



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 07:57 AM EDT

PDB ID : 1VQL
Title : The structure of the transition state analogue "DCSN" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

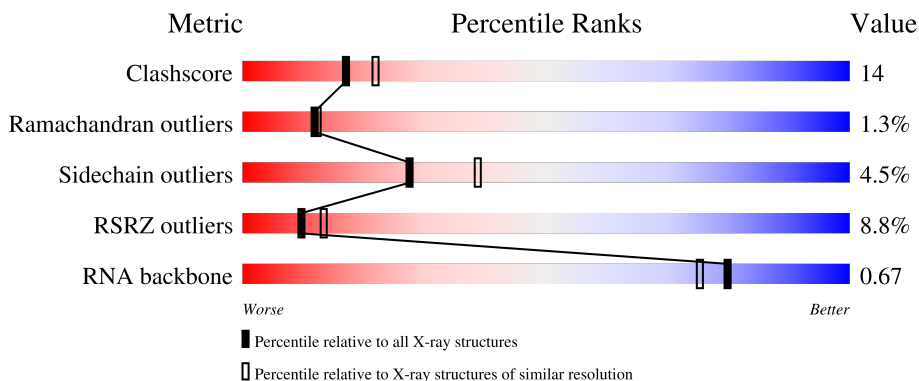
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



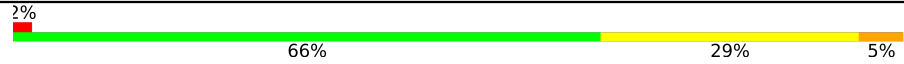
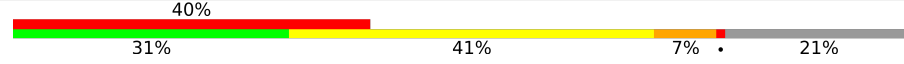
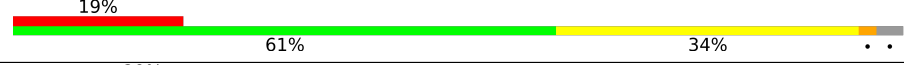

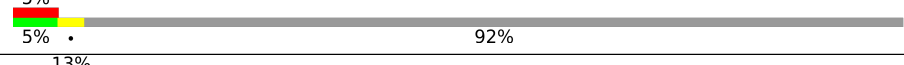
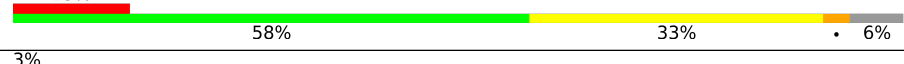
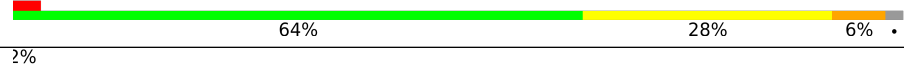

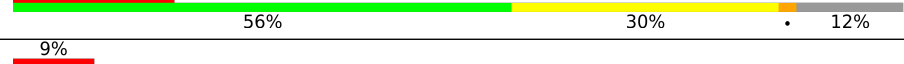


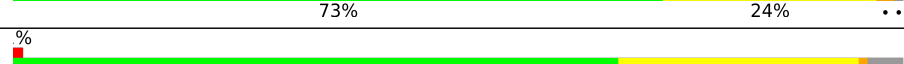
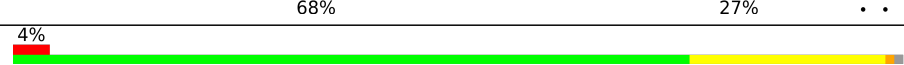
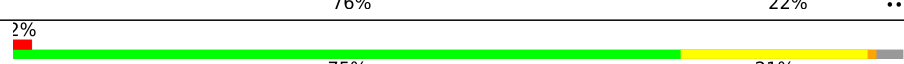

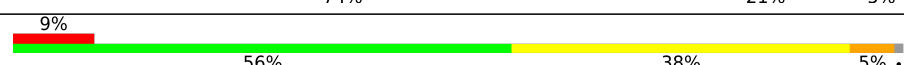


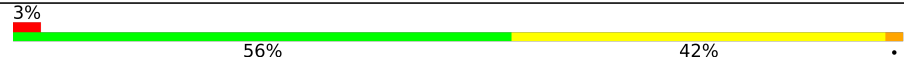

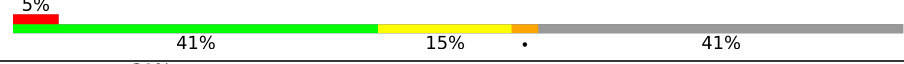

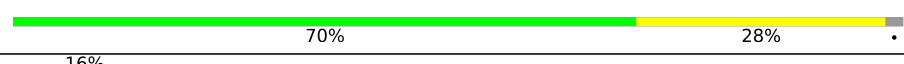


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
2	9	122	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div>
3	4	7	<div style="display: flex; align-items: center;"> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange;"></div> </div>
4	A	240	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div>
5	B	338	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> </div>

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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	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
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	8059	-	-	-	X
33	MG	0	8094	-	-	-	X
35	NA	0	9169	-	-	-	X
35	NA	0	9185	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99053 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*(PPU)*(TSE)*(DA)*CP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
3	4	7	138	70	24	38	5	1	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	89	Total	Mg	0	0
			89	89		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	9	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
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	Y	1	Total Cl 1 1	0	0

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

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	98	Total Sr 98 98	0	0
37	9	3	Total Sr 3 3	0	0
37	A	3	Total Sr 3 3	0	0
37	B	1	Total Sr 1 1	0	0
37	C	1	Total Sr 1 1	0	0
37	F	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	L	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	1	2	Total Sr 2 2	0	0
37	3	1	Total Sr 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	3	1	Total 1	Cd 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5735	Total 5735	O 5735	0	0
39	9	136	Total 136	O 136	0	0
39	4	6	Total 6	O 6	0	0
39	A	128	Total 128	O 128	0	0
39	B	139	Total 139	O 139	0	0
39	C	174	Total 174	O 174	0	0
39	D	50	Total 50	O 50	0	0
39	E	43	Total 43	O 43	0	0
39	F	28	Total 28	O 28	0	0
39	G	16	Total 16	O 16	0	0
39	H	71	Total 71	O 71	0	0
39	J	52	Total 52	O 52	0	0
39	K	59	Total 59	O 59	0	0
39	L	80	Total 80	O 80	0	0
39	M	127	Total 127	O 127	0	0
39	N	60	Total 60	O 60	0	0
39	O	37	Total 37	O 37	0	0
39	P	58	Total 58	O 58	0	0

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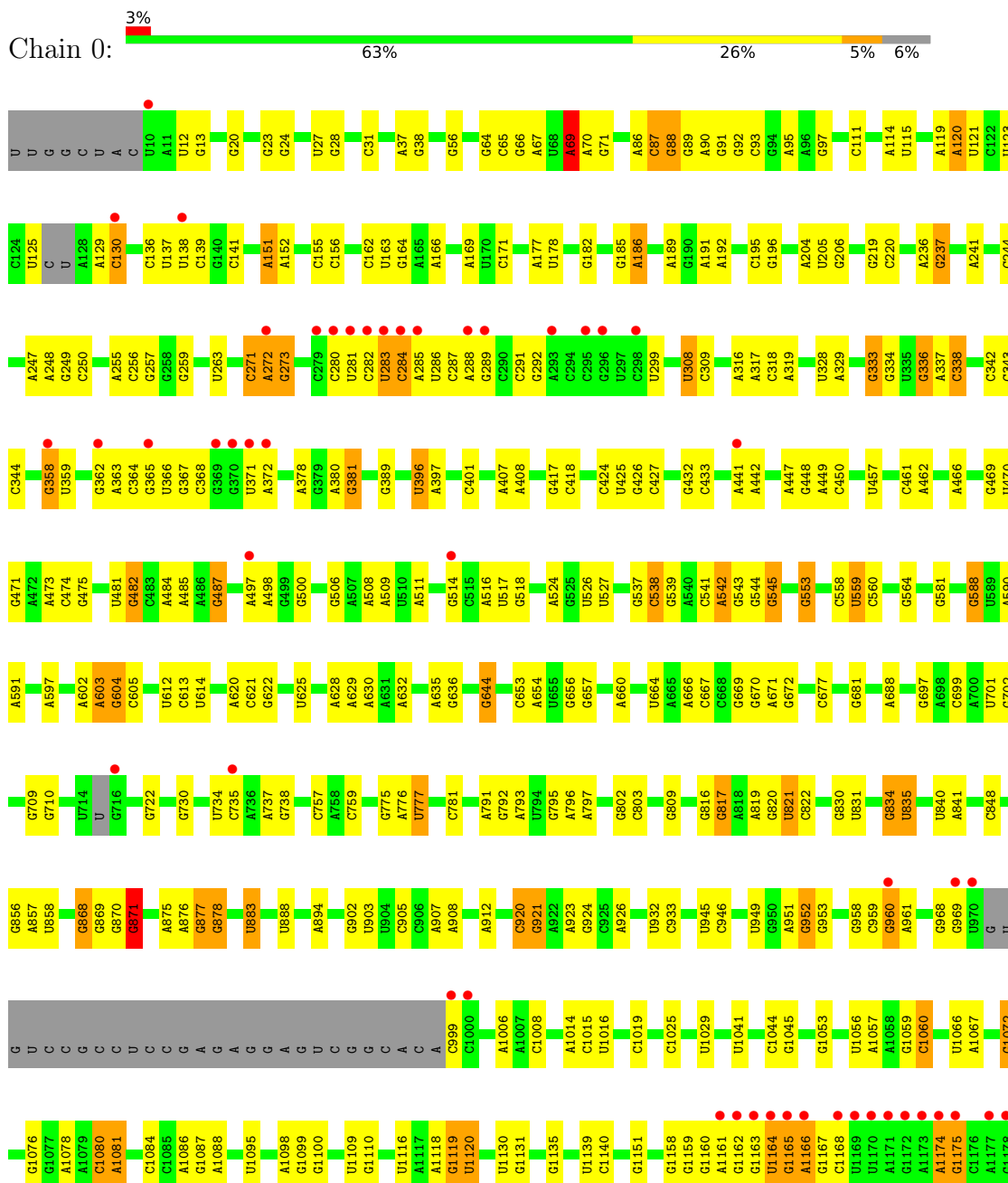
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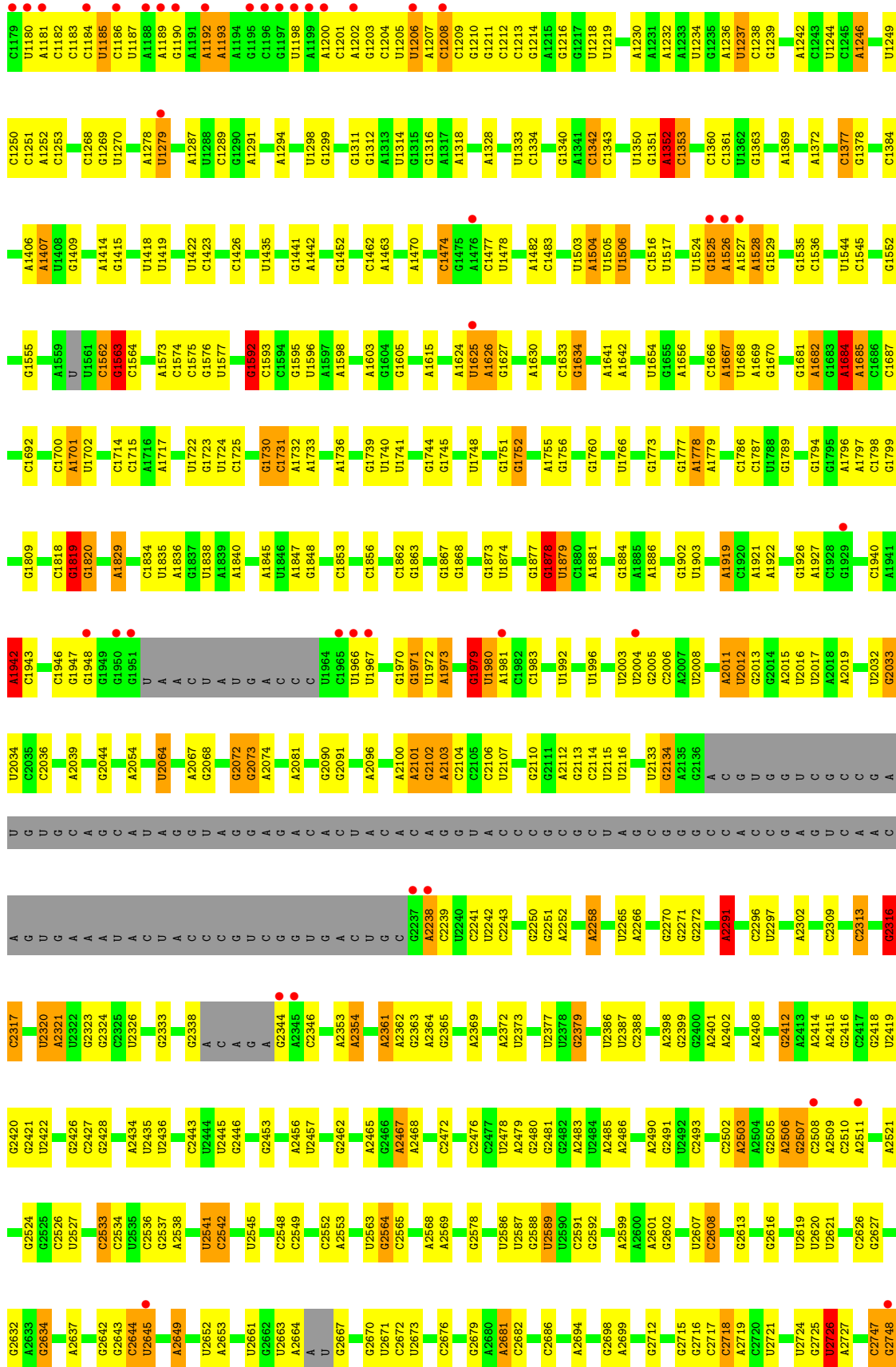
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	48	Total 48	O 48	0	0
39	R	87	Total 87	O 87	0	0
39	S	29	Total 29	O 29	0	0
39	T	36	Total 36	O 36	0	0
39	U	27	Total 27	O 27	0	0
39	V	11	Total 11	O 11	0	0
39	W	69	Total 69	O 69	0	0
39	X	24	Total 24	O 24	0	0
39	Y	87	Total 87	O 87	0	0
39	Z	31	Total 31	O 31	0	0
39	1	55	Total 55	O 55	0	0
39	2	42	Total 42	O 42	0	0
39	3	65	Total 65	O 65	0	0
39	I	9	Total 9	O 9	0	0

