3:31:THR:O	2.09	0.52
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.91	0.52
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.91	0.52
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.52
1:0:777:U:O2'	29:1:11:LYS:HG2	2.10	0.52
1:0:1537:C:H1'	38:0:6819:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1787:C:H2'	1:0:1788:U:H6	1.74	0.52
1:0:2839:C:H4'	5:B:18:ARG:NH2	2.24	0.52
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.40	0.52
1:0:1462:C:H2'	1:0:1463:A:H8	1.74	0.52
1:0:1535:G:H2'	1:0:1536:C:C6	2.45	0.52
1:0:2094:G:C4'	5:B:245:SER:HB3	2.36	0.52
38:O:7247:HOH:O	4:A:211:LYS:HG2	2.08	0.52
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.39	0.52
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.39	0.52
17:O:87:THR:O	17:O:91:GLN:HG3	2.09	0.52
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.52
1:0:1482:A:O2'	1:0:1483:C:H5'	2.10	0.52
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.10	0.52
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.92	0.52
30:2:5:LYS:O	30:2:9:LYS:HG3	2.10	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.73	0.52
38:O:9868:HOH:O	25:W:119:HIS:HE1	1.93	0.52
2:9:3114:G:O6	16:N:11:ARG:HD3	2.10	0.52
11:H:46:GLN:HG3	11:H:137:TYR:CE2	2.44	0.52
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.24	0.52
16:N:23:ARG:HG2	16:N:23:ARG:HH11	1.75	0.52
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.83	0.52
32:I:92:PRO:C	32:I:94:GLU:H	2.13	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.09	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.76	0.52
1:0:1741:U:H3'	38:O:3073:HOH:O	2.10	0.52
1:0:2252:A:C5	1:0:2253:G:H1'	2.45	0.52
1:0:2372:A:H2'	1:0:2373:U:C6	2.45	0.52
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.52
1:0:2730:G:O2'	1:0:2731:G:H5'	2.10	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
11:H:27:LYS:H	11:H:59:HIS:CD2	2.21	0.52
14:L:136:ALA:HB3	38:L:9370:HOH:O	2.09	0.52
1:0:290:C:O2'	1:0:291:C:H5'	2.10	0.51
2:9:3050:G:H2'	2:9:3051:A:C8	2.45	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.45	0.51
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.51
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.92	0.51
14:L:10:SER:O	14:L:12:THR:N	2.41	0.51
20:R:82:GLU:HG3	20:R:83:LYS:N	2.25	0.51
1:0:185:G:O3'	1:0:186:A:H4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:188:C:H5'	15:M:163:LEU:HD21	1.92	0.51
1:0:1130:U:H2'	1:0:1131:G:O4'	2.10	0.51
1:0:1173:A:H4'	1:0:1174:A:C8	2.45	0.51
1:0:1427:A:H61	1:0:1440:U:H1'	1.76	0.51
38:0:5678:HOH:O	4:A:164:ARG:CZ	2.58	0.51
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.91	0.51
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.10	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
25:W:122:ARG:NH1	25:W:152:ALA:O	2.43	0.51
29:1:28:HIS:HD2	29:1:30:LYS:H	1.57	0.51
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.10	0.51
4:A:35:GLY:O	4:A:36:ASP:CB	2.58	0.51
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.44	0.51
5:B:171:VAL:HG23	5:B:172:SER:N	2.24	0.51
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.11	0.51
1:0:2064:U:H5'	1:0:2652:U:H4'	1.93	0.51
1:0:2090:G:H2'	1:0:2091:G:C8	2.45	0.51
5:B:119:HIS:O	5:B:121:PRO:HD3	2.09	0.51
12:J:45:VAL:HG23	12:J:130:VAL:O	2.10	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG12	1.91	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
14:L:104:ASP:O	14:L:105:TYR:HB3	2.09	0.51
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.43	0.51
25:W:65:VAL:HA	25:W:68:THR:CG2	2.37	0.51
38:0:7630:HOH:O	22:T:9:LYS:HD2	2.09	0.51
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.93	0.51
6:C:1:MET:HG2	6:C:2:GLN:NE2	2.25	0.51
16:N:64:SER:C	16:N:66:LEU:H	2.14	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.40	0.51
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.25	0.51
32:I:131:THR:O	32:I:131:THR:HG22	2.11	0.51
1:0:2526:C:O2'	1:0:2527:U:H5'	2.09	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.10	0.51
22:T:4:PRO:O	22:T:8:ARG:HG3	2.10	0.51
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.41	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.10	0.51
32:I:75:THR:HA	32:I:112:LYS:NZ	2.25	0.51
1:0:1166:A:H61	1:0:1180:U:H3	1.57	0.51
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.51
1:0:2720:C:O2	13:K:87:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3064:C:H2'	2:9:3065:A:H5'	1.93	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
6:C:236:THR:HG22	6:C:239:ALA:CB	2.41	0.51
7:D:67:ASP:O	7:D:69:ILE:HG13	2.11	0.51
11:H:9:ILE:HD12	11:H:54:THR:CG2	2.38	0.51
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.41	0.51
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.51
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.09	0.51
5:B:254:GLN:NE2	38:B:9395:HOH:O	2.43	0.51
20:R:99:ALA:CB	20:R:109:MET:HE1	2.32	0.51
27:Y:100:ARG:NH1	27:Y:215:GLU:HA	2.26	0.51
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.91	0.51
31:3:62:THR:HB	38:3:9350:HOH:O	2.11	0.51
1:0:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
1:0:1942:A:O2'	1:0:1943:C:H5'	2.11	0.51
1:0:2748:G:H5'	38:0:7739:HOH:O	2.11	0.51
9:F:99:THR:HG23	9:F:99:THR:O	2.11	0.51
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.54	0.51
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.51
1:0:2072:G:C6	1:0:2533:C:H1'	2.46	0.51
1:0:2073:G:H5''	38:0:4132:HOH:O	2.11	0.51
15:M:164:THR:HG22	15:M:167:GLY:N	2.13	0.51
18:P:115:SER:C	18:P:117:SER:H	2.14	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.16	0.51
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.50
1:0:1733:A:H4'	5:B:212:GLN:HA	1.92	0.50
1:0:1878:G:O2'	1:0:1879:U:OP2	2.29	0.50
1:0:2325:C:H1'	38:0:4453:HOH:O	2.11	0.50
11:H:28:ILE:HG23	38:H:9178:HOH:O	2.10	0.50
11:H:66:ARG:HD3	38:H:9178:HOH:O	2.11	0.50
14:L:79:ASP:HB3	38:L:9357:HOH:O	2.11	0.50
1:0:156:C:H5''	15:M:171:ARG:CD	2.21	0.50
1:0:200:U:H2'	38:0:3752:HOH:O	2.10	0.50
1:0:2862:G:H4'	5:B:336:GLN:O	2.11	0.50
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.93	0.50
12:J:19:MET:CE	12:J:132:LEU:HD11	2.41	0.50
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.50
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.11	0.50
24:V:58:THR:O	24:V:62:GLU:HG3	2.11	0.50
25:W:1:MET:N	25:W:37:GLU:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:544:G:C2'	1:0:545:G:H5''	2.40	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.50
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.41	0.50
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.11	0.50
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.12	0.50
24:V:49:LEU:O	24:V:53:ILE:HG13	2.10	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.46	0.50
1:0:2851:G:C2'	1:0:2852:A:H5'	2.40	0.50
22:T:71:VAL:HG12	22:T:72:ILE:N	2.26	0.50
1:0:536:A:H3'	38:0:5332:HOH:O	2.10	0.50
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.50
1:0:1185:U:OP1	32:I:126:LYS:HD3	2.11	0.50
1:0:1515:A:H2'	1:0:1516:C:C6	2.46	0.50
1:0:2717:C:O2'	1:0:2718:C:H5''	2.11	0.50
16:N:154:LEU:C	16:N:156:GLU:H	2.15	0.50
23:U:44:ARG:HB3	38:U:3805:HOH:O	2.11	0.50
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.94	0.50
1:0:588:G:O6	25:W:154:ARG:NH1	2.44	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
38:0:5260:HOH:O	11:H:58:ARG:HG3	2.11	0.50
4:A:88:ILE:O	4:A:88:ILE:HG22	2.12	0.50
9:F:101:ALA:HA	38:F:5413:HOH:O	2.11	0.50
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.50
1:0:130:C:H2'	38:0:3469:HOH:O	2.11	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.12	0.50
1:0:424:C:H2'	1:0:425:U:C6	2.46	0.50
1:0:1528:A:H2'	1:0:1529:G:O4'	2.11	0.50
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.40	0.50
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.25	0.50
16:N:183:ASP:O	16:N:184:ILE:O	2.28	0.50
25:W:4:LEU:O	25:W:32:CYS:HA	2.11	0.50
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.65	0.50
1:0:1180:U:H4'	32:I:91:GLU:OE2	2.11	0.50
1:0:2270:G:C4'	4:A:223:ARG:HH12	2.22	0.50
38:0:9535:HOH:O	4:A:11:ARG:HD3	2.12	0.50
4:A:36:ASP:CG	4:A:85:SER:HB2	2.30	0.50
5:B:280:VAL:HG13	5:B:334:SER:HA	1.94	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.12	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:65:VAL:O	25:W:68:THR:HG22	2.12	0.50
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
1:0:2387:U:H2'	1:0:2388:C:C6	2.47	0.50
1:0:2524:G:H21	1:0:2526:C:H41	1.59	0.50
4:A:17:ARG:HD2	38:A:9339:HOH:O	2.12	0.50
4:A:215:ILE:HG13	4:A:216:SER:N	2.27	0.50
5:B:109:LEU:HG	5:B:113:LEU:HD12	1.94	0.50
5:B:148:PRO:HB2	5:B:156:LYS:O	2.12	0.50
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.26	0.50
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.44	0.50
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.92	0.50
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.76	0.50
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.50
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.39	0.50
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.49
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.77	0.49
5:B:139:ASP:HB2	5:B:165:ARG:NE	2.24	0.49
6:C:65:ARG:HG3	6:C:67:GLN:HB2	1.93	0.49
21:S:37:VAL:O	21:S:41:VAL:HG23	2.12	0.49
26:X:34:ARG:NH1	26:X:48:VAL:O	2.44	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.28	0.49
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.49
1:0:2472:C:O2'	1:0:2634:G:H4'	2.12	0.49
8:E:11:VAL:HG13	8:E:76:VAL:HG21	1.94	0.49
9:F:113:ASP:O	9:F:117:GLU:HG3	2.12	0.49
12:J:107:ASN:HD22	12:J:107:ASN:C	2.15	0.49
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.49
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.94	0.49
1:0:284:C:H4'	1:0:285:A:O5'	2.12	0.49
1:0:1150:A:C2	10:G:20:VAL:HG21	2.47	0.49
1:0:2385:G:H2'	1:0:2386:U:C6	2.48	0.49
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.77	0.49
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.76	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.41	0.49
32:I:139:ILE:HG22	32:I:140:GLU:N	2.27	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.48	0.49
2:9:3006:C:C5'	16:N:37:ARG:HH12	2.16	0.49
6:C:111:VAL:HB	38:C:9121:HOH:O	2.11	0.49
12:J:131:THR:HG22	12:J:134:GLU:N	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:59:GLN:HE22	25:W:98:PHE:CA	2.25	0.49
1:0:380:A:OP2	15:M:9:ARG:HD2	2.12	0.49
1:0:512:G:O3'	1:0:513:A:H8	1.95	0.49
1:0:2004:U:H2'	1:0:2004:U:O2	2.12	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
20:R:33:ARG:NH1	38:R:9341:HOH:O	2.45	0.49
26:X:43:VAL:CG1	26:X:44:ASP:N	2.74	0.49
1:0:1681:G:H5''	1:0:1682:A:H5'	1.93	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
1:0:2681:A:H4'	1:0:2682:C:H5'	1.95	0.49
38:0:3270:HOH:O	31:3:84:ARG:HB2	2.11	0.49
4:A:130:THR:HG22	4:A:131:HIS:O	2.11	0.49
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.95	0.49
27:Y:133:HIS:HD2	38:Y:8170:HOH:O	1.94	0.49
1:0:21:G:H4'	20:R:2:ILE:HG22	1.95	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:834:G:H4'	1:0:835:U:OP2	2.13	0.49
1:0:2054:A:H2	20:R:128:ARG:HH22	1.57	0.49
1:0:2883:A:H2'	1:0:2884:G:O4'	2.13	0.49
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.39	0.49
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.79	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.13	0.49
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.26	0.49
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.48	0.49
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.76	0.49
1:0:177:A:H2'	1:0:178:U:O4'	2.12	0.49
1:0:1666:C:H2'	1:0:1667:A:H5'	1.94	0.49
1:0:1697:G:O2'	1:0:1698:U:H5'	2.12	0.49
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.49
1:0:2821:C:H4'	5:B:116:PRO:HB3	1.95	0.49
38:0:4910:HOH:O	17:O:39:THR:HB	2.13	0.49
38:0:5799:HOH:O	15:M:58:GLN:HG3	2.13	0.49
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.94	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
7:D:128:LEU:C	7:D:128:LEU:HD23	2.33	0.49
13:K:41:LYS:O	13:K:42:ASN:HB2	2.13	0.49
1:0:2338:G:H1'	7:D:105:SER:OG	2.12	0.49
1:0:2780:C:H2'	1:0:2781:U:C6	2.48	0.49
2:9:3029:C:H2'	2:9:3030:C:C5'	2.39	0.49
4:A:95:PRO:HA	4:A:153:ARG:HA	1.95	0.49
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.95	0.49
16:N:163:PHE:O	16:N:164:ASP:OD1	2.31	0.49
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.16	0.49
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.43	0.49
1:0:2335:C:H2'	1:0:2336:G:C8	2.48	0.49
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.49
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.49
6:C:20:ASP:O	6:C:23:GLU:HB2	2.13	0.49
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.28	0.49
11:H:166:SER:CB	11:H:167:PRO:CD	2.82	0.49
15:M:64:ARG:HD2	38:M:9382:HOH:O	2.13	0.49
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.49
1:0:1415:G:H5'	29:1:12:ASN:O	2.12	0.48
38:0:3957:HOH:O	17:O:3:THR:HG21	2.12	0.48
2:9:3049:G:H2'	2:9:3050:G:O4'	2.13	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
10:G:64:ASN:N	10:G:64:ASN:ND2	2.60	0.48
12:J:75:PRO:HD3	12:J:136:SER:OG	2.13	0.48
27:Y:144:ARG:NH1	38:Y:8164:HOH:O	2.45	0.48
1:0:485:A:N3	1:0:487:G:H5''	2.28	0.48
1:0:1624:A:H5'	1:0:1626:A:O4'	2.13	0.48
1:0:1734:C:OP1	5:B:234:ARG:HD3	2.13	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.94	0.48
4:A:93:THR:HG23	4:A:154:ALA:O	2.12	0.48
5:B:255:GLY:O	5:B:257:THR:HG23	2.13	0.48
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.95	0.48
8:E:21:THR:HG23	8:E:30:THR:OG1	2.12	0.48
14:L:80:ASP:HB2	14:L:90:ARG:O	2.13	0.48
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.13	0.48
16:N:154:LEU:O	16:N:155:GLU:HB3	2.13	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
20:R:113:HIS:O	20:R:145:LEU:HD12	2.13	0.48
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.27	0.48
31:3:65:THR:HB	31:3:83:TRP:H	1.78	0.48
1:0:820:G:H5'	1:0:821:U:H5'	1.95	0.48
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.34	0.48
18:P:41:ARG:O	18:P:44:VAL:HB	2.13	0.48
1:0:90:A:H2'	1:0:91:G:O4'	2.13	0.48
1:0:474:C:O3'	6:C:73:LEU:CD2	2.61	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.48
4:A:132:ASP:OD1	4:A:133:ARG:N	2.47	0.48
5:B:277:GLU:N	5:B:278:PRO:HD2	2.28	0.48
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.96	0.48
7:D:135:VAL:HG22	7:D:136:ARG:N	2.28	0.48
11:H:167:PRO:O	11:H:168:ALA:HB2	2.13	0.48
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.95	0.48
17:O:35:LYS:O	17:O:40:HIS:NE2	2.47	0.48
21:S:11:THR:O	21:S:15:MET:HG2	2.13	0.48
26:X:75:ALA:O	26:X:83:ALA:HA	2.14	0.48
1:0:638:C:H2'	1:0:639:A:C8	2.48	0.48
38:O:6529:HOH:O	27:Y:158:LYS:HD3	2.13	0.48
5:B:251:VAL:HG23	5:B:252:PRO:HD2	1.95	0.48
6:C:19:PRO:HD2	6:C:240:LEU:HD21	1.95	0.48
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.43	0.48
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.48
14:L:114:VAL:HG11	38:L:9370:HOH:O	2.12	0.48
14:L:134:GLU:HA	14:L:138:GLY:O	2.13	0.48
16:N:100:ALA:O	16:N:129:ILE:HG23	2.13	0.48
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.13	0.48
30:2:41:HIS:O	30:2:45:ASN:HB2	2.13	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
1:0:251:C:H5''	15:M:143:ASN:HD22	1.77	0.48
1:0:661:G:C5	1:0:686:A:C2	3.02	0.48
1:0:2361:A:H2'	1:0:2362:A:C8	2.47	0.48
2:9:3001:U:H5''	2:9:3003:A:OP1	2.14	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.61	0.48
25:W:7:LEU:CD1	25:W:53:ALA:HB2	2.44	0.48
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.14	0.48
1:0:545:G:H5'	1:0:545:G:C8	2.40	0.48
1:0:2073:G:OP2	1:0:2490:A:H5'	2.14	0.48
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.95	0.48
14:L:21:ARG:N	38:L:9329:HOH:O	2.46	0.48
14:L:143:THR:HG22	14:L:145:LEU:H	1.79	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.95	0.48
18:P:16:VAL:CG1	18:P:17:GLY:N	2.76	0.48
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.48
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.96	0.48
20:R:8:ALA:CB	20:R:13:THR:HG21	2.39	0.48