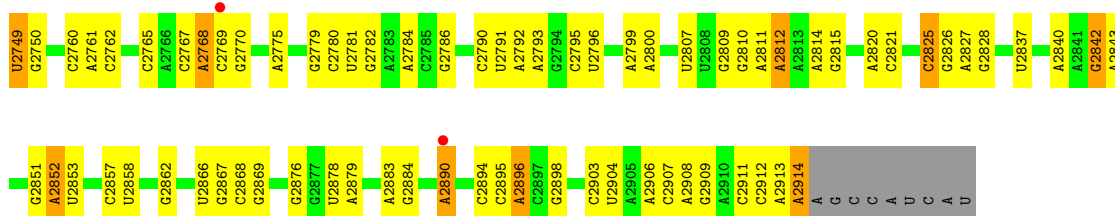
3 Residue-property plots [i](#)

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.

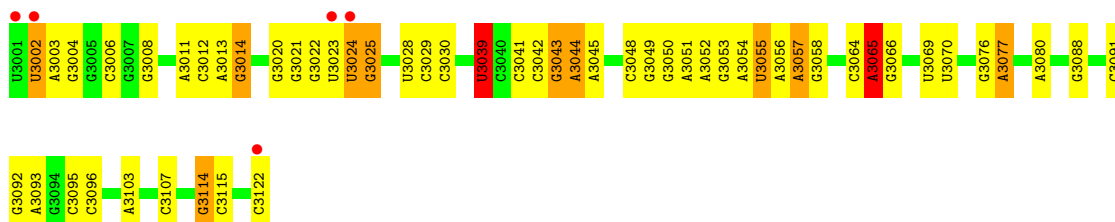
- Molecule 1: 23S ribosomal rna



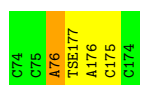




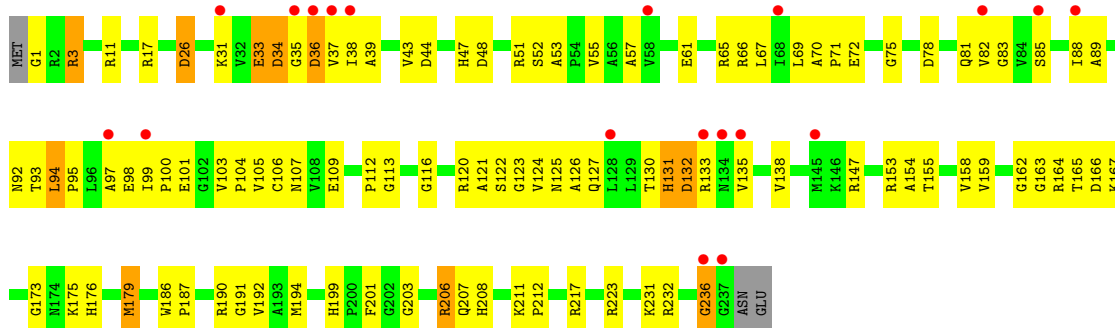
• Molecule 2: 5S ribosomal RNA



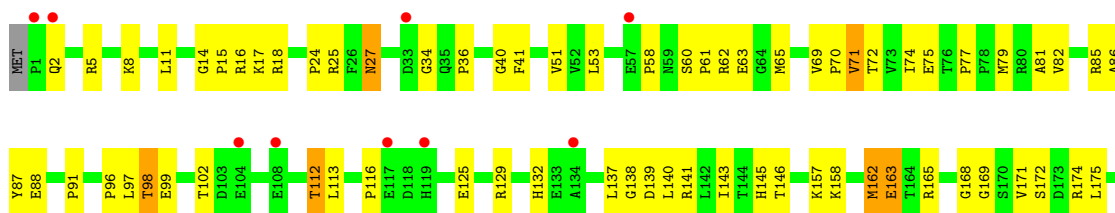
• Molecule 3: 5'-R(*CP*CP*(PPU)*(TSE)*(DA)*CP*C)-3'

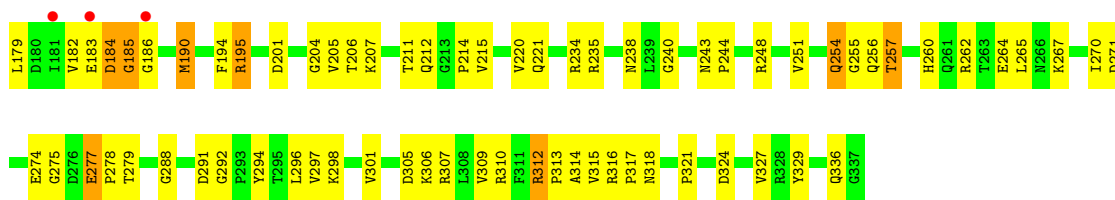


• Molecule 4: 50S ribosomal protein L2P

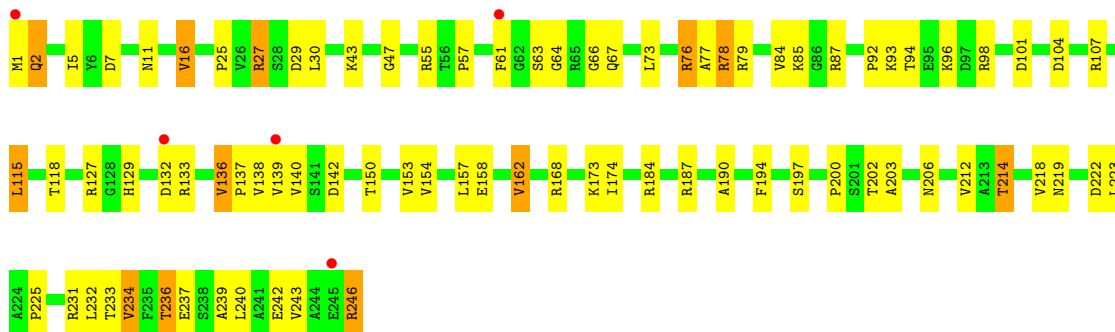


• Molecule 5: 50S ribosomal protein L3P

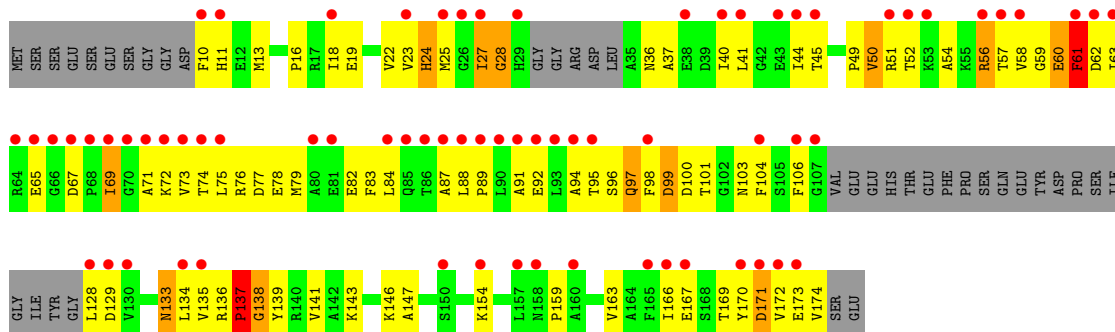




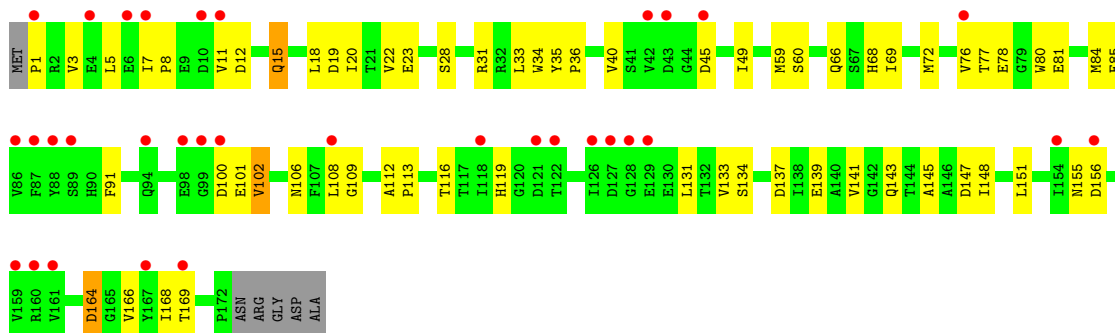
• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P

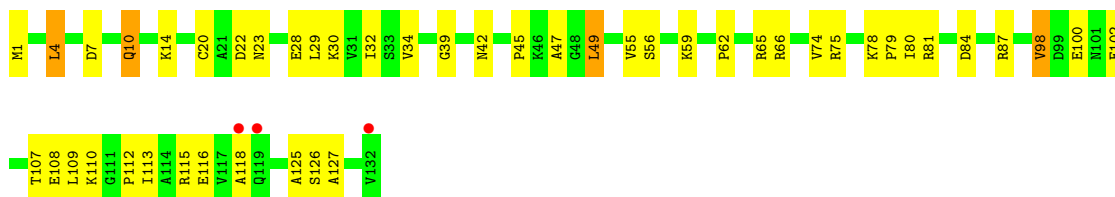


• Molecule 8: 50S ribosomal protein L6P

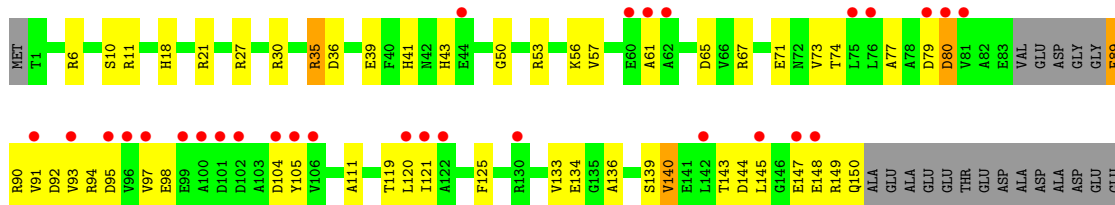




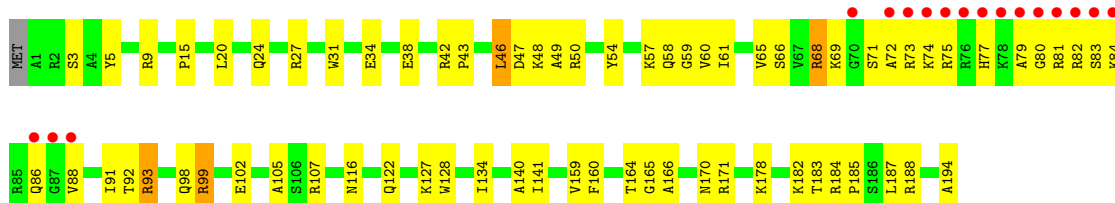
- Molecule 13: 50S ribosomal protein L14P



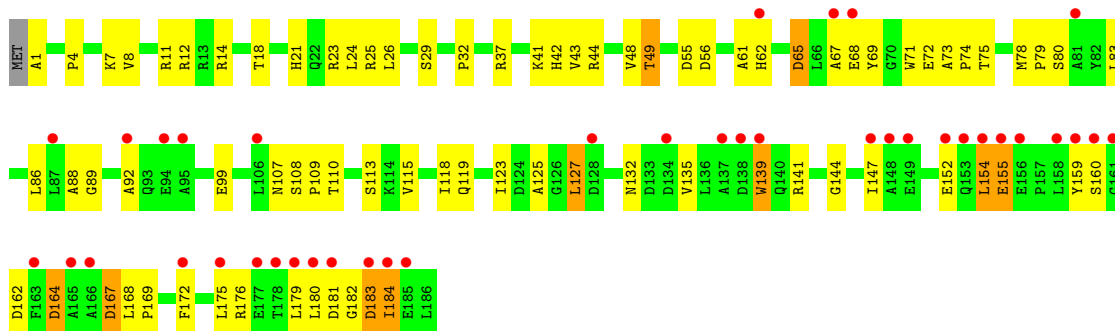
- Molecule 14: 50S ribosomal protein L15P



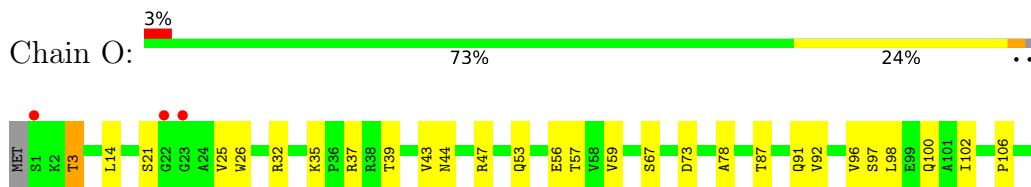
- Molecule 15: 50S Ribosomal Protein L15E



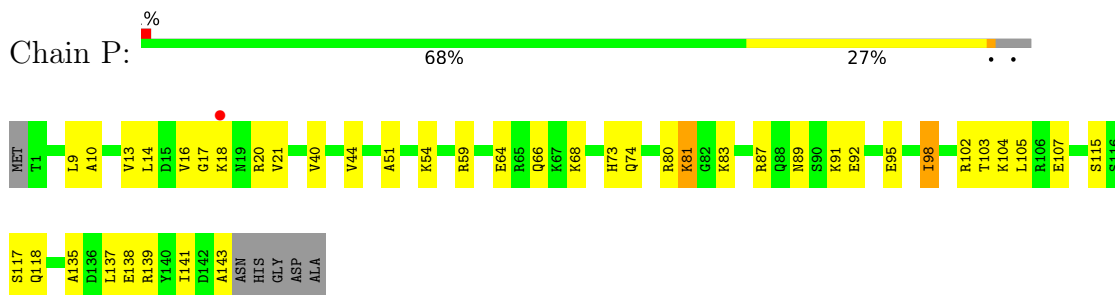
- Molecule 16: 50S ribosomal protein L18P



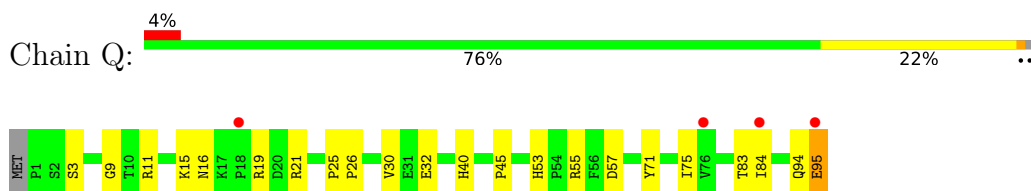
- Molecule 17: 50S ribosomal protein L18e



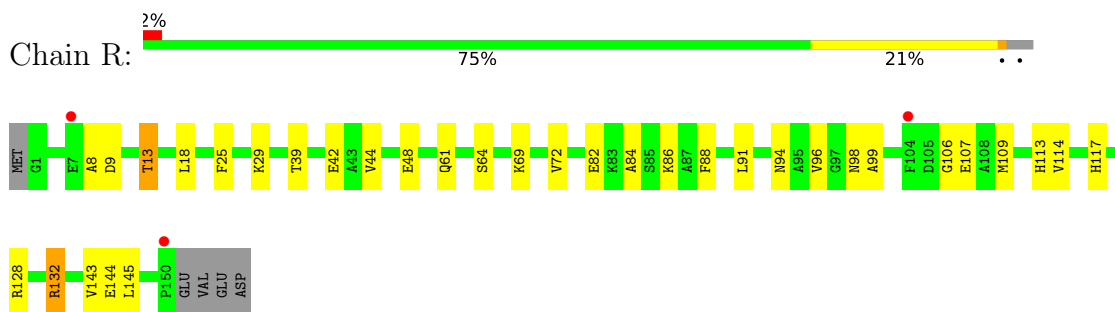
- Molecule 18: 50S ribosomal protein L19E



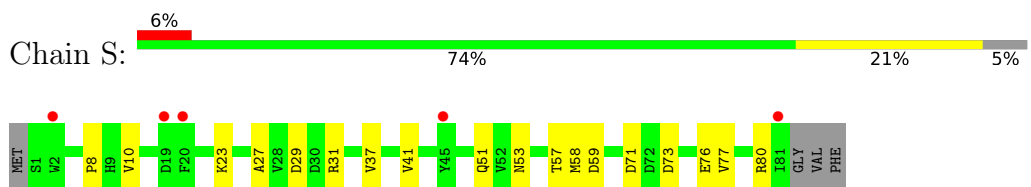
- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

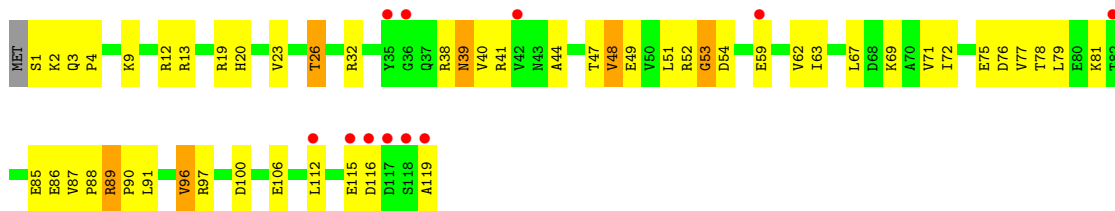


- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

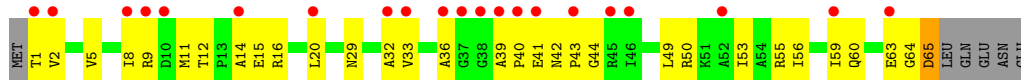




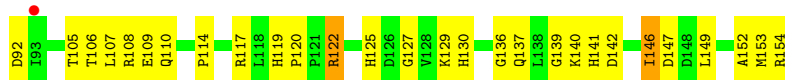
• Molecule 23: 50S ribosomal protein L24E



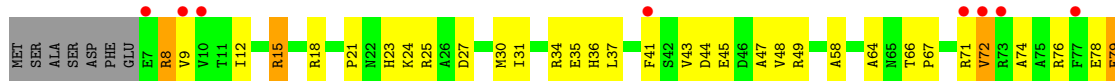
• Molecule 24: 50S ribosomal protein L29P