25:W:137:GLN:HG3	25:W:137:GLN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:67:LEU:HD21	31:3:88:LEU:CD2	2.43	0.48
32:I:102:VAL:O	32:I:106:LYS:HG3	2.14	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.49	0.48
1:0:1919:A:H4'	38:0:5141:HOH:O	2.13	0.48
1:0:2900:G:H2'	1:0:2901:C:O4'	2.14	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.49	0.48
4:A:36:ASP:HB2	4:A:85:SER:H	1.78	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.14	0.48
4:A:210:GLY:HA3	38:A:9383:HOH:O	2.13	0.48
8:E:84:MET:HE3	8:E:131:LEU:HD13	1.94	0.48
16:N:15:GLU:HB3	16:N:17:ARG:CG	2.42	0.48
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.95	0.48
25:W:7:LEU:HD12	25:W:53:ALA:HB2	1.96	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
1:0:1119:G:H22	1:0:1246:A:H2	1.52	0.48
1:0:1201:C:H2'	1:0:1202:A:H5'	1.95	0.48
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.48
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.14	0.48
1:0:2866:U:H4'	1:0:2867:G:H5'	1.94	0.48
1:0:1163:G:H2'	1:0:1164:U:C5	2.49	0.48
1:0:2421:G:H4'	38:0:5073:HOH:O	2.14	0.48
1:0:2909:G:H2'	1:0:2910:A:H8	1.79	0.48
4:A:39:ALA:O	4:A:61:GLU:HG3	2.14	0.48
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.95	0.48
5:B:305:ASP:O	5:B:306:LYS:CB	2.61	0.48
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.44	0.48
9:F:58:GLU:HA	9:F:61:MET:HG3	1.95	0.48
10:G:67:LEU:O	10:G:71:LEU:HG	2.13	0.48
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.48	0.48
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.28	0.48
1:0:189:A:OP1	15:M:171:ARG:NH2	2.47	0.47
1:0:794:U:H3	1:0:819:A:H61	1.63	0.47
1:0:1086:A:N6	25:W:11:VAL:HG11	2.29	0.47
1:0:1811:A:C2	1:0:2752:C:H1'	2.49	0.47
1:0:2807:U:P	5:B:27:ASN:HD21	2.36	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.43	0.47
4:A:51:ARG:NH1	4:A:120:ARG:O	2.47	0.47
5:B:275:GLY:O	5:B:291:ASP:HA	2.14	0.47
16:N:42:HIS:HB3	16:N:62:HIS:CE1	2.49	0.47
21:S:57:THR:CG2	21:S:58:MET:N	2.77	0.47
26:X:78:GLU:CG	26:X:79:GLU:H	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:1805:G:H2'	1:0:1806:G:H8	1.78	0.47
1:0:2078:U:O2'	1:0:2079:G:H5'	2.14	0.47
1:0:2445:U:H2'	1:0:2446:G:C8	2.49	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.14	0.47
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.14	0.47
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.95	0.47
10:G:63:ARG:N	38:G:2569:HOH:O	2.46	0.47
11:H:63:GLU:O	11:H:67:LEU:HB2	2.14	0.47
12:J:8:ALA:HA	12:J:35:THR:CG2	2.44	0.47
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2424:U:H1'	19:Q:7:LEU:HD12	1.96	0.47
1:0:2838:A:H2'	1:0:2839:C:C6	2.50	0.47
5:B:140:LEU:HA	38:B:9384:HOH:O	2.14	0.47
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.96	0.47
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.96	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.27	0.47
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.13	0.47
23:U:9:CYS:HA	23:U:52:THR:CG2	2.38	0.47
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.47
1:0:392:U:O2'	15:M:182:LYS:HE2	2.15	0.47
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.14	0.47
6:C:214:THR:HG23	38:C:9236:HOH:O	2.14	0.47
6:C:237:GLU:HA	38:C:9228:HOH:O	2.13	0.47
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.21	0.47
11:H:58:ARG:NH1	11:H:58:ARG:HG3	2.30	0.47
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.96	0.47
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.47
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.35	0.47
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.95	0.47
31:3:65:THR:HG21	31:3:83:TRP:CZ3	2.49	0.47
1:0:128:A:O2'	1:0:129:A:H5'	2.14	0.47
1:0:1191:A:H2'	1:0:1193:A:H5'	1.96	0.47
1:0:1450:C:C4'	1:0:1451:C:OP2	2.59	0.47
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.47	0.47
38:0:3544:HOH:O	32:I:92:PRO:HD2	2.13	0.47
15:M:107:ARG:NH1	38:M:9374:HOH:O	2.48	0.47
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.47
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:39:G:H2'	1:0:40:C:O4'	2.15	0.47
1:0:960:G:C2'	1:0:960:G:N3	2.78	0.47
1:0:1023:C:O2'	1:0:1024:G:H5'	2.15	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
2:9:3052:A:H2'	2:9:3053:G:O4'	2.15	0.47
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.28	0.47
21:S:53:ASN:HD22	21:S:53:ASN:N	2.12	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
1:0:1132:A:N6	1:0:1229:C:H2'	2.30	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.45	0.47
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.96	0.47
1:0:2252:A:C6	1:0:2253:G:H1'	2.48	0.47
1:0:2314:G:C2'	1:0:2315:C:H5'	2.45	0.47
1:0:2768:A:O2'	1:0:2769:C:H5'	2.14	0.47
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.48	0.47
38:0:3999:HOH:O	8:E:143:GLN:HG2	2.14	0.47
2:9:3041:C:H4'	7:D:48:MET:HB2	1.95	0.47
5:B:238:ASN:ND2	5:B:240:GLY:H	1.98	0.47
6:C:22:PHE:HA	6:C:116:ALA:HA	1.96	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.79	0.47
6:C:233:THR:HG22	6:C:234:VAL:N	2.30	0.47
12:J:52:GLN:HG3	12:J:53:ILE:H	1.78	0.47
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.45	0.47
20:R:47:LEU:O	20:R:51:ILE:HG13	2.14	0.47
20:R:96:VAL:O	20:R:99:ALA:HB3	2.15	0.47
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.97	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.47
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.30	0.47
1:0:10:U:O4	1:0:532:A:OP2	2.33	0.47
1:0:561:G:H2'	1:0:562:A:H8	1.79	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
1:0:1820:G:C6	1:0:2030:A:C2	3.02	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.15	0.47
2:9:3023:U:O2'	2:9:3024:U:H4'	2.14	0.47
4:A:128:LEU:HD21	4:A:131:HIS:CE1	2.50	0.47
5:B:139:ASP:CB	5:B:165:ARG:HE	2.26	0.47
5:B:307:ARG:HH11	5:B:307:ARG:CB	2.25	0.47
6:C:165:ASP:O	6:C:168:ARG:HB3	2.15	0.47
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.13	0.47
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.47
1:0:407:A:H2'	1:0:408:A:C8	2.50	0.47
1:0:790:A:H2'	1:0:791:A:O4'	2.15	0.47
1:0:1060:C:H6	1:0:1060:C:H5'	1.80	0.47
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.47	0.47
1:0:1165:G:O2'	1:0:1174:A:H1'	2.15	0.47
1:0:1687:C:O2	29:1:9:GLY:HA2	2.15	0.47
4:A:179:MET:HA	4:A:179:MET:HE2	1.96	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
10:G:12:ILE:N	10:G:13:PRO:CD	2.78	0.47
32:I:132:CYS:C	32:I:134:SER:H	2.16	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.48	0.47
1:0:1787:C:H4'	1:0:2883:A:O4'	2.15	0.47
4:A:51:ARG:HB2	38:A:9402:HOH:O	2.15	0.47
5:B:48:MET:HG2	5:B:72:THR:HA	1.97	0.47
5:B:271:ASP:OD1	5:B:272:ILE:N	2.48	0.47
7:D:166:ILE:HB	38:D:6326:HOH:O	2.13	0.47
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.47
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.45	0.47
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.49	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.50	0.47
1:0:317:A:OP1	22:T:52:ARG:O	2.33	0.46
1:0:1118:A:C8	1:0:1118:A:C3'	2.94	0.46
1:0:1375:A:H2'	1:0:1376:G:H5'	1.97	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
1:0:1855:G:H4'	1:0:1856:C:O5'	2.15	0.46
1:0:2135:A:O2'	1:0:2136:G:H5'	2.15	0.46
1:0:2613:G:O2'	1:0:2614:C:H5'	2.15	0.46
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.80	0.46
9:F:26:THR:HG21	9:F:102:GLY:C	2.35	0.46
23:U:52:THR:HG21	23:U:54:THR:HB	1.96	0.46
24:V:8:ILE:HA	24:V:11:MET:CE	2.44	0.46
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.15	0.46
1:0:249:G:O2'	1:0:250:C:H5'	2.15	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.15	0.46
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.96	0.46
16:N:67:ALA:C	16:N:69:TYR:H	2.17	0.46
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.16	0.46
1:0:656:G:H5'	17:O:3:THR:CG2	2.45	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.46
1:0:1747:A:C8	13:K:44:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2335:C:H2'	1:0:2336:G:H8	1.81	0.46
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.50	0.46
14:L:24:ALA:HB2	14:L:30:ARG:HD2	1.97	0.46
16:N:152:GLU:C	16:N:154:LEU:H	2.17	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.95	0.46
22:T:48:VAL:HG22	22:T:96:VAL:HG13	1.97	0.46
25:W:35:VAL:CG2	25:W:41:TYR:CD2	2.98	0.46
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.56	0.46
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.46
1:0:538:C:H5''	1:0:539:G:C8	2.51	0.46
1:0:571:C:O5'	1:0:571:C:H6	1.98	0.46
1:0:589:U:H2'	1:0:590:A:H8	1.79	0.46
1:0:899:C:H5'	38:0:3511:HOH:O	2.14	0.46
1:0:1413:A:H2'	1:0:1414:A:O4'	2.15	0.46
1:0:1790:C:H2'	1:0:1791:U:H6	1.80	0.46
1:0:2255:A:H2'	1:0:2256:G:O4'	2.16	0.46
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.46
4:A:94:LEU:HD23	4:A:94:LEU:N	2.30	0.46
16:N:164:ASP:OD1	16:N:167:ASP:CA	2.60	0.46
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.16	0.46
32:I:98:ALA:O	32:I:137:VAL:HA	2.16	0.46
1:0:960:G:N3	1:0:960:G:H3'	2.31	0.46
1:0:1380:U:O4	1:0:2043:U:H4'	2.16	0.46
2:9:3039:U:H3'	2:9:3040:C:H5''	1.98	0.46
5:B:157:LYS:HG2	38:B:9467:HOH:O	2.16	0.46
8:E:68:HIS:O	8:E:72:MET:HG3	2.15	0.46
15:M:164:THR:HB	38:M:9319:HOH:O	2.15	0.46
18:P:14:LEU:HD13	18:P:51:ALA:HB2	1.96	0.46
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.16	0.46
23:U:20:MET:CG	23:U:28:THR:HG23	2.46	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
1:0:949:U:H4'	19:Q:95:GLU:HA	1.97	0.46
1:0:1342:C:C2'	1:0:1343:C:H5'	2.46	0.46
1:0:2897:C:H2'	1:0:2898:G:H8	1.80	0.46
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.45	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46
7:D:37:ALA:O	7:D:40:ILE:HG12	2.16	0.46
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.48	0.46
16:N:108:SER:HA	16:N:109:PRO:HD3	1.72	0.46
25:W:13:MET:HE1	25:W:18:GLN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:83:TRP:CZ3	25:W:112:LEU:HD21	2.51	0.46
1:O:241:A:C2	1:O:378:A:H4'	2.51	0.46
1:O:797:A:O4'	28:Z:10:ARG:N	2.49	0.46
1:O:1375:A:C2'	1:O:1376:G:H5'	2.45	0.46
1:O:1530:U:H2'	1:O:1531:U:O4'	2.16	0.46
1:O:2507:G:H2'	1:O:2510:C:H42	1.81	0.46
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.37	0.46
6:C:147:LEU:HA	38:C:9210:HOH:O	2.15	0.46
7:D:81:GLU:C	7:D:83:PHE:H	2.19	0.46
8:E:77:THR:OG1	8:E:78:GLU:N	2.43	0.46
13:K:49:LEU:HD21	13:K:74:VAL:O	2.16	0.46
22:T:75:GLU:O	22:T:76:ASP:HB2	2.15	0.46
22:T:78:THR:HB	22:T:87:VAL:O	2.16	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.16	0.46
1:O:314:G:N2	1:O:316:A:H3'	2.31	0.46
1:O:1181:A:N1	1:O:1192:A:O2'	2.46	0.46
1:O:1309:U:O2'	1:O:1310:U:H5'	2.16	0.46
1:O:1874:U:OP1	4:A:51:ARG:HD2	2.16	0.46
1:O:2413:A:H2'	1:O:2414:A:O4'	2.15	0.46
1:O:2819:C:H2'	1:O:2820:A:C8	2.50	0.46
4:A:105:VAL:CG1	4:A:106:CYS:N	2.79	0.46
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.46
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.83	0.46
22:T:40:VAL:HG23	22:T:119:ALA:OXT	2.16	0.46
24:V:29:ASN:O	24:V:33:VAL:HG23	2.16	0.46
24:V:57:LYS:HA	24:V:60:GLN:NE2	2.28	0.46
1:O:31:C:H2'	38:O:7883:HOH:O	2.15	0.46
1:O:660:A:H4'	1:O:661:G:O5'	2.16	0.46
1:O:1168:C:H4'	38:I:5128:HOH:O	2.16	0.46
1:O:1849:G:H1'	1:O:2011:A:N1	2.31	0.46
1:O:2846:C:OP1	5:B:158:LYS:HD2	2.15	0.46
14:L:130:ARG:HA	38:L:9356:HOH:O	2.16	0.46
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.31	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.98	0.46
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.36	0.46
1:O:926:A:O2'	14:L:41:HIS:CD2	2.69	0.46
1:O:1164:U:H3	1:O:1192:A:H2	1.64	0.46
1:O:1768:C:H2'	1:O:1769:C:O4'	2.15	0.46
5:B:66:GLU:O	5:B:67:GLU:HB2	2.16	0.46
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.97	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.46
13:K:90:PHE:N	13:K:90:PHE:CD1	2.84	0.46
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.36	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.46	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.45
1:0:1120:U:H5'	1:0:1121:G:OP2	2.15	0.45
1:0:1419:U:H5'	1:0:1420:C:OP2	2.16	0.45
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.45
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
38:0:3205:HOH:O	12:J:46:ILE:HA	2.15	0.45
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.45
7:D:173:GLU:HG3	7:D:174:VAL:H	1.81	0.45
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.34	0.45
25:W:90:TYR:CD1	25:W:90:TYR:N	2.84	0.45
31:3:65:THR:HG23	31:3:67:LEU:HG	1.98	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.45
1:0:1634:G:H2'	1:0:1635:U:C6	2.51	0.45
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.98	0.45
1:0:2346:C:O2'	7:D:52:THR:HG21	2.16	0.45
1:0:2795:C:O2'	1:0:2796:U:H5'	2.15	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
13:K:98:VAL:HG13	13:K:99:ASP:N	2.30	0.45
14:L:117:GLU:HB3	14:L:137:GLY:O	2.17	0.45
22:T:12:ARG:O	22:T:19:ARG:NH2	2.49	0.45
32:I:132:CYS:C	32:I:134:SER:N	2.69	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.45
1:0:1139:U:H2'	1:0:1140:C:C6	2.51	0.45
1:0:2379:G:N3	1:0:2418:G:H2'	2.32	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.17	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
5:B:24:PRO:O	5:B:25:ARG:HD3	2.15	0.45
5:B:270:ILE:O	5:B:271:ASP:HB2	2.17	0.45
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.98	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.14	0.45
32:I:97:VAL:O	32:I:97:VAL:HG12	2.16	0.45
1:0:292:G:H2'	1:0:358:G:N2	2.31	0.45
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.45
1:0:671:A:O2'	1:0:672:G:H2'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
9:F:32:GLY:N	38:F:3111:HOH:O	2.49	0.45
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.45	0.45
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.52	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
25:W:13:MET:HE2	25:W:18:GLN:N	2.31	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.51	0.45
32:I:101:SER:OG	32:I:104:GLN:HG3	2.16	0.45
32:I:131:THR:O	32:I:135:LEU:HG	2.16	0.45
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.45
1:0:816:G:C6	1:0:817:G:N1	2.84	0.45
1:0:2428:G:N7	31:3:60:LYS:NZ	2.61	0.45
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.97	0.45
17:O:96:VAL:HA	38:O:4258:HOH:O	2.17	0.45
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.03	0.45
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.45
32:I:75:THR:CA	32:I:112:LYS:NZ	2.79	0.45
1:0:21:G:H5''	20:R:2:ILE:HA	1.95	0.45
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.45
1:0:1118:A:H62	1:0:1244:U:H3	1.63	0.45
1:0:1269:G:H2'	1:0:1270:U:C6	2.52	0.45
1:0:1299:G:N7	14:L:6:ARG:NH1	2.64	0.45
1:0:2508:C:H2'	38:0:6980:HOH:O	2.15	0.45
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.98	0.45
4:A:48:ASP:HB3	38:A:9402:HOH:O	2.15	0.45
4:A:211:LYS:NZ	38:A:9415:HOH:O	2.43	0.45
5:B:17:LYS:O	5:B:260:HIS:HD2	1.99	0.45
5:B:33:ASP:O	5:B:34:GLY:O	2.34	0.45
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.35	0.45
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.17	0.45
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	1.98	0.45
1:0:1595:G:O2'	1:0:1596:U:H5'	2.16	0.45
1:0:1891:G:H1'	1:0:1972:U:C2	2.51	0.45
1:0:2101:A:H2'	6:C:63:SER:OG	2.17	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.17	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.84	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.46	0.45
9:F:91:VAL:CG1	9:F:92:GLY:N	2.79	0.45
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.45
14:L:57:VAL:HG12	14:L:57:VAL:O	2.17	0.45
21:S:30:ASP:HA	21:S:62:LYS:HE3	1.99	0.45
21:S:52:VAL:C	21:S:53:ASN:HD22	2.19	0.45
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.82	0.45
31:3:48:ASN:ND2	31:3:50:GLY:H	2.14	0.45
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.32	0.45
1:0:960:G:N3	1:0:960:G:H2'	2.31	0.45
1:0:1477:C:O2'	1:0:1478:U:H5'	2.17	0.45
1:0:2266:A:H2'	1:0:2267:G:C8	2.52	0.45
1:0:2637:A:N6	3:4:176:A:H2'	2.32	0.45
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.16	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.51	0.45
8:E:71:ASN:ND2	8:E:138:ILE:HD13	2.31	0.45
13:K:103:ASP:O	13:K:104:PRO:C	2.56	0.45
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.47	0.45
25:W:132:VAL:C	25:W:134:GLU:H	2.20	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
27:Y:189:ASN:C	27:Y:189:ASN:ND2	2.68	0.45
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.82	0.45
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.51	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.45
1:0:1829:A:H2'	1:0:1830:C:H5'	1.99	0.45
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.45
1:0:2401:A:H2'	1:0:2402:A:C8	2.52	0.45
1:0:2541:U:C2	1:0:2620:U:O4	2.69	0.45
38:0:4963:HOH:O	21:S:67:ARG:HD3	2.16	0.45
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.98	0.45
4:A:139:LYS:HE2	4:A:143:GLY:HA2	1.99	0.45
4:A:213:LYS:NZ	38:A:9362:HOH:O	2.46	0.45
6:C:240:LEU:HD23	6:C:240:LEU:O	2.17	0.45
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.17	0.45
11:H:45:VAL:HA	11:H:167:PRO:O	2.16	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
22:T:71:VAL:CG1	22:T:72:ILE:N	2.79	0.45
26:X:41:PHE:O	26:X:43:VAL:HG23	2.17	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:165:A:H5''	14:L:33:ALA:HB2	1.99	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.45
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.45
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.45
38:0:5788:HOH:O	5:B:298:LYS:HD3	2.15	0.45
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.46	0.45
13:K:20:CYS:HB3	13:K:26:ALA:O	2.17	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.17	0.45
1:0:291:C:H2'	1:0:292:G:O4'	2.17	0.44
1:0:700:A:C2	14:L:71:GLU:HG2	2.52	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.17	0.44
1:0:1058:A:H2'	1:0:1060:C:C5'	2.47	0.44
1:0:1300:G:H1'	38:0:4978:HOH:O	2.17	0.44
1:0:2419:U:H5''	1:0:2420:G:H5'	1.99	0.44
1:0:2435:U:H1'	38:0:5700:HOH:O	2.17	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.50	0.44
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.82	0.44
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.99	0.44
7:D:63:ILE:HG13	7:D:64:ARG:N	2.32	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.44
20:R:124:GLY:HA3	20:R:136:TRP:O	2.17	0.44
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.47	0.44
1:0:500:G:H21	20:R:98:ASN:HD21	1.63	0.44
1:0:1189:A:H1'	1:0:1209:C:H1'	1.97	0.44
1:0:1329:A:N1	36:0:9313:CL:CL	2.87	0.44
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.83	0.44
7:D:140:ARG:O	7:D:140:ARG:HG2	2.17	0.44
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.99	0.44
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.99	0.44
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.47	0.44
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.47	0.44
18:P:108:LEU:HB2	18:P:114:LEU:HD12	2.00	0.44
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.85	0.44
21:S:33:SER:OG	21:S:36:GLU:HG3	2.16	0.44
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.32	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.65	0.44
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.18	0.44
32:I:112:LYS:C	32:I:114:PRO:HD2	2.37	0.44
1:0:447:A:OP1	22:T:2:LYS:HG2	2.17	0.44
1:0:736:A:H2'	1:0:737:A:O4'	2.17	0.44
1:0:1495:C:H2'	1:0:1496:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.44
1:0:2403:C:H3'	38:0:5489:HOH:O	2.18	0.44
1:0:2821:C:H4'	5:B:116:PRO:CB	2.48	0.44
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.44
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.99	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.46	0.44
13:K:106:GLY:HA3	38:K:5264:HOH:O	2.16	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
1:0:396:U:H1'	38:0:7824:HOH:O	2.15	0.44
1:0:1183:C:N4	1:0:1184:C:H41	2.15	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.35	0.44
1:0:2036:C:C1'	13:K:44:LEU:HG	2.47	0.44
1:0:2894:C:O2'	1:0:2895:C:H5'	2.17	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.32	0.44
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.44
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.47	0.44
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.17	0.44
11:H:83:TYR:CD1	11:H:83:TYR:C	2.91	0.44
18:P:55:LYS:CG	18:P:56:GLY:N	2.80	0.44
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.48	0.44
1:0:820:G:H3'	38:0:3359:HOH:O	2.18	0.44
1:0:1309:U:C2'	1:0:1310:U:H5'	2.48	0.44
5:B:294:TYR:HE2	38:B:9456:HOH:O	2.01	0.44
9:F:91:VAL:CG1	9:F:92:GLY:H	2.28	0.44
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.00	0.44
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.17	0.44
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.00	0.44
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.99	0.44
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.83	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.44
1:0:1909:A:N1	1:0:2128:G:H1'	2.33	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.18	0.44
1:0:2281:C:C2'	1:0:2282:U:H5'	2.47	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.33	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.48	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.83	0.44
5:B:138:GLY:O	5:B:139:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:195:ARG:NH2	5:B:323:LEU:HD13	2.33	0.44
6:C:153:VAL:O	6:C:157:LEU:HG	2.17	0.44
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.47	0.44
10:G:20:VAL:O	10:G:24:VAL:HG23	2.18	0.44
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.44
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.82	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.85	0.44
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.18	0.44
1:0:289:G:O2'	1:0:290:C:H5'	2.18	0.44
1:0:1976:G:H1'	1:0:2005:G:N2	2.33	0.44
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.17	0.44
12:J:42:GLU:HG3	12:J:145:TRP:CD1	2.53	0.44
16:N:67:ALA:C	16:N:69:TYR:N	2.71	0.44
17:O:96:VAL:HG12	17:O:97:SER:N	2.33	0.44
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.17	0.44
1:0:553:G:P	27:Y:204:ARG:NH2	2.90	0.44
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.18	0.44
1:0:1202:A:H2'	1:0:1203:G:H5'	1.99	0.44
1:0:2004:U:H2'	1:0:2005:G:OP1	2.18	0.44
1:0:2243:C:H5''	38:0:4058:HOH:O	2.17	0.44
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.44
1:0:2782:G:O6	1:0:2790:C:H5''	2.17	0.44
5:B:251:VAL:HG13	38:B:9371:HOH:O	2.18	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.98	0.44
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.44
17:O:24:ALA:O	17:O:28:ASP:HB2	2.18	0.44
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.48	0.44
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.80	0.44
27:Y:177:LYS:HE2	27:Y:183:GLU:OE2	2.17	0.44
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.53	0.44
1:0:1167:G:O2'	1:0:1168:C:H5'	2.18	0.44
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.44
6:C:7:ASP:C	6:C:9:ASP:H	2.21	0.44
15:M:165:GLY:O	15:M:169:ARG:HG3	2.18	0.44
1:0:100:C:O2	22:T:17:HIS:HB3	2.18	0.43
1:0:508:A:H2'	1:0:509:A:H5''	2.00	0.43
1:0:585:C:H5''	38:0:5161:HOH:O	2.17	0.43
1:0:841:A:OP2	20:R:128:ARG:HD2	2.18	0.43
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.43
1:0:1744:G:H2'	1:0:1745:G:H5'	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.51	0.43
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.53	0.43
8:E:7:ILE:HD11	8:E:11:VAL:HG12	2.00	0.43
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.98	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.17	0.43
1:0:1067:A:H5'	38:0:4650:HOH:O	2.16	0.43
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.43
1:0:1883:U:C2'	1:0:1884:G:H5'	2.48	0.43
1:0:1929:G:H1'	38:0:5438:HOH:O	2.18	0.43
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.33	0.43
6:C:115:LEU:HD21	6:C:243:VAL:CG1	2.38	0.43
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.33	0.43
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.51	0.43
23:U:17:THR:CG2	23:U:18:GLY:N	2.81	0.43
28:Z:13:ARG:NH1	38:Z:9219:HOH:O	2.51	0.43
32:I:118:SER:HB2	32:I:123:ASN:HB2	2.00	0.43
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.43
1:0:2015:A:H2'	1:0:2016:U:O4'	2.18	0.43
1:0:2274:A:O2'	1:0:2275:G:H5'	2.18	0.43
1:0:2775:A:C6	1:0:2799:A:C8	3.06	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
2:9:3042:C:O2	7:D:76:ARG:NH1	2.51	0.43
2:9:3055:U:H4'	2:9:3056:A:C8	2.53	0.43
2:9:3106:C:O2'	2:9:3107:C:H5'	2.18	0.43
5:B:36:PRO:HD3	5:B:169:GLY:H	1.83	0.43
6:C:131:PHE:CD2	6:C:131:PHE:N	2.86	0.43
7:D:142:ALA:HA	7:D:149:ARG:O	2.19	0.43
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.43
11:H:154:TYR:CD1	11:H:154:TYR:C	2.91	0.43
12:J:103:VAL:HG12	38:J:9365:HOH:O	2.19	0.43
16:N:151:ASP:HB3	38:N:9324:HOH:O	2.17	0.43
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.79	0.43
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
1:0:1268:C:O2'	1:0:1269:G:H5'	2.18	0.43
1:0:2039:A:OP2	5:B:234:ARG:NH2	2.51	0.43
1:0:2438:G:H2'	1:0:2439:C:O4'	2.18	0.43
5:B:232:TRP:CD1	5:B:235:ARG:HD2	2.54	0.43
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.00	0.43
18:P:71:TYR:HD2	18:P:73:HIS:CD2	2.36	0.43
23:U:5:GLU:HG3	23:U:10:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:C	24:V:41:GLU:H	2.17	0.43
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.51	0.43
1:0:1423:C:O2'	1:0:1424:A:H5'	2.18	0.43
1:0:1625:U:H5''	38:0:6274:HOH:O	2.18	0.43
1:0:2890:A:C8	23:U:56:ARG:NE	2.87	0.43
38:0:4151:HOH:O	11:H:11:LYS:HE2	2.18	0.43
2:9:3054:A:H2	38:9:3535:HOH:O	2.01	0.43
3:4:176:A:OP1	3:4:175:C:H5''	2.17	0.43
25:W:59:GLN:HE22	25:W:98:PHE:N	2.17	0.43
32:I:138:THR:CG2	32:I:139:ILE:H	2.23	0.43
1:0:1169:U:H2'	1:0:1170:U:O4'	2.18	0.43
1:0:1451:C:H5'	1:0:1505:U:N3	2.34	0.43
5:B:51:VAL:HG22	5:B:53:LEU:CD1	2.49	0.43
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.99	0.43
5:B:254:GLN:HG3	38:B:9331:HOH:O	2.17	0.43
7:D:48:MET:HA	7:D:49:PRO:HD3	1.79	0.43
8:E:11:VAL:HG12	8:E:12:ASP:N	2.34	0.43
16:N:42:HIS:HB3	16:N:62:HIS:HE1	1.82	0.43
16:N:147:ILE:HB	38:N:9342:HOH:O	2.19	0.43
22:T:48:VAL:HG22	22:T:97:ARG:C	2.39	0.43
23:U:6:CYS:C	23:U:8:TYR:H	2.22	0.43
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.43
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.99	0.43
1:0:920:C:H5''	1:0:921:G:O5'	2.19	0.43
1:0:1119:G:H8	12:J:52:GLN:NE2	2.17	0.43
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.43
1:0:2511:A:H2'	1:0:2512:U:O4'	2.19	0.43
6:C:8:LEU:HD13	6:C:147:LEU:HD21	1.99	0.43
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.54	0.43
7:D:139:TYR:N	38:D:3723:HOH:O	2.51	0.43
8:E:49:ILE:HD11	8:E:69:ILE:HD12	2.01	0.43
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.49	0.43
14:L:145:LEU:O	14:L:145:LEU:HD23	2.19	0.43
15:M:30:GLU:O	15:M:34:GLU:HG3	2.18	0.43
15:M:98:GLN:O	15:M:102:GLU:HG3	2.19	0.43
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.33	0.43
24:V:1:THR:CG2	24:V:2:VAL:N	2.79	0.43
27:Y:165:GLU:HB3	38:Y:8182:HOH:O	2.17	0.43
1:0:645:U:OP2	14:L:4:LYS:CE	2.67	0.43
2:9:3052:A:O5'	2:9:3052:A:H8	2.02	0.43
4:A:36:ASP:CB	4:A:85:SER:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.81	0.43
5:B:7:ARG:HD3	5:B:9:GLY:O	2.19	0.43
5:B:26:PHE:CE1	5:B:310:ARG:HB3	2.54	0.43
6:C:98:ARG:NH1	38:C:9154:HOH:O	2.50	0.43
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.18	0.43
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
22:T:40:VAL:HG23	22:T:119:ALA:C	2.38	0.43
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.43
1:0:1206:U:H2'	1:0:1207:A:O4'	2.18	0.43
1:0:2382:A:H5'	38:3:9334:HOH:O	2.18	0.43
2:9:3056:A:C3'	2:9:3057:A:H5''	2.49	0.43
7:D:81:GLU:C	7:D:83:PHE:N	2.72	0.43
18:P:55:LYS:HG2	18:P:56:GLY:N	2.33	0.43
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.01	0.43
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.01	0.43
1:0:721:A:H4'	17:O:51:TYR:CD1	2.53	0.43
1:0:1942:A:H3'	38:0:7554:HOH:O	2.19	0.43
1:0:2816:A:H5''	1:0:2817:G:H5'	2.01	0.43
5:B:88:GLU:HB3	5:B:97:LEU:HG	2.00	0.43
15:M:159:VAL:HG13	15:M:160:PHE:N	2.33	0.43
18:P:6:GLN:OE1	18:P:6:GLN:N	2.47	0.43
18:P:40:VAL:O	18:P:44:VAL:HG23	2.19	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
1:0:282:C:H2'	1:0:283:U:O4'	2.18	0.42
1:0:969:G:H1	1:0:999:C:H42	1.67	0.42
1:0:1118:A:C8	1:0:1119:G:H5''	2.51	0.42
1:0:1331:A:OP2	27:Y:142:SER:OG	2.27	0.42
1:0:1654:U:H5''	38:0:7627:HOH:O	2.18	0.42
1:0:1705:C:C5'	18:P:59:ARG:HH12	2.32	0.42
1:0:1942:A:H4'	38:A:9312:HOH:O	2.19	0.42
1:0:2740:G:H2'	1:0:2741:A:O4'	2.19	0.42
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.84	0.42
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
7:D:57:THR:HG23	7:D:63:ILE:HG22	2.00	0.42
9:F:22:VAL:CG2	9:F:104:ALA:HB2	2.49	0.42
15:M:46:LEU:HG	38:M:9413:HOH:O	2.18	0.42
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.18	0.42
30:2:19:SER:HB3	38:2:4479:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:544:G:H2'	1:0:545:G:C5'	2.49	0.42
1:0:559:U:H2'	1:0:560:C:O4'	2.19	0.42
1:0:1377:C:H6	1:0:1377:C:C5'	2.31	0.42
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.42
1:0:2708:G:N2	13:K:1:MET:O	2.52	0.42
16:N:44:ARG:HG3	16:N:45:ALA:N	2.34	0.42
16:N:104:ILE:O	16:N:104:ILE:HG13	2.18	0.42
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.23	0.42
20:R:25:PHE:CE2	20:R:29:LYS:CE	3.01	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.42
1:0:1711:A:O2'	1:0:1712:A:H5'	2.19	0.42
1:0:2327:A:H2'	1:0:2328:U:O4'	2.19	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.42
38:0:6997:HOH:O	16:N:5:ARG:HB2	2.19	0.42
7:D:101:THR:HG22	38:D:7400:HOH:O	2.19	0.42
8:E:166:VAL:HB	38:E:6341:HOH:O	2.19	0.42
13:K:45:PRO:HB2	38:K:7169:HOH:O	2.18	0.42
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.52	0.42
16:N:149:GLU:O	16:N:152:GLU:HB2	2.19	0.42
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.33	0.42
1:0:875:A:C2	4:A:194:MET:SD	3.12	0.42
1:0:1167:G:H4'	32:I:135:LEU:HD22	2.01	0.42
1:0:1205:U:H2'	1:0:1206:U:C5'	2.49	0.42
1:0:1544:U:H2'	1:0:1545:C:H6	1.84	0.42
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
1:0:2499:U:O2'	1:0:2500:C:H5'	2.18	0.42
1:0:2719:A:C2	5:B:70:PRO:HG3	2.54	0.42
2:9:3007:G:H5'	38:N:9345:HOH:O	2.17	0.42
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.32	0.42
9:F:83:LEU:HD11	9:F:96:ALA:HB3	2.02	0.42
9:F:107:ASP:O	9:F:111:ILE:HG13	2.20	0.42
12:J:4:ALA:O	12:J:5:GLU:O	2.37	0.42
15:M:123:ASP:OD1	15:M:126:GLN:HG2	2.19	0.42
20:R:39:THR:CG2	20:R:42:GLU:HG3	2.49	0.42
22:T:47:THR:HG22	22:T:99:THR:OG1	2.19	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
1:0:969:G:H1	1:0:999:C:N4	2.17	0.42
1:0:1175:G:H1'	1:0:1193:A:C2'	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1427:A:N6	1:0:1440:U:H1'	2.34	0.42
1:0:1773:G:N2	1:0:1774:G:C8	2.87	0.42
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.20	0.42
1:0:2372:A:H2'	1:0:2373:U:H6	1.84	0.42
1:0:2453:G:H5'	38:0:4985:HOH:O	2.18	0.42
1:0:2728:C:H2'	1:0:2729:C:C6	2.54	0.42
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.19	0.42
5:B:90:THR:C	5:B:92:TYR:H	2.22	0.42
6:C:107:ARG:NE	38:C:9256:HOH:O	2.27	0.42
6:C:124:VAL:HA	6:C:230:GLY:O	2.18	0.42
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.53	0.42
11:H:38:LYS:HE2	11:H:42:ASP:HB2	2.01	0.42
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.02	0.42
16:N:103:ASP:C	16:N:103:ASP:OD1	2.57	0.42
22:T:40:VAL:HA	22:T:119:ALA:O	2.19	0.42
25:W:59:GLN:HE22	25:W:98:PHE:CB	2.30	0.42
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.01	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.72	0.42
1:0:196:G:H2'	38:L:9371:HOH:O	2.18	0.42
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.42
1:0:581:G:O2'	1:0:582:C:H5'	2.19	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.52	0.42
1:0:2415:A:O2'	16:N:29:SER:HB3	2.19	0.42
2:9:3049:G:C2'	2:9:3050:G:H5'	2.50	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.19	0.42
4:A:153:ARG:HD3	38:A:9328:HOH:O	2.18	0.42
4:A:186:TRP:CG	4:A:187:PRO:HA	2.54	0.42
8:E:84:MET:HE3	8:E:148:ILE:HG21	2.02	0.42