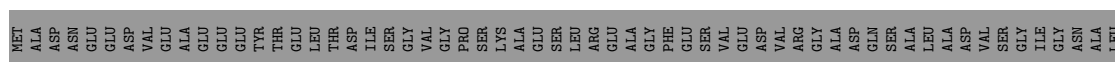
• Molecule 25: 50S ribosomal protein L30P

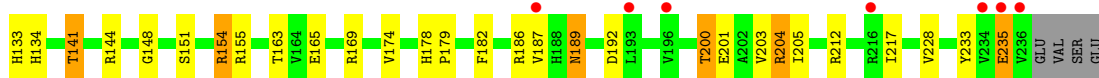
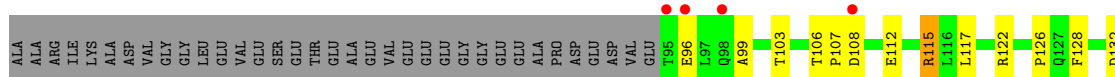


• Molecule 26: 50S ribosomal protein L31e

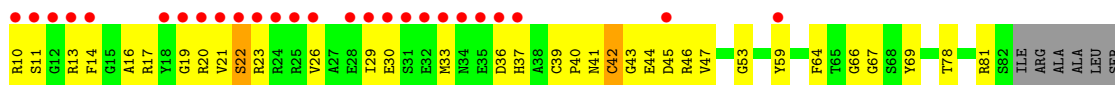


• Molecule 27: 50S ribosomal protein L32E





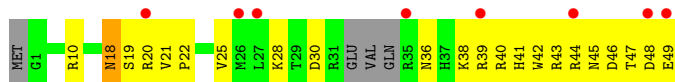
• Molecule 28: 50S ribosomal protein L37Ae



• Molecule 29: 50S ribosomal protein L37e



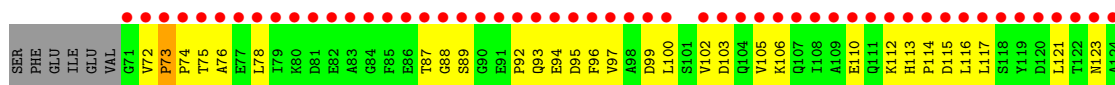
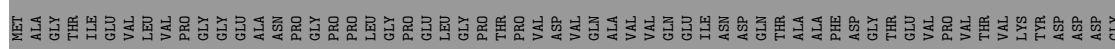
• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P



A125	K126	E127	V128	V129	G130	T131	C132	T133	S134	L135	G136	V137	T138	I139	E140	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	ALA	GLU	ALA	GLN	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.30) 89.4 (49.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.22 (at 2.29Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.251 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99053	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

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

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: OMU, MG, TSE, K, CD, UR3, CL, PPU, SR, NA, 1MA, OMG, PSU

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	27/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.48	0/102	0.65	0/149
4	A	0.33	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.34	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.61	0/1999
17	O	0.32	0/874	0.58	0/1181
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.36	0/749	0.69	0/1005
20	R	0.34	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.29	0/958	0.62	0/1289
23	U	0.35	0/417	0.57	0/562
24	V	0.27	0/502	0.51	0/675
25	W	0.33	0/1219	0.60	0/1655
26	X	0.33	0/664	0.57	0/895
27	Y	0.35	0/1146	0.64	0/1536
28	Z	0.33	0/589	0.58	0/787
29	1	0.44	0/438	0.67	0/578
30	2	0.34	0/401	0.60	0/529
31	3	0.37	0/771	0.57	0/1024
32	I	0.29	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	29/147726 (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	46
2	9	0	2
All	All	1	48

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.71	130.86	109.50
1	0	871	G	C5'-C4'-O4'	-7.68	99.89	109.10
2	9	3039	U	N1-C1'-C2'	7.28	123.46	114.00
1	0	1942	A	C5'-C4'-C3'	7.25	127.60	116.00
1	0	1592	G	N9-C1'-C2'	6.96	123.05	114.00
1	0	1819	G	C5'-C4'-C3'	6.63	126.61	116.00
1	0	1979	G	C2'-C3'-O3'	6.62	124.30	113.70
1	0	1504	A	C1'-O4'-C4'	-6.28	104.88	109.90
1	0	777	U	O4'-C1'-N1	6.11	113.09	108.20
1	0	2467	A	C1'-O4'-C4'	-5.92	105.17	109.90
1	0	883	U	N1-C1'-C2'	5.79	121.53	114.00
1	0	1819	G	C1'-O4'-C4'	-5.69	105.35	109.90
1	0	2726	U	N1-C1'-C2'	5.46	121.09	114.00
1	0	206	G	C5'-C4'-C3'	-5.41	107.35	116.00
1	0	2313	C	C5'-C4'-O4'	5.40	115.58	109.10
1	0	389	G	C5'-C4'-C3'	-5.37	107.41	116.00
1	0	841	A	C1'-O4'-C4'	-5.34	105.63	109.90
1	0	1819	G	C4'-C3'-C2'	-5.33	97.27	102.60
1	0	69	A	C5'-C4'-O4'	-5.28	102.76	109.10
1	0	1504	A	N9-C1'-C2'	5.13	120.67	114.00
1	0	2291	A	N9-C1'-C2'	5.13	120.67	114.00
1	0	1120	U	C5'-C4'-C3'	-5.10	107.85	116.00
1	0	1878	G	O4'-C1'-N9	5.09	112.27	108.20
1	0	2316	G	C5'-C4'-C3'	-5.09	107.86	116.00
1	0	1684	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	0	1352	A	OP1-P-O3'	5.05	116.30	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1615	A	C5'-C4'-C3'	5.05	124.08	116.00
21	S	27	ALA	N-CA-C	-5.04	97.38	111.00
1	0	1452	G	C5'-C4'-C3'	-5.01	107.98	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1361	C	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	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	1970	G	Sidechain
1	0	1979	G	Sidechain
1	0	2036	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2616	G	Sidechain
1	0	2632	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	781	C	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	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	756	0
2	9	2600	0	1326	59	0
3	4	138	0	85	5	0
4	A	1753	0	1765	117	0
5	B	2625	0	2531	135	0
6	C	1859	0	1816	96	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	59	0
9	F	890	0	843	49	0
10	G	240	0	231	13	0
11	H	1266	0	1268	63	0
12	J	1120	0	1098	72	0
13	K	992	0	1031	51	0
14	L	1118	0	1076	51	0
15	M	1560	0	1568	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1445	0	1401	83	0
17	O	865	0	873	35	0
18	P	1136	0	1123	39	0
19	Q	735	0	728	22	0
20	R	1149	0	1122	39	0
21	S	641	0	605	16	0
22	T	950	0	924	54	0
23	U	410	0	364	17	0
24	V	499	0	511	33	0
25	W	1196	0	1137	91	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	47	0
28	Z	578	0	539	34	0
29	1	431	0	426	25	0
30	2	396	0	413	34	0
31	3	755	0	728	29	0
32	I	519	0	500	47	0
33	0	89	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5735	0	0	103	0
39	1	55	0	0	1	0
39	2	42	0	0	2	0
39	3	65	0	0	4	0
39	4	6	0	0	0	0
39	9	136	0	0	5	0
39	A	128	0	0	10	0
39	B	139	0	0	18	0
39	C	174	0	0	19	0
39	D	50	0	0	8	0
39	E	43	0	0	3	0
39	F	28	0	0	2	0
39	G	16	0	0	2	0
39	H	71	0	0	6	0
39	I	9	0	0	1	0
39	J	52	0	0	3	0
39	K	59	0	0	4	0
39	L	80	0	0	9	0
39	M	127	0	0	5	0
39	N	60	0	0	10	0
39	O	37	0	0	0	0
39	P	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Q	48	0	0	4	0
39	R	87	0	0	5	0
39	S	29	0	0	2	0
39	T	36	0	0	6	0
39	U	27	0	0	2	0
39	V	11	0	0	1	0
39	W	69	0	0	4	0
39	X	24	0	0	5	0
39	Y	87	0	0	8	0
39	Z	31	0	0	5	0
All	All	99053	0	59982	2116	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 14.