12:J:80:LYS:NZ	38:J:9370:HOH:O	2.52	0.42
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.02	0.42
18:P:143:ALA:HA	38:P:190:HOH:O	2.20	0.42
1:0:970:U:H2'	38:0:6568:HOH:O	2.19	0.42
1:0:1185:U:H2'	1:0:1186:C:H6	1.82	0.42
1:0:1562:C:N4	38:0:6127:HOH:O	2.53	0.42
1:0:1587:U:H2'	1:0:1588:G:O4'	2.19	0.42
1:0:2474:A:N6	3:4:176:A:OP2	2.53	0.42
38:0:4910:HOH:O	17:O:35:LYS:HD3	2.20	0.42
2:9:3107:C:H2'	2:9:3108:C:H6	1.83	0.42
7:D:56:ARG:N	38:D:6752:HOH:O	2.53	0.42
8:E:43:ASP:HA	38:E:5864:HOH:O	2.19	0.42
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.42
16:N:163:PHE:O	16:N:164:ASP:O	2.38	0.42
16:N:171:HIS:CE1	38:N:9364:HOH:O	2.73	0.42
18:P:92:GLU:HA	18:P:95:GLU:OE1	2.20	0.42
30:2:36:ASN:O	30:2:39:ARG:HG3	2.19	0.42
1:0:462:A:N3	30:2:37:HIS:HB3	2.35	0.42
1:0:581:G:H5'	38:0:7877:HOH:O	2.19	0.42
1:0:603:A:H4'	1:0:604:G:O5'	2.19	0.42
1:0:1471:A:H2'	1:0:1472:C:C6	2.55	0.42
1:0:2728:C:H2'	1:0:2729:C:H6	1.83	0.42
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.54	0.42
5:B:279:THR:CG2	5:B:280:VAL:N	2.83	0.42
6:C:115:LEU:HD12	6:C:115:LEU:HA	1.92	0.42
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.19	0.42
8:E:107:PHE:CD2	8:E:108:LEU:HD13	2.55	0.42
12:J:22:VAL:O	12:J:26:VAL:HG23	2.20	0.42
13:K:75:ARG:HH21	13:K:94:ALA:CB	2.32	0.42
25:W:84:VAL:HG21	25:W:93:ILE:HG12	2.00	0.42
1:0:371:U:H2'	1:0:372:A:H8	1.85	0.42
1:0:484:A:N1	1:0:506:G:H4'	2.35	0.42
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.42
1:0:1187:U:O2'	1:0:1189:A:H2	1.82	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.42
1:0:2333:G:P	7:D:56:ARG:HH22	2.42	0.42
1:0:2786:G:H2'	38:0:7404:HOH:O	2.20	0.42
4:A:86:ALA:HB3	4:A:94:LEU:HD13	2.02	0.42
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.50	0.42
5:B:210:GLY:HA2	5:B:256:GLN:NE2	2.35	0.42
6:C:173:LYS:O	6:C:186:TYR:HA	2.20	0.42
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.20	0.42
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.38	0.42
24:V:1:THR:HG22	24:V:48:GLU:OE1	2.20	0.42
24:V:12:THR:CG2	24:V:15:GLU:H	2.33	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
1:0:731:U:O2'	1:0:732:C:H5'	2.20	0.42
1:0:1163:G:N2	38:0:6299:HOH:O	2.53	0.42
1:0:1312:G:OP1	27:Y:213:LYS:NZ	2.46	0.42
1:0:1594:C:O2'	1:0:1595:G:H5'	2.20	0.42
1:0:1684:A:O2'	1:0:1685:A:H5''	2.19	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.55	0.42
1:0:2254:G:O2'	1:0:2255:A:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.42
8:E:31:ARG:NH1	8:E:68:HIS:ND1	2.66	0.42
11:H:50:ILE:HG23	11:H:131:GLU:O	2.20	0.42
14:L:133:VAL:HB	38:L:9356:HOH:O	2.18	0.42
28:Z:81:ARG:O	28:Z:82:SER:C	2.57	0.42
1:0:569:A:H5''	1:0:587:A:N1	2.35	0.41
1:0:1878:G:H5''	38:0:3103:HOH:O	2.19	0.41
1:0:2271:G:N3	1:0:2271:G:H2'	2.35	0.41
4:A:93:THR:HA	4:A:154:ALA:O	2.19	0.41
6:C:35:VAL:HG21	6:C:227:GLY:HA2	2.02	0.41
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.19	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.50	0.41
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.53	0.41
27:Y:134:HIS:H	27:Y:134:HIS:CD2	2.38	0.41
1:0:1028:U:H5'	1:0:1031:G:O4'	2.20	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.87	0.41
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.88	0.41
1:0:1593:C:O2'	1:0:1594:C:H5'	2.20	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.41
5:B:279:THR:HG22	5:B:280:VAL:N	2.35	0.41
13:K:132:VAL:O	13:K:132:VAL:HG12	2.20	0.41
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.20	0.41
15:M:182:LYS:NZ	38:M:9325:HOH:O	2.53	0.41
16:N:181:ASP:O	16:N:184:ILE:HG22	2.20	0.41
25:W:21:LEU:HD21	25:W:48:VAL:HG13	2.01	0.41
1:0:288:A:H61	1:0:364:C:H42	1.69	0.41
1:0:705:C:O2	1:0:705:C:H2'	2.20	0.41
1:0:1776:A:C8	1:0:1778:A:O4'	2.73	0.41
1:0:2541:U:O2'	1:0:2542:C:H5'	2.19	0.41
1:0:2754:G:O2'	1:0:2755:G:H5'	2.20	0.41
1:0:2780:C:H2'	1:0:2781:U:H6	1.84	0.41
4:A:179:MET:HG2	4:A:186:TRP:CG	2.55	0.41
5:B:53:LEU:HD11	5:B:327:VAL:HG22	2.01	0.41
5:B:87:TYR:OH	5:B:163:GLU:OE2	2.27	0.41
5:B:168:GLY:H	5:B:174:ARG:HD2	1.85	0.41
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.43	0.41
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HD2	30:2:49:GLU:N	2.34	0.41
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.20	0.41
32:I:129:VAL:O	32:I:129:VAL:HG12	2.21	0.41
1:0:2269:C:C2'	1:0:2270:G:H5'	2.50	0.41
1:0:2832:C:H5	38:0:7429:HOH:O	2.03	0.41
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.34	0.41
5:B:247:VAL:HG13	5:B:251:VAL:HG11	2.03	0.41
12:J:45:VAL:CG2	12:J:46:ILE:N	2.83	0.41
14:L:128:GLY:O	14:L:132:LYS:HG3	2.20	0.41
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	2.02	0.41
29:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.20	0.41
1:0:1044:C:H5''	38:0:9342:HOH:O	2.21	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.09	0.41
1:0:1180:U:H2'	1:0:1181:A:O4'	2.21	0.41
1:0:1921:A:O2'	1:0:1922:A:H5'	2.20	0.41
1:0:2072:G:H3'	1:0:2073:G:C5'	2.51	0.41
1:0:2464:C:H5''	1:0:2465:A:OP1	2.20	0.41
1:0:2670:G:O2'	1:0:2671:U:H5'	2.21	0.41
38:9:1056:HOH:O	16:N:7:LYS:HE2	2.21	0.41
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.85	0.41
11:H:80:GLU:HA	38:H:9182:HOH:O	2.20	0.41
14:L:34:GLY:C	14:L:36:ASP:H	2.24	0.41
14:L:140:VAL:O	14:L:140:VAL:HG12	2.19	0.41
16:N:154:LEU:O	16:N:155:GLU:CB	2.68	0.41
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.21	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
23:U:6:CYS:HA	23:U:13:ILE:HD11	2.03	0.41
25:W:13:MET:CE	25:W:18:GLN:HA	2.51	0.41
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.41
26:X:7:GLU:HA	26:X:74:ALA:O	2.19	0.41
31:3:30:GLN:HE21	31:3:30:GLN:HB3	1.61	0.41
1:0:1006:A:N1	1:0:2311:A:H1'	2.35	0.41
1:0:1355:A:H2'	38:0:4429:HOH:O	2.21	0.41
1:0:1477:C:H5'	1:0:1868:G:H5''	2.03	0.41
1:0:2564:G:OP2	1:0:2565:C:H5''	2.21	0.41
1:0:2812:A:C2	1:0:2814:A:N6	2.75	0.41
1:0:2842:G:H2'	1:0:2843:A:H5'	2.03	0.41
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.13	0.41
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.85	0.41
6:C:130:GLU:OE1	6:C:130:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:16:ASP:O	8:E:17:HIS:HB2	2.19	0.41
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.41
16:N:37:ARG:NH2	38:N:9331:HOH:O	2.53	0.41
1:0:120:A:N3	1:0:120:A:H2'	2.36	0.41
1:0:204:A:C2'	1:0:205:U:H5'	2.51	0.41
1:0:250:C:H2'	1:0:251:C:C6	2.55	0.41
1:0:825:U:H5''	1:0:826:U:OP1	2.21	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.56	0.41
1:0:1762:C:H4'	38:0:4949:HOH:O	2.19	0.41
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.41
1:0:2379:G:N7	1:0:2408:A:N1	2.68	0.41
1:0:2455:A:H2'	1:0:2456:A:O4'	2.20	0.41
1:0:2668:G:H2'	1:0:2669:U:C6	2.56	0.41
1:0:2735:U:H2'	1:0:2736:U:C6	2.55	0.41
38:0:7175:HOH:O	19:Q:16:ASN:HB2	2.21	0.41
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.41
5:B:217:ARG:CG	5:B:257:THR:HG22	2.48	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.20	0.41
7:D:27:ILE:HG22	7:D:28:GLY:N	2.34	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.03	0.41
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.36	0.41
11:H:51:VAL:HG21	11:H:127:VAL:HG11	2.03	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.44	0.41
1:0:377:C:H5	38:0:3616:HOH:O	2.03	0.41
1:0:451:C:O2'	1:0:452:G:H5'	2.21	0.41
1:0:1307:A:H2'	1:0:1308:A:C8	2.56	0.41
1:0:2255:A:C6	1:0:2256:G:C5	3.09	0.41
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.90	0.41
5:B:184:ASP:HB2	5:B:185:GLY:H	1.71	0.41
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.03	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.91	0.41
17:O:81:PHE:CD1	17:O:81:PHE:N	2.88	0.41
18:P:59:ARG:O	18:P:63:ARG:HG3	2.21	0.41
25:W:5:VAL:HG11	25:W:153:MET:CE	2.51	0.41
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.20	0.41
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.55	0.41
32:I:132:CYS:O	32:I:135:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:200:U:O2'	1:0:201:G:H5'	2.21	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:432:G:O2'	1:0:433:C:H5'	2.20	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.36	0.41
1:0:645:U:O2	1:0:761:A:H2	2.04	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.35	0.41
1:0:894:A:C2	6:C:87:ARG:NH2	2.88	0.41
1:0:1119:G:P	12:J:49:ARG:HH11	2.44	0.41
1:0:1386:G:O2'	1:0:1387:G:H5'	2.21	0.41
1:0:1396:C:H4'	18:P:2:ASP:OD1	2.21	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.21	0.41
1:0:1778:A:H2'	1:0:1779:A:H5'	2.02	0.41
1:0:2079:G:H2'	1:0:2080:G:O4'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.41
4:A:36:ASP:C	4:A:38:ILE:N	2.71	0.41
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.85	0.41
6:C:19:PRO:HG2	6:C:22:PHE:CD1	2.56	0.41
6:C:39:GLN:O	6:C:43:LYS:HD3	2.20	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.03	0.41
8:E:75:GLY:HA2	8:E:79:GLY:HA2	2.03	0.41
9:F:111:ILE:O	9:F:115:VAL:HG23	2.21	0.41
10:G:12:ILE:HG13	38:G:6833:HOH:O	2.21	0.41
12:J:39:VAL:CG1	12:J:40:ASN:N	2.84	0.41
12:J:131:THR:CG2	12:J:134:GLU:HG3	2.51	0.41
13:K:10:GLN:NE2	13:K:10:GLN:N	2.43	0.41
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.55	0.41
15:M:65:VAL:HG21	15:M:105:ALA:HB2	2.03	0.41
18:P:115:SER:C	18:P:117:SER:N	2.74	0.41
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.55	0.41
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.20	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.86	0.41
22:T:19:ARG:NH1	22:T:68:ASP:O	2.54	0.41
23:U:49:LEU:HG	38:U:3805:HOH:O	2.20	0.41
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.85	0.41
1:0:710:G:OP1	17:O:24:ALA:HB3	2.21	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.56	0.41
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
2:9:3041:C:H5''	7:D:48:MET:SD	2.61	0.41
5:B:57:GLU:OE1	5:B:60:SER:HB2	2.21	0.41
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.51	0.41
6:C:77:ALA:O	6:C:78:ARG:HG3	2.21	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.56	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
11:H:99:LYS:CG	11:H:119:LYS:HD3	2.51	0.41
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.53	0.41
15:M:72:ALA:HB2	15:M:93:ARG:HG2	2.03	0.41
22:T:41:ARG:O	22:T:43:ASN:ND2	2.53	0.41
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.21	0.41
1:0:353:G:O2'	1:0:354:A:H5'	2.22	0.40
1:0:475:G:H5'	6:C:73:LEU:CD2	2.50	0.40
1:0:542:A:O2'	1:0:543:G:H5'	2.21	0.40
1:0:907:A:H4'	1:0:1328:A:C2	2.56	0.40
1:0:1370:G:O5'	20:R:62:HIS:HB3	2.21	0.40
1:0:1543:G:N1	1:0:1641:A:OP2	2.41	0.40
1:0:1682:A:H5''	38:0:9769:HOH:O	2.20	0.40
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.40
1:0:2615:U:C5	1:0:2616:G:C6	3.09	0.40
38:0:4650:HOH:O	25:W:14:HIS:HA	2.20	0.40
2:9:3033:U:H2'	38:9:3797:HOH:O	2.21	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
8:E:73:PHE:O	8:E:76:VAL:HG22	2.21	0.40
11:H:154:TYR:C	11:H:154:TYR:HD1	2.24	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.63	0.40
15:M:164:THR:HG22	15:M:166:ALA:N	2.36	0.40
16:N:164:ASP:CG	16:N:167:ASP:HA	2.39	0.40
1:0:10:U:H1'	1:0:532:A:H62	1.86	0.40
1:0:354:A:H2'	1:0:355:C:C6	2.56	0.40
1:0:474:C:O2'	6:C:73:LEU:HD21	2.21	0.40
1:0:702:G:O2'	1:0:703:G:H5'	2.22	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
1:0:1730:G:N3	1:0:1730:G:H2'	2.36	0.40
1:0:1739:G:O2'	1:0:1740:U:H5'	2.21	0.40
1:0:2506:A:O2'	1:0:2507:G:P	2.79	0.40
1:0:2690:U:H4'	8:E:111:LYS:CE	2.51	0.40
1:0:2765:C:H2'	1:0:2766:A:H8	1.87	0.40
4:A:30:ARG:HE	4:A:30:ARG:HB3	1.73	0.40
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:86:THR:HG23	38:D:7477:HOH:O	2.21	0.40
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.56	0.40
16:N:63:SER:HB2	16:N:75:THR:HB	2.03	0.40
16:N:101:VAL:HG12	38:N:9327:HOH:O	2.22	0.40
16:N:157:PRO:HA	38:N:9322:HOH:O	2.21	0.40
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.04	0.40
20:R:99:ALA:CB	20:R:109:MET:CE	2.95	0.40
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.41	0.40
23:U:35:LYS:HE2	23:U:51:TRP:CH2	2.56	0.40
27:Y:197:ASP:C	27:Y:197:ASP:OD1	2.60	0.40
1:O:566:A:H2'	1:O:567:U:O4'	2.21	0.40
1:O:999:C:H2'	1:O:1000:C:O4'	2.21	0.40
1:O:1139:U:H2'	1:O:1140:C:H6	1.85	0.40
1:O:1613:C:H2'	1:O:1614:G:O4'	2.21	0.40
1:O:1985:U:C2	1:O:1996:U:O4'	2.75	0.40
1:O:2061:C:H2'	1:O:2062:A:H5'	2.04	0.40
1:O:2453:G:H4'	14:L:50:GLY:C	2.41	0.40
1:O:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
4:A:194:MET:CE	4:A:199:HIS:HB2	2.51	0.40
4:A:223:ARG:CZ	38:A:9317:HOH:O	2.69	0.40
5:B:53:LEU:HD12	5:B:327:VAL:HA	2.04	0.40
7:D:104:PHE:CE2	7:D:166:ILE:CD1	3.04	0.40
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.93	0.40
8:E:87:PHE:O	8:E:93:MET:HE3	2.21	0.40
12:J:51:GLU:O	12:J:55:GLU:HG3	2.20	0.40
12:J:130:VAL:CG1	12:J:131:THR:N	2.85	0.40
16:N:67:ALA:O	16:N:69:TYR:N	2.54	0.40
18:P:135:ALA:O	18:P:139:ARG:HG3	2.22	0.40
20:R:76:ASP:OD1	20:R:76:ASP:N	2.53	0.40
23:U:37:GLU:O	23:U:40:ALA:HB3	2.22	0.40
25:W:85:ALA:HB2	25:W:91:ASP:O	2.21	0.40
1:O:338:C:H4'	6:C:174:ILE:HD12	2.03	0.40
1:O:601:G:O2'	1:O:602:A:H5'	2.21	0.40
1:O:615:G:H2'	1:O:616:U:C6	2.56	0.40
1:O:1079:A:H4'	1:O:2078:U:H5'	2.04	0.40
1:O:1158:G:O2'	1:O:1159:G:H5'	2.21	0.40
1:O:1194:A:C2'	1:O:1195:G:H5'	2.51	0.40
1:O:1196:C:H2'	1:O:1197:G:H5'	2.04	0.40
1:O:1311:G:C2	1:O:1312:G:C8	3.09	0.40
1:O:2067:A:H2'	1:O:2068:G:O4'	2.21	0.40
1:O:2456:A:H2'	1:O:2457:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3034:A:H2'	2:9:3035:C:O4'	2.21	0.40
5:B:175:LEU:HD23	5:B:175:LEU:O	2.21	0.40
11:H:20:ILE:CG2	11:H:120:ILE:HD11	2.52	0.40
11:H:63:GLU:OE1	11:H:66:ARG:NH1	2.54	0.40
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.40
14:L:125:PHE:CE2	14:L:140:VAL:HG22	2.56	0.40
21:S:81:ILE:HG12	38:S:9134:HOH:O	2.21	0.40
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.94	0.40
28:Z:67:GLY:N	28:Z:70:LYS:O	2.54	0.40
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.62	0.40
1:0:912:A:C4	1:0:1294:A:C2	3.10	0.40
1:0:1335:C:H2'	1:0:1336:U:C6	2.57	0.40
1:0:2093:G:H5''	38:B:9326:HOH:O	2.21	0.40
4:A:65:ARG:C	4:A:66:ARG:HG3	2.42	0.40
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	2.04	0.40
5:B:76:THR:N	5:B:77:PRO:HD3	2.37	0.40
5:B:307:ARG:HH11	5:B:307:ARG:CG	2.35	0.40
5:B:316:ARG:N	5:B:317:PRO:HD3	2.37	0.40
7:D:173:GLU:CG	7:D:174:VAL:H	2.35	0.40
8:E:102:VAL:HG11	8:E:148:ILE:HG12	2.03	0.40
11:H:88:ARG:H	11:H:88:ARG:HG2	1.68	0.40
12:J:39:VAL:HG12	12:J:40:ASN:CG	2.42	0.40
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.22	0.40
20:R:61:GLN:CD	38:R:9338:HOH:O	2.60	0.40
20:R:106:GLY:HA2	20:R:109:MET:HE3	2.02	0.40
25:W:130:HIS:O	25:W:136:GLY:HA3	2.22	0.40
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.34	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	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	9	16
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	8	14
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	34	54
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	1	1
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100	100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	2	2
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	8	13
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	11	20
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	6	10
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	5	7
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	3	4
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	17	31
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	22	39
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17	31
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4	5
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	22	39
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	12	21
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	5	7
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	6	9
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	6	10
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	10	18
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	9	17

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	34	GLY
5	B	139	ASP
5	B	184	ASP
7	D	173	GLU
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	81	ARG
32	I	138	THR
4	A	34	ASP
4	A	132	ASP
6	C	8	LEU
7	D	27	ILE
14	L	80	ASP
16	N	164	ASP
31	3	57	GLY
5	B	169	GLY
7	D	137	PRO
7	D	171	ASP
9	F	61	MET
13	K	39	GLY
13	K	126	SER
14	L	143	THR
16	N	167	ASP
17	O	108	GLY
22	T	53	GLY
24	V	43	PRO
25	W	49	ASN
30	2	37	HIS
31	3	56	PRO
5	B	2	GLN
7	D	16	PRO
7	D	28	GLY
7	D	65	GLU
7	D	97	GLN
7	D	147	ALA
12	J	143	LYS

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Mol	Chain	Res	Type
13	K	111	GLY
16	N	65	ASP
26	X	78	GLU
28	Z	43	GLY
5	B	67	GLU
9	F	44	SER
9	F	64	PRO
11	H	140	VAL
14	L	11	ARG
14	L	35	ARG
16	N	68	GLU
18	P	116	SER
9	F	100	ASP
9	F	104	ALA
7	D	69	ILE
24	V	40	PRO

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	A	179/182 (98%)	170 (95%)	9 (5%)	24	46
5	B	282/283 (100%)	266 (94%)	16 (6%)	20	39
6	C	193/193 (100%)	178 (92%)	15 (8%)	12	24
7	D	117/148 (79%)	111 (95%)	6 (5%)	24	45
8	E	152/156 (97%)	151 (99%)	1 (1%)	84	94
9	F	93/94 (99%)	93 (100%)	0	100	100
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	124 (94%)	8 (6%)	18	36
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	25
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	58
14	L	113/127 (89%)	107 (95%)	6 (5%)	22	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	M	158/158 (100%)	153 (97%)	5 (3%)	39	65
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	49
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	53
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	71
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	58
20	R	117/122 (96%)	115 (98%)	2 (2%)	60	82
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	86
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	39
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	32	57
25	W	130/130 (100%)	126 (97%)	4 (3%)	40	67
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	36
27	Y	120/196 (61%)	112 (93%)	8 (7%)	16	31
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	74
31	3	79/79 (100%)	77 (98%)	2 (2%)	47	73
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2967 (96%)	126 (4%)	30	55