All (2116) 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)
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.11
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.32	1.06
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.22	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.73	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.40	1.00
6:C:236:THR:HG22	6:C:239:ALA:H	1.26	1.00
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.44	1.00
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.42	0.99
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.39	0.99
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.41	0.99
9:F:91:VAL:HG12	9:F:92:GLY:H	1.21	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.48	0.96
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.80	0.96
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.26	0.95
30:2:41:HIS:H	30:2:45:ASN:HD22	1.07	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	1.15	0.93
1:0:871:G:C8	1:0:871:G:H5'	2.04	0.93
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.51	0.93
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.82	0.93
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.49	0.93
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.51	0.93
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.13	0.93
1:0:1160:G:H5'	1:0:1161:A:H5''	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1242:A:H5'	12:J:82:THR:HG23	1.50	0.92
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.85	0.92
5:B:140:LEU:HA	39:B:9512:HOH:O	1.68	0.92
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.51	0.92
1:0:2717:C:H2'	1:0:2718:C:H5''	1.51	0.91
5:B:86:ALA:HA	39:B:9512:HOH:O	1.71	0.91
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.35	0.91
29:1:25:LYS:HD2	30:2:49:GLU:H	1.34	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.91
7:D:25:MET:HE2	7:D:41:LEU:HG	1.50	0.90
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.18	0.90
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.54	0.90
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.50	0.90
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.07	0.90
1:0:542:A:H5'	1:0:542:A:H8	1.36	0.90
17:O:57:THR:HB	17:O:111:VAL:HG23	1.52	0.90
13:K:10:GLN:HE21	13:K:10:GLN:H	0.90	0.90
1:0:1372:A:H3'	39:0:7654:HOH:O	1.72	0.89
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.19	0.89
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.35	0.89
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.54	0.89
1:0:2812:A:H2	1:0:2814:A:H62	1.18	0.89
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.53	0.89
1:0:2506:A:HO2'	1:0:2507:G:H8	0.92	0.88
16:N:113:SER:HB2	39:N:9354:HOH:O	1.73	0.88
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.53	0.88
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.55	0.88
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.54	0.88
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.89	0.88
6:C:1:MET:HG2	6:C:2:GLN:H	1.39	0.88
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.88
13:K:10:GLN:HE21	13:K:10:GLN:N	1.72	0.87
13:K:10:GLN:H	13:K:10:GLN:NE2	1.72	0.87
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.89	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.03	0.87
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.74	0.87
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.56	0.87
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.57	0.86
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.56	0.86
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.86
4:A:192:VAL:HG22	39:A:9625:HOH:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:131:THR:HG22	12:J:134:GLU:H	1.41	0.85
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.40	0.85
16:N:144:GLY:O	16:N:147:ILE:HG22	1.77	0.84
25:W:88:THR:HB	39:W:6679:HOH:O	1.77	0.84
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.59	0.84
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.60	0.84
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.77	0.84
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.41	0.84
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.58	0.84
1:O:541:C:H2'	1:O:542:A:H5''	1.59	0.84
39:O:5375:HOH:O	12:J:47:THR:HB	1.77	0.83
1:O:1474:C:H6	1:O:1474:C:H5'	1.42	0.83
1:O:288:A:H61	1:O:364:C:H42	1.25	0.82
1:O:1838:U:H1'	1:O:2644:C:H5'	1.61	0.82
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.43	0.82
1:O:1116:U:HO2'	1:O:1118:A:H2	0.83	0.82
1:O:1041:U:H5'	39:L:9488:HOH:O	1.79	0.82
1:O:2851:G:C2'	1:O:2852:A:H5'	2.10	0.82
1:O:870:G:H2'	1:O:871:G:H5''	1.60	0.81
1:O:1979:G:H2'	39:O:3881:HOH:O	1.80	0.81
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.61	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.45	0.81
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.59	0.81
25:W:122:ARG:HG2	25:W:152:ALA:O	1.79	0.81
4:A:206:ARG:H	4:A:206:ARG:HD3	1.45	0.81
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.45	0.81
1:O:1593:C:OP1	18:P:117:SER:HB3	1.81	0.80
7:D:154:LYS:H	7:D:154:LYS:HD2	1.46	0.80
30:2:18:ASN:HD21	30:2:40:ARG:H	1.24	0.80
6:C:246:ARG:HB3	6:C:246:ARG:HH11	1.46	0.80
1:O:1159:G:H21	1:O:1189:A:H8	1.30	0.80
1:O:1667:A:H8	1:O:1667:A:H5'	1.47	0.80
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.64	0.80
1:O:1116:U:O2'	1:O:1118:A:H2	1.64	0.80
9:F:91:VAL:HG12	9:F:92:GLY:N	1.97	0.80
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.64	0.80
7:D:57:THR:HG23	7:D:63:ILE:HA	1.65	0.79
2:9:3039:U:H1'	2:9:3044:A:H61	1.48	0.79
4:A:191:GLY:HA2	4:A:194:MET:CE	2.13	0.79
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.63	0.79
1:O:1603:A:H5'	1:O:1605:G:O4'	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.62	0.79
1:0:871:G:H5'	1:0:871:G:H8	1.47	0.79
1:0:111:C:O2'	29:1:20:ARG:HG2	1.82	0.78
1:0:289:G:H22	1:0:363:A:H2	1.26	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.13	0.78
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.65	0.78
1:0:2073:G:H5''	39:0:4393:HOH:O	1.84	0.78
21:S:57:THR:HG22	21:S:59:ASP:H	1.48	0.78
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.65	0.78
18:P:115:SER:OG	18:P:118:GLN:HG3	1.82	0.78
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.65	0.78
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.66	0.78
1:0:2851:G:H2'	1:0:2852:A:H5'	1.66	0.77
1:0:871:G:C8	1:0:871:G:C5'	2.68	0.77
1:0:796:A:HO2'	28:Z:10:ARG:N	1.82	0.77
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.65	0.77
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.84	0.77
1:0:1119:G:N2	1:0:1246:A:C2	2.51	0.77
9:F:96:ALA:HA	39:F:3111:HOH:O	1.85	0.77
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.77
1:0:481:U:H5''	39:0:6177:HOH:O	1.85	0.77
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.65	0.76
11:H:27:LYS:H	11:H:59:HIS:HD2	1.32	0.76
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.67	0.76
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.76
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.66	0.76
1:0:2840:A:OP1	5:B:211:THR:HG23	1.86	0.76
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.68	0.76
9:F:58:GLU:HA	9:F:61:MET:HE2	1.68	0.76
15:M:164:THR:HG22	15:M:166:ALA:H	1.51	0.76
1:0:381:G:H5''	39:M:9375:HOH:O	1.86	0.76
6:C:246:ARG:HB3	6:C:246:ARG:NH1	2.01	0.76
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.68	0.75
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.88	0.75
1:0:559:U:H6	1:0:559:U:H5'	1.52	0.75
1:0:1563:G:H4'	39:0:4791:HOH:O	1.87	0.75
39:0:7895:HOH:O	5:B:211:THR:HG21	1.86	0.75
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.17	0.75
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.67	0.75
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.02	0.75
1:0:2468:A:H61	31:3:48:ASN:HD21	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.68	0.74
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.85	0.74
25:W:122:ARG:NH2	25:W:154:ARG:HG2	2.02	0.74
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.68	0.74
5:B:179:LEU:O	5:B:183:GLU:HG2	1.86	0.74
16:N:132:ASN:O	16:N:135:VAL:HG12	1.88	0.74
1:O:282:C:H1'	1:O:368:C:N4	2.02	0.74
1:O:2054:A:N3	20:R:128:ARG:NH2	2.35	0.74
1:O:2748:G:H2'	39:O:7977:HOH:O	1.88	0.74
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.50	0.74
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.74
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.74
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.69	0.74
1:O:2534:C:H1'	39:O:4077:HOH:O	1.87	0.74
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.74
1:O:1377:C:H5'	1:O:1377:C:H6	1.52	0.74
1:O:1701:A:H4'	1:O:1702:U:H5''	1.70	0.74
7:D:172:VAL:HG12	7:D:173:GLU:H	1.53	0.73
1:O:1118:A:H62	1:O:1244:U:H3	1.35	0.73
29:1:25:LYS:HD2	30:2:49:GLU:N	2.02	0.73
1:O:2506:A:O2'	1:O:2507:G:H8	1.68	0.73
16:N:80:SER:HB2	39:N:9334:HOH:O	1.89	0.73
2:9:3014:G:H5'	2:9:3014:G:H8	1.54	0.73
1:O:1878:G:H1'	39:O:6632:HOH:O	1.88	0.73
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.04	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.86	0.73
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.03	0.73
1:O:1118:A:H8	1:O:1118:A:H3'	1.53	0.73
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.54	0.73
18:P:115:SER:H	18:P:118:GLN:NE2	1.84	0.73
24:V:39:ALA:N	24:V:40:PRO:HD2	2.04	0.73
1:O:1165:G:H4'	1:O:1174:A:O2'	1.89	0.73
1:O:2291:A:C8	1:O:2309:C:H5'	2.24	0.73
1:O:281:U:H2'	1:O:282:C:O4'	1.89	0.72
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.70	0.72
6:C:236:THR:HG22	6:C:239:ALA:N	2.03	0.72
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.71	0.72
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.19	0.72
1:O:506:G:H22	1:O:509:A:C5'	2.02	0.72
1:O:1160:G:C5'	1:O:1161:A:H5'	2.20	0.72
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.53	0.72
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.54	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.72
25:W:52:VAL:HG22	25:W:53:ALA:H	1.53	0.72
1:0:560:C:H42	1:0:597:A:H61	1.35	0.72
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.54	0.72
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.70	0.72
5:B:16:ARG:NH1	39:B:9547:HOH:O	2.22	0.72
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.53	0.72
1:0:1118:A:H3'	1:0:1118:A:C8	2.24	0.72
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.70	0.72
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.25	0.72
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.23	0.72
5:B:275:GLY:O	5:B:291:ASP:HA	1.89	0.72
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.72	0.72
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.70	0.72
15:M:80:GLY:O	15:M:81:ARG:HD2	1.90	0.72
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.05	0.72
17:O:32:ARG:O	17:O:32:ARG:HD3	1.88	0.72
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.07	0.71
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.55	0.71
1:0:1751:G:H2'	1:0:1752:G:H5''	1.72	0.71
1:0:2073:G:OP2	1:0:2490:A:H5'	1.91	0.71
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.89	0.71
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.86	0.71
4:A:33:GLU:H	4:A:33:GLU:CD	1.92	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.90	0.71
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.35	0.71