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	36	ASP
4	A	69	LEU
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN

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Mol	Chain	Res	Type
5	B	53	LEU
5	B	97	LEU
5	B	139	ASP
5	B	162	MET
5	B	195	ARG
5	B	234	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	131	PHE
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	86	THR
7	D	133	ASN
7	D	136	ARG
7	D	149	ARG
8	E	164	ASP
11	H	18	GLU
11	H	30	GLN
11	H	62	LEU
11	H	84	LYS
11	H	88	ARG
11	H	111	ASP
11	H	154	TYR
11	H	170	ASN

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Mol	Chain	Res	Type
12	J	46	ILE
12	J	47	THR
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	99	GLU
14	L	102	ASP
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	47	LEU
16	N	49	THR
16	N	135	VAL
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	98	LEU
17	O	115	ARG
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR

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Mol	Chain	Res	Type
20	R	39	THR
21	S	53	ASN
22	T	39	ASN
22	T	48	VAL
22	T	73	HIS
22	T	89	ARG
22	T	96	VAL
22	T	112	LEU
24	V	43	PRO
24	V	65	ASP
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	72	VAL
26	X	79	GLU
27	Y	117	LEU
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	191	ASP
27	Y	200	THR
27	Y	235	GLU
30	2	18	ASN
31	3	56	PRO
31	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	92	ASN
4	A	125	ASN
4	A	127	GLN
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN

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Mol	Chain	Res	Type
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	71	ASN
8	E	90	HIS
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	132	GLN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN

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Mol	Chain	Res	Type
20	R	113	HIS
20	R	117	HIS
20	R	123	GLN
21	S	9	HIS
21	S	25	GLN
21	S	53	ASN
22	T	39	ASN
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	2	HIS
25	W	6	GLN
25	W	27	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	98	GLN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	251 (8%)	33 (1%)

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G

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Mol	Chain	Res	Type
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	905	C
1	0	920	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

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Mol	Chain	Res	Type
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G

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Mol	Chain	Res	Type
1	0	1980	U
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A

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Mol	Chain	Res	Type
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A

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Mol	Chain	Res	Type
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	87	C
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	0	2588	3,1	18,26,27	1.04	2 (11%)	19,38,41	0.71	1 (5%)
1	OMU	0	2587	1	19,22,23	0.24	0	26,31,34	0.35	0
1	1MA	0	628	1	16,25,26	1.37	3 (18%)	18,37,40	1.15	2 (11%)
3	5AA	4	76	3,1	18,26,27	1.09	1 (5%)	15,38,41	0.80	1 (6%)
1	PSU	0	2621	1	18,21,22	1.49	2 (11%)	22,30,33	1.31	3 (13%)
1	UR3	0	2619	1	19,22,23	0.36	0	26,32,35	0.66	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	3,1	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	5AA	4	76	3,1	-	0/7/29/30	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.97	1.43	1.36
1	0	628	1MA	C2-N3	3.67	1.33	1.29
3	4	76	5AA	C3'-N3'	-3.38	1.42	1.47
1	0	628	1MA	C6-N6	2.67	1.34	1.27
1	0	2621	PSU	C6-C5	2.59	1.38	1.35
1	0	2588	OMG	C8-N7	-2.54	1.30	1.35
1	0	2588	OMG	C5-C6	-2.46	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	628	1MA	C8-N7	-2.05	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.66	120.75	118.20
1	0	2621	PSU	C6-N1-C2	-3.02	119.60	122.68
1	0	628	1MA	N1-C2-N3	2.83	129.32	126.02
1	0	2621	PSU	O2-C2-N1	2.61	125.66	122.79
1	0	628	1MA	C5-C6-N1	2.46	117.56	113.90
1	0	2619	UR3	C4-N3-C2	2.45	126.88	124.56
1	0	2588	OMG	O6-C6-C5	2.10	128.48	124.37
3	4	76	5AA	C9-N6-C6	2.01	125.59	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	0	2749/2922 (94%)	-0.49	48 (1%) 70 72	24, 49, 93, 155	0
2	9	122/122 (100%)	-0.29	5 (4%) 37 40	45, 66, 91, 152	0
3	4	5/8 (62%)	-0.71	0 100 100	41, 45, 47, 49	0
4	A	237/240 (98%)	0.39	17 (7%) 15 16	30, 51, 89, 114	0
5	B	337/338 (99%)	0.30	11 (3%) 46 50	31, 61, 90, 100	0
6	C	246/246 (100%)	-0.05	4 (1%) 72 74	28, 48, 71, 82	0
7	D	140/177 (79%)	2.54	74 (52%) 0 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.10	27 (15%) 2 1	52, 76, 101, 111	0
9	F	119/120 (99%)	0.99	27 (22%) 0 0	52, 74, 100, 116	0
10	G	29/348 (8%)	2.64	19 (65%) 0 0	74, 92, 104, 108	0
11	H	160/171 (93%)	0.39	8 (5%) 28 30	42, 60, 91, 100	0
12	J	142/145 (97%)	0.13	0 100 100	40, 56, 76, 99	0
13	K	132/132 (100%)	0.20	3 (2%) 60 63	35, 58, 80, 85	0
14	L	145/165 (87%)	0.85	28 (19%) 1 1	28, 69, 114, 127	0
15	M	194/194 (100%)	0.04	2 (1%) 82 84	32, 43, 59, 66	0
16	N	186/187 (99%)	0.84	36 (19%) 1 1	40, 64, 113, 119	0
17	O	115/116 (99%)	0.15	3 (2%) 56 59	39, 58, 75, 90	0
18	P	143/149 (95%)	0.30	5 (3%) 44 47	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.14	2 (2%) 63 66	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.07	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.19	2 (2%) 57 61	45, 59, 78, 88	0
22	T	119/120 (99%)	0.42	3 (2%) 57 61	40, 58, 85, 96	0
23	U	53/66 (80%)	0.28	2 (3%) 40 43	46, 62, 76, 86	0
24	V	65/71 (91%)	1.62	22 (33%) 0 0	56, 76, 112, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.07	0 100 100	39, 55, 74, 86	0
26	X	82/92 (89%)	0.65	12 (14%) 2 2	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.27	8 (5%) 24 25	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.18	5 (6%) 17 17	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.35	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.61	14 (30%) 0 0	36, 65, 120, 122	0
31	3	92/92 (100%)	0.32	5 (5%) 25 27	35, 55, 71, 87	0
32	I	70/162 (43%)	4.52	59 (84%) 0 0	108, 126, 148, 149	0
All	All	6651/7482 (88%)	0.11	451 (6%) 17 17	24, 55, 103, 155	0

All (451) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	96	PHE	15.2
32	I	133	THR	13.6
24	V	1	THR	13.1
32	I	102	VAL	12.5
32	I	93	GLN	11.6
7	D	63	ILE	9.7
30	2	38	LYS	9.3
16	N	166	ALA	9.2
2	9	3001	U	9.0
7	D	88	LEU	8.7
32	I	116	LEU	8.7
7	D	69	ILE	8.4
32	I	71	GLY	8.3
10	G	23	ILE	8.2
32	I	79	ILE	8.0
10	G	27	ILE	7.5
32	I	117	LEU	7.4
7	D	57	THR	7.4
32	I	109	ALA	7.4
7	D	26	GLY	7.3
24	V	39	ALA	7.3
30	2	41	HIS	7.2
7	D	44	ILE	7.2
7	D	64	ARG	7.0
4	A	37	VAL	6.9
32	I	113	HIS	6.9

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Mol	Chain	Res	Type	RSRZ
24	V	40	PRO	6.8
32	I	137	VAL	6.7
7	D	84	LEU	6.6
32	I	118	SER	6.6
24	V	38	GLY	6.5
32	I	75	THR	6.5
7	D	85	GLN	6.4
30	2	44	ARG	6.4
7	D	58	VAL	6.2
32	I	105	VAL	6.2
7	D	172	VAL	6.2
7	D	170	TYR	6.1
7	D	61	PHE	6.0
32	I	88	GLY	5.9
7	D	66	GLY	5.8
32	I	85	PHE	5.8
32	I	103	ASP	5.6
30	2	42	TRP	5.5
10	G	24	VAL	5.5
32	I	111	GLN	5.5
7	D	75	LEU	5.5
32	I	77	GLU	5.5
30	2	45	ASN	5.3
30	2	48	ASP	5.3
1	0	2237	G	5.3
30	2	49	GLU	5.3
7	D	10	PHE	5.3
30	2	37	HIS	5.3
24	V	43	PRO	5.2
26	X	88	GLU	5.2
2	9	3024	U	5.2
32	I	129	VAL	5.1
1	0	1173	A	5.1
7	D	23	VAL	5.1
8	E	42	VAL	5.1
7	D	41	LEU	5.1
8	E	44	GLY	5.0
7	D	40	ILE	4.9
2	9	3023	U	4.8
32	I	119	TYR	4.8
7	D	87	ALA	4.8
32	I	115	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
32	I	81	ASP	4.7
32	I	114	PRO	4.7
32	I	94	GLU	4.6
7	D	165	PHE	4.6
32	I	126	LYS	4.6
32	I	92	PRO	4.5
7	D	56	ARG	4.5
32	I	74	PRO	4.5
16	N	159	TYR	4.4
32	I	78	LEU	4.4
1	0	1177	A	4.4
1	0	960	G	4.4
32	I	97	VAL	4.4
16	N	160	SER	4.4
1	0	282	C	4.3
32	I	72	VAL	4.3
4	A	31	LYS	4.3
21	S	81	ILE	4.3
7	D	98	PHE	4.3
7	D	68	PRO	4.3
11	H	73	LEU	4.3
7	D	90	LEU	4.2
1	0	1172	G	4.2
32	I	106	LYS	4.2
1	0	2238	A	4.2
7	D	18	ILE	4.2
9	F	17	LEU	4.2
10	G	71	LEU	4.2
14	L	97	VAL	4.1
32	I	89	SER	4.1
9	F	119	ARG	4.1
32	I	121	LEU	4.1
24	V	37	GLY	4.1
7	D	89	PRO	4.1
7	D	51	ARG	4.1
30	2	39	ARG	4.1
30	2	36	ASN	4.0
7	D	65	GLU	4.0
14	L	106	VAL	4.0
16	N	67	ALA	4.0
14	L	60	GLU	4.0
24	V	41	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
7	D	166	ILE	4.0
8	E	11	VAL	4.0
8	E	87	PHE	4.0
16	N	152	GLU	4.0
7	D	86	THR	4.0
32	I	136	GLY	4.0
1	0	970	U	3.9
32	I	73	PRO	3.9
30	2	47	THR	3.9
10	G	26	MET	3.9
32	I	76	ALA	3.9
7	D	59	GLY	3.9
7	D	62	ASP	3.9
32	I	107	GLN	3.9
1	0	1951	G	3.8
32	I	91	GLU	3.8
7	D	128	LEU	3.8
9	F	16	ALA	3.8
7	D	49	PRO	3.8
7	D	106	PHE	3.8
7	D	92	GLU	3.8
7	D	93	LEU	3.8
16	N	158	LEU	3.8
7	D	104	PHE	3.8
7	D	27	ILE	3.7
32	I	139	ILE	3.7
7	D	134	LEU	3.7
32	I	135	LEU	3.7
1	0	1199	A	3.7
14	L	80	ASP	3.7
32	I	95	ASP	3.7
32	I	125	ALA	3.7
8	E	76	VAL	3.6
9	F	106	ALA	3.6
14	L	105	TYR	3.6
1	0	1171	A	3.6
27	Y	236	VAL	3.6
1	0	1525	G	3.6
8	E	100	ASP	3.6
7	D	81	GLU	3.6
27	Y	235	GLU	3.6
32	I	104	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
7	D	73	VAL	3.6
4	A	35	GLY	3.6
7	D	135	VAL	3.6
8	E	8	PRO	3.5
7	D	25	MET	3.5
9	F	45	ALA	3.5
32	I	98	ALA	3.5
8	E	88	TYR	3.5
7	D	70	GLY	3.5
1	0	10	U	3.5
32	I	132	CYS	3.5
8	E	45	ASP	3.5
9	F	117	GLU	3.4
30	2	43	ARG	3.4
9	F	44	SER	3.4
32	I	128	VAL	3.4
5	B	119	HIS	3.4
26	X	41	PHE	3.4
17	O	22	GLY	3.4
7	D	71	ALA	3.4
14	L	142	LEU	3.3
16	N	175	LEU	3.3
32	I	86	GLU	3.3
32	I	138	THR	3.3
1	0	735	C	3.3
7	D	167	GLU	3.3
23	U	47	ARG	3.3
4	A	36	ASP	3.3
11	H	45	VAL	3.3
14	L	149	ARG	3.3
14	L	104	ASP	3.2
16	N	164	ASP	3.2
24	V	8	ILE	3.2
4	A	85	SER	3.2
1	0	1279	U	3.2
26	X	85	VAL	3.2
16	N	149	GLU	3.2
27	Y	98	GLN	3.2
26	X	71	ARG	3.2
7	D	130	VAL	3.2
32	I	110	GLU	3.1
7	D	29	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
16	N	148	ALA	3.1
26	X	10	VAL	3.1
9	F	49	PHE	3.1
32	I	122	THR	3.1
14	L	96	VAL	3.1
7	D	17	ARG	3.1
9	F	22	VAL	3.1
1	0	280	C	3.0
32	I	124	ALA	3.0
11	H	37	GLN	3.0
18	P	114	LEU	3.0
14	L	130	ARG	3.0
4	A	38	ILE	3.0
16	N	143	ARG	3.0
7	D	157	LEU	3.0
16	N	157	PRO	3.0
7	D	171	ASP	3.0
7	D	45	THR	3.0
9	F	103	GLU	3.0
9	F	26	THR	3.0
30	2	20	ARG	2.9
10	G	73	ASP	2.9
10	G	20	VAL	2.9
1	0	2004	U	2.9
30	2	35	ARG	2.9
14	L	145	LEU	2.9
6	C	61	PHE	2.9
26	X	72	VAL	2.9
26	X	80	GLU	2.9
7	D	24	HIS	2.9
22	T	35	TYR	2.9
4	A	33	GLU	2.8
9	F	18	GLU	2.8
14	L	102	ASP	2.8
8	E	48	VAL	2.8
7	D	53	LYS	2.8
14	L	150	GLN	2.8
26	X	77	PHE	2.8
32	I	108	ILE	2.8
22	T	119	ALA	2.8
8	E	5	LEU	2.8
8	E	108	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
9	F	12	LEU	2.8
14	L	76	LEU	2.8
16	N	154	LEU	2.8
14	L	133	VAL	2.8
10	G	67	LEU	2.8
14	L	120	LEU	2.8
1	0	2254	G	2.8
10	G	28	GLU	2.8
5	B	181	ILE	2.8
14	L	121	ILE	2.8
1	0	2769	C	2.8
8	E	10	ASP	2.8
26	X	73	ARG	2.8
1	0	272	A	2.8
1	0	2508	C	2.8
16	N	180	LEU	2.8
4	A	34	ASP	2.8
1	0	370	G	2.8
22	T	112	LEU	2.8
16	N	140	GLN	2.7
8	E	118	ILE	2.7
32	I	87	THR	2.7
1	0	2250	G	2.7
7	D	55	LYS	2.7
1	0	497	A	2.7
2	9	3122	C	2.7
16	N	182	GLY	2.7
1	0	283	U	2.7
14	L	81	VAL	2.7
24	V	33	VAL	2.7
16	N	139	TRP	2.7
11	H	146	VAL	2.7
5	B	106	HIS	2.7
9	F	107	ASP	2.7
31	3	92	GLU	2.6
24	V	59	ILE	2.6
16	N	138	ASP	2.6
4	A	32	VAL	2.6
16	N	95	ALA	2.6
4	A	237	GLY	2.6
24	V	3	LEU	2.6
7	D	94	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
9	F	108	VAL	2.6
27	Y	95	THR	2.6
5	B	105	PHE	2.6
18	P	141	ILE	2.6
1	0	999	C	2.6
16	N	183	ASP	2.6
8	E	7	ILE	2.6
6	C	135	GLU	2.6
7	D	48	MET	2.6
7	D	129	ASP	2.6
9	F	19	ALA	2.6
14	L	108	VAL	2.6
27	Y	108	ASP	2.6
4	A	97	ALA	2.6
9	F	98	VAL	2.6
1	0	1169	U	2.6
2	9	3002	U	2.6
1	0	1163	G	2.6
4	A	133	ARG	2.6
1	0	2251	G	2.5
1	0	284	C	2.5
7	D	173	GLU	2.5
7	D	164	ALA	2.5
1	0	2850	C	2.5
10	G	66	LEU	2.5
16	N	68	GLU	2.5
1	0	281	U	2.5
1	0	1198	U	2.5
28	Z	11	SER	2.5
18	P	71	TYR	2.5
7	D	11	HIS	2.5
11	H	47	ILE	2.5
7	D	47	GLN	2.5
23	U	54	THR	2.5
32	I	100	LEU	2.5
1	0	285	A	2.5
24	V	36	ALA	2.5
8	E	95	VAL	2.5
8	E	161	VAL	2.5
9	F	118	LEU	2.5
1	0	1179	C	2.5
10	G	69	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
28	Z	59	TYR	2.4
32	I	112	LYS	2.4
5	B	117	GLU	2.4
10	G	25	GLU	2.4
24	V	9	ARG	2.4
11	H	50	ILE	2.4
16	N	155	GLU	2.4
8	E	170	ARG	2.4
1	0	2239	C	2.4
8	E	128	GLY	2.4
9	F	20	LEU	2.4
14	L	118	LEU	2.4
7	D	67	ASP	2.4
28	Z	21	VAL	2.4
16	N	150	TYR	2.4
7	D	83	PHE	2.4
28	Z	20	ARG	2.4
31	3	22	VAL	2.4
1	0	1625	U	2.4
8	E	126	ILE	2.4
24	V	46	ILE	2.4
14	L	125	PHE	2.4
1	0	1162	G	2.4
10	G	65	THR	2.4
24	V	45	ARG	2.4
7	D	43	GLU	2.4
16	N	147	ILE	2.4
16	N	145	ALA	2.4
4	A	94	LEU	2.4
5	B	1	PRO	2.3
31	3	1	MET	2.3
16	N	165	ALA	2.3
16	N	162	ASP	2.3
16	N	184	ILE	2.3
7	D	80	ALA	2.3
15	M	194	ALA	2.3
19	Q	95	GLU	2.3
7	D	105	SER	2.3
1	0	1000	C	2.3
14	L	100	ALA	2.3
10	G	21	ASP	2.3
1	0	1948	G	2.3

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Mol	Chain	Res	Type	RSRZ
24	V	2	VAL	2.3
9	F	99	THR	2.3
4	A	96	LEU	2.3
5	B	104	GLU	2.3
19	Q	76	VAL	2.2
32	I	84	GLY	2.2
14	L	99	GLU	2.2
8	E	93	MET	2.2
14	L	73	VAL	2.2
27	Y	96	GLU	2.2
5	B	123	ALA	2.2
17	O	24	ALA	2.2
9	F	47	LEU	2.2
10	G	15	TRP	2.2
4	A	82	VAL	2.2
7	D	72	LYS	2.2
31	3	13	HIS	2.2
27	Y	97	LEU	2.2
16	N	181	ASP	2.2
26	X	9	VAL	2.2
5	B	35	GLN	2.2
21	S	20	PHE	2.2
1	0	1190	G	2.2
9	F	109	GLU	2.2
18	P	77	ALA	2.2
24	V	52	ALA	2.2
26	X	74	ALA	2.2
6	C	132	ASP	2.2
1	0	2249	G	2.2
7	D	50	VAL	2.2
10	G	12	ILE	2.2
11	H	74	ILE	2.2
10	G	63	ARG	2.2
1	0	372	A	2.2
31	3	2	GLN	2.1
9	F	15	ASP	2.1
9	F	100	ASP	2.1
10	G	72	ASP	2.1
32	I	120	ASP	2.1
18	P	67	LYS	2.1
24	V	11	MET	2.1
10	G	70	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
13	K	132	VAL	2.1
14	L	91	VAL	2.1
14	L	93	VAL	2.1
28	Z	24	ARG	2.1
8	E	6	GLU	2.1
15	M	164	THR	2.1
1	0	1950	G	2.1
16	N	172	PHE	2.1
16	N	186	LEU	2.1
14	L	144	ASP	2.1
1	0	1130	U	2.1
24	V	49	LEU	2.1
4	A	65	ARG	2.1
8	E	2	ARG	2.1
13	K	101	ASN	2.1
24	V	44	GLY	2.1
1	0	1180	U	2.1
14	L	61	ALA	2.1
17	O	111	VAL	2.1
7	D	74	THR	2.1
8	E	46	THR	2.1
16	N	178	THR	2.1
6	C	237	GLU	2.1
16	N	179	LEU	2.1
8	E	72	MET	2.1
1	0	138	U	2.1
8	E	86	VAL	2.1
11	H	171	ALA	2.1
32	I	83	ALA	2.1
24	V	62	GLU	2.1
4	A	99	ILE	2.1
26	X	82	GLU	2.1
27	Y	216	ARG	2.1
5	B	121	PRO	2.1
9	F	29	VAL	2.1
9	F	110	ASP	2.1
7	D	38	GLU	2.1
16	N	177	GLU	2.0
1	0	279	C	2.0
13	K	108	GLU	2.0
9	F	27	GLY	2.0
7	D	52	THR	2.0

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Mol	Chain	Res	Type	RSRZ
8	E	94	GLN	2.0
16	N	92	ALA	2.0
16	N	126	GLY	2.0
5	B	118	ASP	2.0
24	V	10	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMU	0	2587	21/22	0.98	0.13	31,34,37,38	0
1	OMG	0	2588	24/25	0.98	0.13	30,34,37,38	0
1	PSU	0	2621	20/21	0.98	0.13	28,31,39,40	0
1	UR3	0	2619	21/22	0.99	0.15	33,38,40,43	0
1	1MA	0	628	23/24	0.99	0.16	31,35,37,38	0
3	5AA	4	76	24/25	0.99	0.14	39,44,45,46	0