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.06	0.71
1:0:2491:G:H1'	39:O:7345:HOH:O	1.89	0.71
15:M:69:LYS:O	15:M:73:ARG:NH2	2.24	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.25	0.71
1:0:1182:C:H1'	1:0:1192:A:H8	1.55	0.71
6:C:236:THR:CG2	6:C:239:ALA:H	2.02	0.71
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.71
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.90	0.71
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.91	0.71
1:0:1206:U:H5'	1:0:1206:U:H6	1.56	0.71
1:0:2541:U:H4'	1:0:2542:C:OP1	1.90	0.70
25:W:13:MET:HE1	25:W:18:GLN:HA	1.73	0.70
1:0:93:C:H5''	24:V:1:THR:HB	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:HO2'	1:0:1189:A:H2	1.40	0.70
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.70
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.21	0.70
23:U:14:GLU:O	23:U:17:THR:HB	1.91	0.70
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.21	0.70
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.92	0.70
1:0:1175:G:H1'	1:0:1193:A:H2'	1.73	0.70
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.72	0.70
39:0:7683:HOH:O	4:A:11:ARG:HA	1.90	0.70
24:V:56:ILE:O	24:V:60:GLN:HG3	1.90	0.70
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.73	0.70
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.73	0.70
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.74	0.70
11:H:30:GLN:H	11:H:66:ARG:NH1	1.90	0.70
14:L:73:VAL:HG23	14:L:74:THR:H	1.56	0.70
1:0:1184:C:H1'	39:0:7904:HOH:O	1.92	0.70
25:W:88:THR:HG22	25:W:89:ASP:N	2.06	0.70
1:0:1474:C:H5'	1:0:1474:C:C6	2.25	0.70
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.74	0.69
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.74	0.69
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.57	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.91	0.69
27:Y:165:GLU:HB3	39:Y:9386:HOH:O	1.91	0.69
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.26	0.69
25:W:125:HIS:HD2	25:W:127:GLY:H	1.41	0.69
1:0:553:G:P	27:Y:204:ARG:HH22	2.15	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.22	0.69
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.57	0.69
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.23	0.69
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.89	0.69
1:0:544:G:H2'	1:0:545:G:H5''	1.73	0.69
1:0:1700:C:H5''	1:0:1701:A:OP2	1.93	0.69
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.56	0.69
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.74	0.69
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.17	0.69
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.57	0.69
32:I:99:ASP:OD1	32:I:138:THR:HB	1.93	0.69
26:X:25:ARG:HD3	26:X:64:ALA:O	1.92	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.91	0.69
1:0:236:A:H4'	1:0:237:G:H5'	1.75	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:960:G:H4'	39:0:7871:HOH:O	1.93	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.93	0.68
14:L:143:THR:HG22	14:L:144:ASP:N	2.08	0.68
1:0:1206:U:H2'	1:0:1207:A:O4'	1.93	0.68
6:C:132:ASP:HB3	39:C:9562:HOH:O	1.94	0.68
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.09	0.68
14:L:143:THR:HG22	14:L:144:ASP:H	1.56	0.68
25:W:48:VAL:O	25:W:48:VAL:HG12	1.93	0.68
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.75	0.68
25:W:88:THR:HG22	25:W:89:ASP:H	1.56	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.68
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.94	0.68
10:G:12:ILE:N	10:G:13:PRO:HD3	2.08	0.68
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.76	0.68
6:C:107:ARG:NE	39:C:9655:HOH:O	2.26	0.68
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.76	0.68
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.23	0.68
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.24	0.68
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.94	0.68
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.68
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.09	0.68
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.76	0.68
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.67
4:A:48:ASP:HB3	39:A:9597:HOH:O	1.93	0.67
5:B:51:VAL:HG23	5:B:329:TYR:O	1.93	0.67
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.91	0.67
21:S:57:THR:HG22	21:S:59:ASP:N	2.08	0.67
2:9:3039:U:H1'	2:9:3044:A:N6	2.09	0.67
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.76	0.67
1:0:542:A:H5'	1:0:542:A:C8	2.25	0.67
6:C:2:GLN:HB3	39:C:9585:HOH:O	1.93	0.67
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.76	0.67
1:0:506:G:H22	1:0:509:A:H5''	1.59	0.67
4:A:51:ARG:HB2	39:A:9597:HOH:O	1.93	0.67
1:0:545:G:H5'	1:0:545:G:H8	1.60	0.67
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.74	0.67
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.67
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.76	0.67
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.75	0.67
1:0:2716:G:H5''	5:B:206:THR:HG21	1.77	0.67
2:9:3029:C:H2'	2:9:3030:C:H5'	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2480:G:H3'	39:0:4747:HOH:O	1.95	0.67
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.75	0.67
1:0:524:A:H5''	20:R:29:LYS:HD3	1.77	0.67
1:0:1666:C:O2'	1:0:1667:A:H5''	1.94	0.67
2:9:3056:A:C2'	2:9:3057:A:H5''	2.24	0.67
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.10	0.67
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.94	0.67
1:0:1973:A:H5'	1:0:1973:A:H8	1.59	0.66
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.10	0.66
2:9:3020:G:O2'	2:9:3021:G:H5'	1.95	0.66
1:0:470:U:O2'	29:1:16:HIS:HD2	1.79	0.66
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.43	0.66
1:0:338:C:H4'	6:C:174:ILE:CD1	2.25	0.66
16:N:11:ARG:HA	16:N:14:ARG:NH1	2.10	0.66
1:0:1555:G:H4'	1:0:1630:A:H2	1.60	0.66
1:0:2524:G:H21	1:0:2526:C:N4	1.93	0.66
1:0:2661:U:H3	1:0:2812:A:H62	1.42	0.66
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.78	0.66
1:0:1528:A:H2'	1:0:1529:G:O4'	1.95	0.66
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.08	0.66
14:L:67:ARG:O	14:L:71:GLU:HG3	1.95	0.66
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.57	0.66
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.59	0.66
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.92	0.66
1:0:1209:C:H2'	1:0:1210:G:H8	1.59	0.66
5:B:112:THR:HG23	5:B:158:LYS:HE3	1.77	0.66
1:0:282:C:O2'	1:0:283:U:H5'	1.94	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:2896:A:H5''	39:0:6611:HOH:O	1.95	0.66
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.26	0.66
1:0:69:A:H5'	1:0:69:A:C8	2.31	0.66
5:B:162:MET:CE	5:B:310:ARG:HD3	2.25	0.66
7:D:159:PRO:O	7:D:163:VAL:HG23	1.95	0.66
25:W:130:HIS:O	25:W:136:GLY:HA3	1.96	0.66
1:0:2878:U:H2'	1:0:2879:A:O4'	1.95	0.66
9:F:60:VAL:O	9:F:60:VAL:HG12	1.96	0.66
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.77	0.66
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.95	0.65
27:Y:115:ARG:HB3	27:Y:115:ARG:HH11	1.62	0.65
1:0:380:A:OP2	15:M:9:ARG:HD2	1.96	0.65
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.12	0.65
1:O:1201:C:H2'	1:O:1202:A:H5'	1.76	0.65
1:O:1426:C:H2'	39:O:3202:HOH:O	1.94	0.65
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.60	0.65
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.10	0.65
1:O:280:C:H2'	1:O:281:U:O4'	1.97	0.65
6:C:1:MET:HG2	6:C:2:GLN:N	2.09	0.65
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.65
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.12	0.65
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.94	0.65
27:Y:144:ARG:CZ	39:Y:9403:HOH:O	2.43	0.65
14:L:80:ASP:HB2	14:L:90:ARG:O	1.96	0.65
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.65
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.32	0.65
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.79	0.65
1:O:1160:G:H5'	1:O:1161:A:C5'	2.26	0.65
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.11	0.65
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.77	0.65
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.78	0.65
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.11	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.41	0.65
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.12	0.65
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.79	0.65
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.79	0.65
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.78	0.65
1:O:544:G:C2'	1:O:545:G:H5''	2.27	0.64
9:F:91:VAL:CG1	9:F:92:GLY:H	2.05	0.64
1:O:2505:G:O2'	1:O:2506:A:H5'	1.97	0.64
1:O:2748:G:H1'	39:O:8415:HOH:O	1.96	0.64
1:O:2749:U:H5'	39:O:8438:HOH:O	1.95	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.27	0.64
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.27	0.64
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.97	0.64
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.62	0.64
22:T:26:THR:HA	22:T:39:ASN:HB3	1.80	0.64
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.79	0.64
1:O:949:U:H4'	19:Q:95:GLU:HA	1.77	0.64
1:O:1116:U:O2'	1:O:1118:A:C2	2.45	0.64
1:O:2426:G:H1'	39:O:6604:HOH:O	1.97	0.64
4:A:199:HIS:CD2	4:A:201:PHE:H	2.14	0.64
12:J:19:MET:CE	12:J:132:LEU:HD11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:HG22	15:M:166:ALA:N	2.11	0.64
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.24	0.64
1:0:138:U:H5''	1:0:139:C:OP2	1.97	0.64
1:0:220:C:H1'	39:0:6283:HOH:O	1.97	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.98	0.64
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.28	0.64
1:0:2649:A:H5'	1:0:2649:A:H8	1.61	0.64
12:J:45:VAL:HG23	12:J:130:VAL:O	1.98	0.64
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.64
25:W:125:HIS:CD2	25:W:127:GLY:H	2.16	0.64
1:0:1730:G:H5'	1:0:1731:C:C5	2.33	0.64
5:B:254:GLN:HG2	5:B:255:GLY:N	2.12	0.64
8:E:15:GLN:HG2	8:E:19:ASP:O	1.98	0.64
1:0:1819:G:H2'	1:0:1820:G:H4'	1.79	0.64
39:0:6051:HOH:O	5:B:298:LYS:HG2	1.96	0.64
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.33	0.64
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.12	0.64
11:H:170:ASN:HD22	11:H:170:ASN:N	1.95	0.64
1:0:1183:C:N4	1:0:1184:C:H41	1.96	0.64
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.80	0.64
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.79	0.63
7:D:99:ASP:HB2	7:D:103:ASN:H	1.63	0.63
1:0:2908:A:H2'	1:0:2909:G:O4'	1.98	0.63
2:9:3051:A:H5'	16:N:160:SER:HB3	1.79	0.63
7:D:172:VAL:HG12	7:D:173:GLU:N	2.13	0.63
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.27	0.63
1:0:263:U:O4'	9:F:59:ILE:HD13	1.97	0.63
25:W:13:MET:CE	25:W:17:ILE:HG22	2.28	0.63
1:0:1299:G:O6	14:L:6:ARG:HD3	1.99	0.63
1:0:2643:G:H5''	39:0:4494:HOH:O	1.97	0.63
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.64	0.63
1:0:316:A:H5'	22:T:54:ASP:OD2	1.98	0.63
39:0:5990:HOH:O	10:G:12:ILE:HA	1.98	0.63
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.79	0.63
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.32	0.63
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.28	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.63
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.33	0.63
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.63
1:0:1687:C:O2	29:1:9:GLY:HA2	1.99	0.63
4:A:131:HIS:O	4:A:132:ASP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.80	0.63
1:0:12:U:H2'	1:0:13:G:H5'	1.81	0.63