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
35	NA	9	9151	1/1	0.51	0.14	76,76,76,76	0
34	K	0	9003	1/1	0.62	0.31	82,82,82,82	0
33	MG	9	8095	1/1	0.63	0.11	72,72,72,72	0
35	NA	0	9182	1/1	0.65	0.28	74,74,74,74	0
33	MG	0	8092	1/1	0.76	0.48	95,95,95,95	0
35	NA	S	9112	1/1	0.78	0.49	76,76,76,76	0
33	MG	0	8085	1/1	0.79	0.25	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8114	1/1	0.80	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.80	0.23	65,65,65,65	0
35	NA	H	9122	1/1	0.81	0.25	77,77,77,77	0
35	NA	0	9172	1/1	0.82	0.31	59,59,59,59	0
35	NA	0	9171	1/1	0.82	0.26	60,60,60,60	0
35	NA	0	9184	1/1	0.82	0.10	75,75,75,75	0
35	NA	0	9163	1/1	0.83	0.35	71,71,71,71	0
33	MG	0	8090	1/1	0.83	0.39	80,80,80,80	0
35	NA	0	9186	1/1	0.84	0.32	75,75,75,75	0
35	NA	0	9174	1/1	0.84	0.25	59,59,59,59	0
35	NA	0	9116	1/1	0.84	0.13	36,36,36,36	0
33	MG	0	8082	1/1	0.84	0.14	66,66,66,66	0
35	NA	0	9124	1/1	0.85	0.09	59,59,59,59	0
35	NA	0	9141	1/1	0.85	0.12	46,46,46,46	0
33	MG	0	8049	1/1	0.85	0.39	90,90,90,90	0
35	NA	0	9117	1/1	0.86	0.21	72,72,72,72	0
35	NA	0	9185	1/1	0.86	0.36	60,60,60,60	0
33	MG	0	8047	1/1	0.86	0.18	102,102,102,102	0
33	MG	0	8071	1/1	0.87	0.08	53,53,53,53	0
35	NA	R	9137	1/1	0.87	0.08	42,42,42,42	0
33	MG	0	8104	1/1	0.87	0.17	53,53,53,53	0
33	MG	0	8107	1/1	0.88	0.06	45,45,45,45	0
35	NA	0	9150	1/1	0.88	0.21	44,44,44,44	0
33	MG	0	8030	1/1	0.88	0.11	35,35,35,35	0
35	NA	0	9165	1/1	0.88	0.18	39,39,39,39	0
35	NA	0	9113	1/1	0.88	0.14	59,59,59,59	0
33	MG	0	8076	1/1	0.89	0.11	57,57,57,57	0
35	NA	0	9126	1/1	0.89	0.14	40,40,40,40	0
33	MG	0	8053	1/1	0.89	0.09	51,51,51,51	0
35	NA	0	9142	1/1	0.89	0.22	52,52,52,52	0
33	MG	0	8050	1/1	0.89	0.07	63,63,63,63	0
33	MG	3	8078	1/1	0.89	0.07	46,46,46,46	0
35	NA	0	9166	1/1	0.90	0.12	77,77,77,77	0
35	NA	0	9129	1/1	0.90	0.14	53,53,53,53	0
33	MG	0	8043	1/1	0.90	0.09	42,42,42,42	0
36	CL	J	9302	1/1	0.90	0.13	70,70,70,70	0
37	CD	O	9205	1/1	0.90	0.07	137,137,137,137	0
33	MG	0	8101	1/1	0.91	0.17	69,69,69,69	0
33	MG	0	8051	1/1	0.91	0.12	56,56,56,56	0
35	NA	B	9158	1/1	0.91	1.05	69,69,69,69	0
35	NA	0	9119	1/1	0.91	0.13	42,42,42,42	0
35	NA	0	9176	1/1	0.91	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8048	1/1	0.91	0.13	60,60,60,60	0
36	CL	0	9315	1/1	0.91	0.21	69,69,69,69	0
36	CL	0	9322	1/1	0.91	0.31	76,76,76,76	0
35	NA	0	9107	1/1	0.91	0.13	43,43,43,43	0
33	MG	0	8057	1/1	0.91	0.13	39,39,39,39	0
37	CD	3	9204	1/1	0.91	0.10	62,62,62,62	0
33	MG	0	8059	1/1	0.92	0.09	51,51,51,51	0
34	K	0	9001	1/1	0.92	0.09	66,66,66,66	0
35	NA	J	9146	1/1	0.92	0.14	37,37,37,37	0
35	NA	0	9167	1/1	0.92	0.09	40,40,40,40	0
33	MG	0	8014	1/1	0.92	0.10	42,42,42,42	0
35	NA	0	9138	1/1	0.93	0.12	51,51,51,51	0
33	MG	0	8072	1/1	0.93	0.20	51,51,51,51	0
33	MG	0	8113	1/1	0.93	0.10	45,45,45,45	0
35	NA	L	9180	1/1	0.93	0.38	50,50,50,50	0
33	MG	0	8042	1/1	0.93	0.07	45,45,45,45	0
35	NA	0	9181	1/1	0.93	0.14	51,51,51,51	0
36	CL	0	9314	1/1	0.93	0.09	50,50,50,50	0
35	NA	0	9155	1/1	0.93	0.25	60,60,60,60	0
33	MG	0	8116	1/1	0.93	0.07	50,50,50,50	0
36	CL	J	9301	1/1	0.93	0.12	72,72,72,72	0
35	NA	0	9105	1/1	0.93	0.13	35,35,35,35	0
36	CL	L	9310	1/1	0.93	0.09	58,58,58,58	0
36	CL	O	9308	1/1	0.93	0.11	68,68,68,68	0
33	MG	0	8118	1/1	0.93	0.10	63,63,63,63	0
35	NA	0	9111	1/1	0.93	0.24	65,65,65,65	0
35	NA	0	9108	1/1	0.94	0.12	48,48,48,48	0
35	NA	0	9175	1/1	0.94	0.23	42,42,42,42	0
35	NA	0	9156	1/1	0.94	0.21	50,50,50,50	0
35	NA	0	9177	1/1	0.94	0.22	55,55,55,55	0
35	NA	0	9159	1/1	0.94	0.19	50,50,50,50	0
33	MG	0	8080	1/1	0.94	0.06	37,37,37,37	0
33	MG	0	8001	1/1	0.94	0.07	36,36,36,36	0
35	NA	0	9114	1/1	0.94	0.16	66,66,66,66	0
33	MG	0	8075	1/1	0.94	0.05	39,39,39,39	0
33	MG	0	8106	1/1	0.94	0.10	51,51,51,51	0
35	NA	9	9183	1/1	0.94	0.11	55,55,55,55	0
36	CL	3	9304	1/1	0.94	0.06	47,47,47,47	0
33	MG	0	8040	1/1	0.94	0.09	45,45,45,45	0
35	NA	0	9173	1/1	0.94	0.14	42,42,42,42	0
35	NA	0	9164	1/1	0.95	0.16	52,52,52,52	0
35	NA	0	9125	1/1	0.95	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	MG	0	8062	1/1	0.95	0.10	53,53,53,53	0
33	MG	0	8063	1/1	0.95	0.09	53,53,53,53	0
35	NA	0	9169	1/1	0.95	0.15	46,46,46,46	0
35	NA	0	9170	1/1	0.95	0.41	61,61,61,61	0
35	NA	0	9135	1/1	0.95	0.20	43,43,43,43	0
33	MG	0	8013	1/1	0.95	0.23	33,33,33,33	0
35	NA	0	9140	1/1	0.95	0.33	49,49,49,49	0
33	MG	0	8008	1/1	0.95	0.08	35,35,35,35	0
35	NA	0	9115	1/1	0.95	0.14	37,37,37,37	0
33	MG	0	8041	1/1	0.95	0.23	59,59,59,59	0
35	NA	0	9102	1/1	0.95	0.13	42,42,42,42	0
33	MG	0	8115	1/1	0.95	0.14	52,52,52,52	0
35	NA	0	9157	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	9121	1/1	0.95	0.26	50,50,50,50	0
35	NA	0	9161	1/1	0.95	0.25	49,49,49,49	0
33	MG	0	8046	1/1	0.95	0.04	52,52,52,52	0
35	NA	0	9106	1/1	0.96	0.17	34,34,34,34	0
35	NA	A	9145	1/1	0.96	0.18	39,39,39,39	0
33	MG	0	8023	1/1	0.96	0.20	53,53,53,53	0
35	NA	C	9104	1/1	0.96	0.09	32,32,32,32	0
35	NA	0	9136	1/1	0.96	0.08	53,53,53,53	0
33	MG	0	8093	1/1	0.96	0.13	56,56,56,56	0
33	MG	0	8094	1/1	0.96	0.16	62,62,62,62	0
33	MG	0	8100	1/1	0.96	0.10	68,68,68,68	0
33	MG	0	8027	1/1	0.96	0.12	44,44,44,44	0
36	CL	0	9303	1/1	0.96	0.15	54,54,54,54	0
36	CL	0	9313	1/1	0.96	0.14	62,62,62,62	0
33	MG	9	8052	1/1	0.96	0.07	50,50,50,50	0
33	MG	0	8103	1/1	0.96	0.20	66,66,66,66	0
36	CL	0	9316	1/1	0.96	0.09	56,56,56,56	0
33	MG	0	8006	1/1	0.96	0.09	32,32,32,32	0
36	CL	B	9319	1/1	0.96	0.14	47,47,47,47	0
33	MG	0	8088	1/1	0.96	0.06	39,39,39,39	0
34	K	0	9002	1/1	0.96	0.06	43,43,43,43	0
35	NA	0	9160	1/1	0.96	0.24	41,41,41,41	0
33	MG	0	8037	1/1	0.96	0.10	46,46,46,46	0
33	MG	0	8111	1/1	0.96	0.08	57,57,57,57	0
33	MG	0	8112	1/1	0.96	0.05	37,37,37,37	0
35	NA	0	9127	1/1	0.96	0.18	39,39,39,39	0
33	MG	0	8039	1/1	0.97	0.08	49,49,49,49	0
33	MG	0	8098	1/1	0.97	0.11	45,45,45,45	0
35	NA	0	9168	1/1	0.97	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9110	1/1	0.97	0.14	37,37,37,37	0
33	MG	0	8019	1/1	0.97	0.10	33,33,33,33	0
33	MG	0	8060	1/1	0.97	0.20	39,39,39,39	0
33	MG	0	8102	1/1	0.97	0.08	51,51,51,51	0
33	MG	0	8020	1/1	0.97	0.14	32,32,32,32	0
33	MG	0	8021	1/1	0.97	0.14	25,25,25,25	0
33	MG	0	8066	1/1	0.97	0.17	114,114,114,114	0
35	NA	0	9118	1/1	0.97	0.12	54,54,54,54	0
33	MG	0	8067	1/1	0.97	0.12	52,52,52,52	0
35	NA	0	9178	1/1	0.97	0.31	53,53,53,53	0
35	NA	0	9179	1/1	0.97	0.20	57,57,57,57	0
33	MG	0	8108	1/1	0.97	0.09	56,56,56,56	0
33	MG	0	8070	1/1	0.97	0.12	53,53,53,53	0
33	MG	0	8022	1/1	0.97	0.06	35,35,35,35	0
33	MG	0	8044	1/1	0.97	0.06	47,47,47,47	0
33	MG	0	8003	1/1	0.97	0.13	26,26,26,26	0
33	MG	0	8024	1/1	0.97	0.15	49,49,49,49	0
35	NA	0	9130	1/1	0.97	0.09	36,36,36,36	0
35	NA	0	9131	1/1	0.97	0.13	35,35,35,35	0
35	NA	0	9133	1/1	0.97	0.16	27,27,27,27	0
35	NA	0	9134	1/1	0.97	0.14	34,34,34,34	0
33	MG	0	8002	1/1	0.97	0.03	28,28,28,28	0
33	MG	0	8007	1/1	0.97	0.08	23,23,23,23	0
33	MG	0	8084	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	8032	1/1	0.97	0.16	39,39,39,39	0
33	MG	4	8119	1/1	0.97	0.08	41,41,41,41	0
33	MG	A	8065	1/1	0.97	0.14	42,42,42,42	0
35	NA	0	9149	1/1	0.97	0.09	36,36,36,36	0
33	MG	B	8055	1/1	0.97	0.20	60,60,60,60	0
35	NA	0	9152	1/1	0.97	0.30	60,60,60,60	0
33	MG	Y	8109	1/1	0.97	0.08	40,40,40,40	0
33	MG	0	8086	1/1	0.97	0.07	50,50,50,50	0
33	MG	0	8087	1/1	0.97	0.21	57,57,57,57	0
33	MG	0	8035	1/1	0.97	0.08	50,50,50,50	0
33	MG	0	8036	1/1	0.97	0.14	39,39,39,39	0
36	CL	J	9321	1/1	0.97	0.15	54,54,54,54	0
35	NA	0	9101	1/1	0.97	0.22	46,46,46,46	0
36	CL	N	9307	1/1	0.97	0.16	61,61,61,61	0
35	NA	0	9162	1/1	0.97	0.26	58,58,58,58	0
33	MG	0	8091	1/1	0.97	0.07	74,74,74,74	0
33	MG	0	8018	1/1	0.97	0.13	40,40,40,40	0
33	MG	0	8054	1/1	0.97	0.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8079	1/1	0.98	0.12	28,28,28,28	0
35	NA	0	9153	1/1	0.98	0.05	17,17,17,17	0
35	NA	0	9154	1/1	0.98	0.09	26,26,26,26	0
33	MG	0	8038	1/1	0.98	0.17	28,28,28,28	0
33	MG	0	8028	1/1	0.98	0.15	43,43,43,43	0
33	MG	B	8056	1/1	0.98	0.15	49,49,49,49	0
35	NA	0	9120	1/1	0.98	0.14	56,56,56,56	0
33	MG	K	8069	1/1	0.98	0.11	41,41,41,41	0
35	NA	H	9109	1/1	0.98	0.13	31,31,31,31	0
33	MG	0	8012	1/1	0.98	0.15	35,35,35,35	0
33	MG	0	8015	1/1	0.98	0.10	30,30,30,30	0
33	MG	0	8033	1/1	0.98	0.08	39,39,39,39	0
35	NA	M	9147	1/1	0.98	0.13	18,18,18,18	0
35	NA	Q	9148	1/1	0.98	0.20	36,36,36,36	0
33	MG	0	8068	1/1	0.98	0.06	58,58,58,58	0
35	NA	0	9128	1/1	0.98	0.08	40,40,40,40	0
33	MG	0	8034	1/1	0.98	0.12	39,39,39,39	0
36	CL	0	9305	1/1	0.98	0.10	52,52,52,52	0
36	CL	0	9311	1/1	0.98	0.14	51,51,51,51	0
33	MG	0	8110	1/1	0.98	0.06	34,34,34,34	0
33	MG	0	8089	1/1	0.98	0.06	60,60,60,60	0
35	NA	0	9132	1/1	0.98	0.09	29,29,29,29	0
35	NA	0	9103	1/1	0.98	0.15	44,44,44,44	0
36	CL	0	9320	1/1	0.98	0.11	48,48,48,48	0
33	MG	0	8016	1/1	0.98	0.19	35,35,35,35	0
36	CL	A	9309	1/1	0.98	0.21	58,58,58,58	0
33	MG	0	8026	1/1	0.98	0.12	24,24,24,24	0
33	MG	0	8074	1/1	0.98	0.07	34,34,34,34	0
33	MG	0	8058	1/1	0.98	0.16	45,45,45,45	0
35	NA	0	9139	1/1	0.98	0.09	22,22,22,22	0
33	MG	0	8017	1/1	0.98	0.10	31,31,31,31	0
33	MG	0	8117	1/1	0.98	0.07	32,32,32,32	0
33	MG	0	8096	1/1	0.98	0.09	38,38,38,38	0
36	CL	R	9306	1/1	0.98	0.12	53,53,53,53	0
35	NA	0	9144	1/1	0.98	0.06	35,35,35,35	0
33	MG	0	8077	1/1	0.98	0.10	29,29,29,29	0
33	MG	0	8099	1/1	0.98	0.14	59,59,59,59	0
33	MG	0	8011	1/1	0.99	0.11	23,23,23,23	0
33	MG	0	8064	1/1	0.99	0.12	25,25,25,25	0
33	MG	0	8005	1/1	0.99	0.09	24,24,24,24	0
36	CL	0	9317	1/1	0.99	0.05	61,61,61,61	0
33	MG	0	8029	1/1	0.99	0.19	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9123	1/1	0.99	0.13	52,52,52,52	0
33	MG	0	8081	1/1	0.99	0.14	43,43,43,43	0
33	MG	0	8004	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	8083	1/1	0.99	0.08	35,35,35,35	0
33	MG	0	8097	1/1	0.99	0.10	45,45,45,45	0
33	MG	T	8073	1/1	0.99	0.05	49,49,49,49	0
33	MG	0	8031	1/1	0.99	0.08	30,30,30,30	0
36	CL	M	9318	1/1	0.99	0.13	36,36,36,36	0
35	NA	T	9143	1/1	0.99	0.06	31,31,31,31	0
33	MG	0	8009	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	8025	1/1	0.99	0.13	48,48,48,48	0
33	MG	0	8061	1/1	0.99	0.09	34,34,34,34	0
36	CL	0	9312	1/1	0.99	0.07	52,52,52,52	0
37	CD	U	9201	1/1	0.99	0.06	73,73,73,73	0
37	CD	Z	9203	1/1	0.99	0.08	61,61,61,61	0
37	CD	1	9202	1/1	0.99	0.02	54,54,54,54	0
33	MG	0	8010	1/1	0.99	0.07	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.