3:4:176:DA:O4'	3:4:175:C:H2'	1.99	0.63
18:P:115:SER:N	18:P:118:GLN:HE21	1.92	0.63
22:T:115:GLU:HG3	22:T:116:ASP:N	2.14	0.63
5:B:143:ILE:HD13	5:B:163:GLU:HG3	1.80	0.63
1:0:1201:C:H5''	39:0:6740:HOH:O	1.97	0.62
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.62
2:9:3006:C:C5'	16:N:37:ARG:HH12	2.10	0.62
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.79	0.62
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.33	0.62
16:N:115:VAL:HG22	39:N:9354:HOH:O	1.98	0.62
1:0:902:G:N7	14:L:18:HIS:HD2	1.97	0.62
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.81	0.62
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.81	0.62
11:H:166:SER:CB	11:H:167:PRO:HD3	2.30	0.62
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.80	0.62
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.97	0.62
1:0:870:G:C2'	1:0:871:G:H5''	2.27	0.62
1:0:1166:A:H61	1:0:1180:U:H3	1.48	0.62
1:0:2346:C:O2'	7:D:52:THR:HG21	1.99	0.62
12:J:130:VAL:HG12	12:J:131:THR:H	1.63	0.62
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.81	0.62
14:L:133:VAL:HA	39:L:9470:HOH:O	2.00	0.62
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.29	0.62
18:P:9:LEU:O	18:P:13:VAL:HG12	1.99	0.62
1:0:681:G:N3	1:0:681:G:H5'	2.15	0.62
1:0:834:G:H4'	1:0:835:U:OP2	2.00	0.62
1:0:1189:A:H3'	39:0:8199:HOH:O	2.00	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.62
39:0:3148:HOH:O	18:P:81:LYS:HG2	1.98	0.62
4:A:33:GLU:O	4:A:34:ASP:HB2	1.99	0.62
17:O:21:SER:OG	17:O:106:PRO:HB2	1.98	0.62
1:0:516:A:H5'	39:0:6177:HOH:O	2.00	0.62
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.30	0.62
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.82	0.62
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.82	0.62
1:0:396:U:O2'	1:0:418:C:H4'	2.00	0.62
1:0:558:C:H2'	1:0:559:U:C5'	2.29	0.62
2:9:3013:A:O2'	2:9:3014:G:H5''	1.99	0.62
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:77:VAL:O	21:S:80:ARG:HG2	1.99	0.62
1:O:474:C:O3'	6:C:73:LEU:HD21	2.00	0.61
1:O:2765:C:H4'	39:O:6051:HOH:O	2.00	0.61
39:O:6988:HOH:O	27:Y:141:THR:HG23	2.00	0.61
30:2:18:ASN:ND2	30:2:40:ARG:H	1.97	0.61
1:O:2524:G:H21	1:O:2526:C:H41	1.47	0.61
4:A:35:GLY:O	4:A:36:ASP:HB3	1.98	0.61
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.29	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	1.98	0.61
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.66	0.61
17:O:87:THR:O	17:O:91:GLN:HG3	2.00	0.61
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.30	0.61
29:1:10:LYS:HG3	39:1:9491:HOH:O	1.99	0.61
1:O:2649:A:H5'	1:O:2649:A:C8	2.36	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
5:B:40:GLY:HA3	39:B:9578:HOH:O	1.99	0.61
12:J:75:PRO:HD3	12:J:136:SER:OG	2.00	0.61
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.81	0.61
1:O:877:G:H5'	1:O:878:G:OP1	1.99	0.61
1:O:2578:G:H5'	1:O:2578:G:H8	1.65	0.61
4:A:192:VAL:HB	39:A:9584:HOH:O	1.99	0.61
1:O:69:A:H5'	1:O:69:A:H8	1.66	0.61
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.81	0.61
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.20	0.61
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.83	0.61
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.61
1:O:123:U:H5'	39:O:7142:HOH:O	1.98	0.61
1:O:289:G:N2	1:O:363:A:H2	1.98	0.61
1:O:1333:U:H2'	1:O:1334:C:C6	2.36	0.61
20:R:44:VAL:O	20:R:48:GLU:HG3	2.00	0.61
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.33	0.61
1:O:2064:U:H5'	1:O:2652:U:H4'	1.82	0.61
11:H:63:GLU:HA	39:H:9545:HOH:O	2.00	0.61
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.83	0.61
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.95	0.61
25:W:149:LEU:HG	25:W:153:MET:CE	2.31	0.61
1:O:2502:C:H2'	1:O:2503:A:H5'	1.83	0.60
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.59	0.60
11:H:27:LYS:N	11:H:59:HIS:HD2	1.98	0.60
27:Y:212:ARG:HD2	39:Y:9394:HOH:O	2.00	0.60
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:447:A:P	22:T:1:SER:HB2	2.41	0.60
1:0:969:G:H1	1:0:999:C:H42	1.46	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.64	0.60
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.85	0.60
1:0:2541:U:H5'	39:0:3021:HOH:O	1.99	0.60
1:0:1681:G:H5''	1:0:1682:A:H5'	1.83	0.60
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.02	0.60
15:M:182:LYS:O	15:M:194:ALA:HB2	2.01	0.60
1:0:558:C:C2'	1:0:559:U:H5''	2.32	0.60
1:0:558:C:O2'	1:0:559:U:H5''	2.02	0.60
1:0:1701:A:H4'	1:0:1702:U:C5'	2.31	0.60
1:0:1748:U:H4'	39:0:7959:HOH:O	2.02	0.60
1:0:2502:C:C2'	1:0:2503:A:H5'	2.32	0.60
39:0:7351:HOH:O	15:M:178:LYS:HB2	2.01	0.60
17:O:97:SER:OG	17:O:100:GLN:HG3	2.01	0.60
28:Z:17:ARG:HD3	39:Z:9220:HOH:O	2.02	0.60
1:0:164:G:H4'	14:L:30:ARG:HD3	1.84	0.60
1:0:1116:U:H3	1:0:1246:A:H62	1.49	0.60
7:D:50:VAL:O	7:D:71:ALA:HA	2.02	0.60
13:K:55:VAL:HG12	13:K:56:SER:N	2.16	0.60
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.66	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.15	0.60
29:1:25:LYS:CD	30:2:49:GLU:H	2.09	0.60
1:0:272:A:H5'	1:0:273:G:OP2	2.01	0.60
1:0:558:C:H2'	1:0:559:U:H5'	1.84	0.60
1:0:1168:C:H4'	39:I:5128:HOH:O	2.01	0.60
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.84	0.60
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.82	0.60
32:I:92:PRO:C	32:I:94:GLU:H	2.04	0.60
1:0:88:G:H2'	1:0:89:G:C8	2.36	0.60
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.31	0.60
18:P:64:GLU:HG2	39:P:163:HOH:O	2.01	0.60
31:3:65:THR:HG22	31:3:67:LEU:HG	1.82	0.60
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.83	0.59
5:B:238:ASN:ND2	5:B:240:GLY:H	1.94	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.32	0.59
1:0:2769:C:C2'	1:0:2770:G:H5'	2.33	0.59
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.84	0.59
11:H:166:SER:HB2	11:H:167:PRO:CD	2.32	0.59
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.59
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.83	0.59
1:0:2718:C:H6	1:0:2718:C:H5'	1.66	0.59
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.15	0.59
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.31	0.59
16:N:164:ASP:CG	16:N:167:ASP:HA	2.22	0.59
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.36	0.59
1:0:291:C:H2'	1:0:292:G:O4'	2.02	0.59
2:9:3049:G:H5''	39:N:9343:HOH:O	2.01	0.59
6:C:107:ARG:HB3	6:C:107:ARG:HH11	1.66	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.59
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.83	0.59
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.67	0.59
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.85	0.59
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.84	0.59
1:0:1119:G:H8	12:J:52:GLN:HE22	1.51	0.59
1:0:1183:C:H2'	39:0:6750:HOH:O	2.02	0.59
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.32	0.59
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.83	0.59
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.18	0.59
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.84	0.59
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.15	0.59
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.83	0.59
11:H:154:TYR:HB2	39:H:9557:HOH:O	2.03	0.59
16:N:162:ASP:HA	39:N:9330:HOH:O	2.03	0.59
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.75	0.59
5:B:297:VAL:HB	39:B:9536:HOH:O	2.02	0.59
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.13	0.59
7:D:59:GLY:O	7:D:61:PHE:N	2.36	0.59
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.85	0.59
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.38	0.59
1:0:244:C:OP2	9:F:38:LYS:HE3	2.02	0.59
1:0:1080:C:H4'	1:0:1081:A:OP1	2.03	0.59
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.85	0.59
1:0:1666:C:H2'	1:0:1667:A:H5'	1.84	0.59
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.59
6:C:236:THR:HG22	6:C:239:ALA:CB	2.32	0.59
8:E:34:TRP:O	12:J:127:ILE:HD11	2.02	0.59
11:H:56:GLN:NE2	11:H:126:ARG:HE	2.01	0.59
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.18	0.59
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:657:G:OP1	6:C:27:ARG:NH2	2.28	0.58
1:0:1189:A:H1'	1:0:1209:C:O4'	2.03	0.58
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.33	0.58
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.02	0.58
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.58
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.32	0.58
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.67	0.58
1:0:1119:G:H8	12:J:52:GLN:NE2	2.00	0.58
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.33	0.58
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.19	0.58
18:P:16:VAL:HG12	18:P:17:GLY:N	2.17	0.58
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.04	0.58
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.68	0.58
1:0:775:G:OP1	29:1:16:HIS:HE1	1.87	0.58
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.58
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.68	0.58
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.86	0.58
24:V:12:THR:HG22	24:V:15:GLU:CG	2.23	0.58
22:T:40:VAL:HG22	22:T:41:ARG:N	2.19	0.58
32:I:138:THR:HG22	32:I:139:ILE:H	1.68	0.58
1:0:1641:A:H2'	1:0:1642:A:H5'	1.84	0.58
1:0:2866:U:H4'	1:0:2867:G:H5'	1.84	0.58
22:T:71:VAL:HG12	22:T:72:ILE:N	2.18	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.86	0.58
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.86	0.58
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.85	0.58
15:M:77:HIS:HD2	15:M:79:ALA:O	1.86	0.58
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.95	0.58
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.69	0.58
25:W:139:GLY:O	25:W:141:HIS:HD2	1.87	0.58
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.04	0.58
1:0:20:G:H21	20:R:117:HIS:HD2	1.52	0.57
1:0:883:U:H2'	1:0:883:U:O2	2.04	0.57
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.57
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.86	0.57
24:V:39:ALA:N	24:V:40:PRO:CD	2.67	0.57
1:0:506:G:H22	1:0:509:A:H5'	1.69	0.57
1:0:2883:A:H2'	1:0:2884:G:O4'	2.04	0.57
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.68	0.57
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.86	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:709:G:O2'	17:O:25:VAL:HG12	2.04	0.57
4:A:163:GLY:HA2	4:A:166:ASP:OD2	2.03	0.57
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.85	0.57
32:I:113:HIS:N	32:I:114:PRO:HD2	2.19	0.57
1:0:441:A:H1'	1:0:442:A:N7	2.19	0.57
39:O:9698:HOH:O	5:B:214:PRO:HD2	2.02	0.57
4:A:105:VAL:HG13	4:A:155:THR:O	2.04	0.57
5:B:125:GLU:O	5:B:129:ARG:HG3	2.03	0.57
6:C:214:THR:HG23	39:C:9635:HOH:O	2.03	0.57
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.85	0.57
9:F:21:GLU:O	9:F:24:ARG:HG3	2.04	0.57
1:0:2807:U:P	5:B:27:ASN:HD21	2.28	0.57
7:D:138:GLY:N	39:D:7597:HOH:O	2.37	0.57
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.18	0.57
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.87	0.57
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.39	0.57
12:J:131:THR:HB	12:J:134:GLU:OE1	2.04	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.42	0.57
16:N:169:PRO:O	16:N:172:PHE:HB3	2.05	0.57
1:0:2769:C:O2'	1:0:2770:G:H5'	2.05	0.57
2:9:3004:G:H21	16:N:44:ARG:NH1	2.02	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.57
1:0:797:A:H5'	28:Z:10:ARG:N	2.20	0.57
5:B:85:ARG:NH1	39:B:9565:HOH:O	2.37	0.57
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.23	0.57
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.05	0.57
16:N:110:THR:HB	16:N:113:SER:OG	2.04	0.57
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.85	0.57
1:0:450:C:OP1	6:C:184:ARG:NH2	2.38	0.56
1:0:475:G:OP1	6:C:73:LEU:HD22	2.05	0.56
1:0:1377:C:H5'	1:0:1377:C:C6	2.36	0.56
5:B:305:ASP:O	5:B:306:LYS:HB2	2.05	0.56
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.86	0.56
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.70	0.56
1:0:1189:A:H1'	1:0:1209:C:C1'	2.35	0.56
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.69	0.56
2:9:3064:C:H2'	2:9:3065:A:H5'	1.87	0.56
4:A:36:ASP:C	4:A:38:ILE:H	2.09	0.56
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.87	0.56
12:J:74:ARG:O	12:J:78:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1972:U:H2'	1:0:1973:A:H5'	1.86	0.56
5:B:62:ARG:HA	5:B:65:MET:HE3	1.87	0.56
6:C:168:ARG:NH2	6:C:190:ALA:O	2.38	0.56
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.35	0.56
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.25	0.56
16:N:37:ARG:NE	39:N:9332:HOH:O	2.38	0.56
17:O:25:VAL:HG23	17:O:26:TRP:H	1.70	0.56
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.06	0.56
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.68	0.56
32:I:102:VAL:O	32:I:106:LYS:HG3	2.05	0.56
1:0:328:U:O4'	6:C:202:THR:HG22	2.05	0.56
1:0:1352:A:O2'	1:0:1353:C:OP1	2.23	0.56
39:0:9968:HOH:O	29:1:1:THR:HA	2.06	0.56
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.88	0.56
1:0:625:U:H5''	1:0:1044:C:N4	2.20	0.56
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.88	0.56
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.87	0.56
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.36	0.56
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.03	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.68	0.56
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.21	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
5:B:96:PRO:HG3	39:B:9565:HOH:O	2.05	0.56
15:M:57:LYS:HE2	15:M:140:ALA:O	2.04	0.56
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.87	0.56
1:0:137:U:H2'	1:0:139:C:C5	2.40	0.56
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.05	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
4:A:34:ASP:OD1	4:A:35:GLY:N	2.39	0.56
4:A:39:ALA:O	4:A:61:GLU:HG3	2.06	0.56
5:B:254:GLN:HG3	39:B:9468:HOH:O	2.05	0.56
18:P:40:VAL:O	18:P:44:VAL:HG23	2.06	0.56
1:0:380:A:H2'	39:0:7690:HOH:O	2.05	0.56
1:0:1773:G:C8	28:Z:16:ALA:HA	2.40	0.56
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.21	0.56
6:C:79:ARG:O	6:C:87:ARG:HG2	2.06	0.56
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.87	0.56
18:P:103:THR:O	18:P:107:GLU:HG3	2.06	0.56
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.40	0.56
1:0:1979:G:O2'	1:0:1980:U:OP1	2.21	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.56
6:C:246:ARG:NE	39:C:9622:HOH:O	2.39	0.56
14:L:119:THR:HG23	14:L:139:SER:OG	2.06	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.06	0.55
2:9:3008:G:O6	16:N:11:ARG:NH1	2.38	0.55
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.21	0.55
12:J:47:THR:HG22	12:J:48:GLY:N	2.22	0.55
13:K:30:LYS:O	13:K:55:VAL:HG13	2.06	0.55
1:0:121:U:OP2	30:2:10:ARG:NH2	2.35	0.55
1:0:1189:A:O2'	1:0:1208:C:H2'	2.05	0.55
15:M:68:ARG:O	15:M:68:ARG:HD3	2.06	0.55
28:Z:13:ARG:HD3	39:Z:9216:HOH:O	2.06	0.55
28:Z:29:ILE:O	28:Z:33:MET:HB2	2.06	0.55
32:I:106:LYS:O	32:I:110:GLU:HG3	2.06	0.55
7:D:103:ASN:ND2	7:D:134:LEU:H	2.03	0.55
7:D:154:LYS:HD2	7:D:154:LYS:N	2.18	0.55
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.71	0.55
11:H:170:ASN:N	11:H:170:ASN:ND2	2.55	0.55
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.36	0.55
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.54	0.55
6:C:104:ASP:CA	6:C:107:ARG:HH12	2.09	0.55
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.88	0.55
15:M:107:ARG:NH1	39:M:9383:HOH:O	2.40	0.55
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.55
32:I:129:VAL:O	32:I:129:VAL:HG12	2.07	0.55
1:0:256:C:H2'	1:0:257:G:O4'	2.07	0.55
1:0:2533:C:H5'	1:0:2533:C:C6	2.41	0.55
4:A:105:VAL:HG12	4:A:106:CYS:N	2.21	0.55
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.88	0.55
21:S:37:VAL:O	21:S:41:VAL:HG23	2.06	0.55
7:D:25:MET:CE	7:D:37:ALA:HB1	2.36	0.55
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.89	0.55
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.87	0.55
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.22	0.55
1:0:1384:C:H5'	26:X:30:MET:HG2	1.86	0.55
39:0:7993:HOH:O	31:3:60:LYS:HG3	2.07	0.55
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.99	0.55
25:W:38:THR:HG22	25:W:39:ASP:N	2.22	0.55
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.06	0.55
1:0:1159:G:H1	1:0:1208:C:H42	1.53	0.55
2:9:3064:C:C2'	2:9:3065:A:H5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.88	0.55
1:0:316:A:N3	1:0:336:G:O2'	2.36	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.88	0.55
1:0:1919:A:H4'	39:0:5389:HOH:O	2.07	0.55
1:0:185:G:H4'	1:0:186:A:H4'	1.88	0.55
1:0:1943:C:H4'	4:A:211:LYS:O	2.07	0.55
1:0:2851:G:O2'	1:0:2852:A:H5'	2.06	0.55
1:0:2896:A:N3	1:0:2896:A:H2'	2.22	0.55
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.89	0.55
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.88	0.55
6:C:115:LEU:O	6:C:118:THR:HB	2.06	0.55
10:G:64:ASN:HD22	10:G:64:ASN:N	2.02	0.55
28:Z:37:HIS:O	28:Z:45:ASP:HA	2.07	0.55
1:0:2645:U:C6	1:0:2645:U:OP2	2.59	0.54
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.07	0.54
5:B:145:HIS:HD2	5:B:146:THR:O	1.90	0.54
6:C:236:THR:HG21	39:C:9574:HOH:O	2.07	0.54
22:T:78:THR:HB	22:T:87:VAL:O	2.08	0.54
1:0:1119:G:N2	1:0:1246:A:N1	2.55	0.54
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.42	0.54
6:C:139:VAL:HG13	39:C:9645:HOH:O	2.07	0.54
6:C:246:ARG:HH11	6:C:246:ARG:CB	2.18	0.54
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.22	0.54
27:Y:144:ARG:NH1	39:Y:9370:HOH:O	2.39	0.54
29:1:25:LYS:HE2	39:2:7213:HOH:O	2.06	0.54
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.36	0.54
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.56	0.54
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.72	0.54
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.54
1:0:475:G:C5'	6:C:73:LEU:HD23	2.38	0.54
2:9:3114:G:O6	16:N:11:ARG:HD3	2.08	0.54
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.89	0.54
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.89	0.54
9:F:46:GLU:O	9:F:73:PRO:HD2	2.06	0.54
26:X:41:PHE:O	26:X:43:VAL:HG23	2.08	0.54
31:3:35:TRP:HB2	39:3:9489:HOH:O	2.08	0.54
1:0:1462:C:H2'	1:0:1463:A:C8	2.43	0.54
1:0:1552:G:N2	1:0:1634:G:H1'	2.23	0.54
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.54
23:U:52:THR:HG22	23:U:55:ALA:H	1.72	0.54
25:W:4:LEU:O	25:W:32:CYS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.90	0.54
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.54
1:0:1634:G:H3'	39:0:4461:HOH:O	2.08	0.54
39:C:9557:HOH:O	17:O:3:THR:HG21	2.06	0.54
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.08	0.54
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.38	0.54
1:0:317:A:H5''	22:T:52:ARG:HD2	1.90	0.54
6:C:233:THR:HG22	6:C:234:VAL:N	2.22	0.54
7:D:135:VAL:HG22	7:D:136:ARG:H	1.72	0.54
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.89	0.54
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.90	0.54
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.90	0.54
24:V:64:GLY:O	24:V:65:ASP:HB2	2.06	0.54
1:0:588:G:O6	25:W:154:ARG:NH1	2.41	0.54
1:0:920:C:H5''	1:0:921:G:O5'	2.08	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.54
7:D:99:ASP:HB3	7:D:101:THR:H	1.73	0.54
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.90	0.54
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.37	0.54
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.36	0.54
13:K:125:ALA:C	13:K:127:ALA:H	2.10	0.54
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.07	0.54
1:0:485:A:N3	1:0:487:G:H5''	2.23	0.54
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.54
39:0:7254:HOH:O	16:N:4:PRO:HD2	2.07	0.54
2:9:3049:G:O2'	2:9:3050:G:H5'	2.07	0.54
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.90	0.54
1:0:1667:A:H5'	1:0:1667:A:C8	2.36	0.53
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.08	0.53
4:A:121:ALA:O	4:A:124:VAL:HG22	2.09	0.53
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.89	0.53
9:F:57:GLU:O	9:F:61:MET:HG3	2.08	0.53
13:K:75:ARG:HD3	13:K:112:PRO:O	2.08	0.53
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.08	0.53
27:Y:133:HIS:HD2	39:Y:9376:HOH:O	1.91	0.53
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.08	0.53
1:0:1477:C:O2'	1:0:1478:U:H5'	2.08	0.53
1:0:2003:U:H4'	1:0:2004:U:H5	1.71	0.53
1:0:2481:G:H5''	39:0:5095:HOH:O	2.07	0.53
5:B:102:THR:HG21	5:B:182:VAL:O	2.09	0.53
12:J:39:VAL:HG13	12:J:106:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:39:THR:HG22	20:R:107:GLU:O	2.09	0.53
1:0:1118:A:H8	1:0:1119:G:H5''	1.73	0.53
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.91	0.53
25:W:52:VAL:HG22	25:W:53:ALA:N	2.23	0.53
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.22	0.53
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.89	0.53
1:0:120:A:H5'	29:1:20:ARG:HH21	1.74	0.53
1:0:288:A:H2'	1:0:289:G:C8	2.43	0.53
1:0:1209:C:H2'	1:0:1210:G:C8	2.43	0.53
1:0:1878:G:O2'	1:0:1879:U:OP2	2.25	0.53
1:0:2779:G:H21	8:E:143:GLN:NE2	2.06	0.53
9:F:38:LYS:NZ	15:M:3:SER:HA	2.23	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.24	0.53
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.89	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
1:0:797:A:H4'	28:Z:10:ARG:N	2.24	0.53
1:0:1666:C:H2'	1:0:1667:A:C5'	2.38	0.53
1:0:2852:A:H5''	39:0:5769:HOH:O	2.06	0.53
39:0:5941:HOH:O	4:A:164:ARG:CZ	2.56	0.53
39:0:9737:HOH:O	15:M:82:ARG:HD2	2.09	0.53
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.91	0.53
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.38	0.53
25:W:64:THR:O	25:W:68:THR:HG22	2.08	0.53
1:0:2815:G:N7	12:J:80:LYS:NZ	2.57	0.53
1:0:2866:U:C4	23:U:50:GLU:HB3	2.44	0.53
39:0:5511:HOH:O	11:H:58:ARG:HG3	2.08	0.53
4:A:89:ALA:HB3	39:A:9617:HOH:O	2.07	0.53
5:B:41:PHE:HA	5:B:79:MET:HE2	1.89	0.53
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.90	0.53
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.23	0.53
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.08	0.53
1:0:1730:G:H5'	1:0:1731:C:C6	2.44	0.53
7:D:94:ALA:HA	7:D:174:VAL:HA	1.91	0.53
17:O:98:LEU:O	17:O:102:ILE:HG13	2.09	0.53
22:T:40:VAL:HG22	22:T:41:ARG:H	1.74	0.53
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.90	0.53
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.08	0.53
1:0:95:A:H5''	1:0:97:G:O4'	2.09	0.53
1:0:482:G:H4'	1:0:508:A:N1	2.24	0.53
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.71	0.53
1:0:1595:G:O2'	1:0:1596:U:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1981:A:H1'	1:0:1983:C:N4	2.24	0.53
16:N:183:ASP:O	16:N:184:ILE:O	2.26	0.53
32:I:102:VAL:HG23	32:I:140:GLU:O	2.09	0.53
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.44	0.53
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.09	0.53
7:D:25:MET:SD	7:D:40:ILE:HD11	2.49	0.53
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.09	0.53
10:G:20:VAL:O	10:G:24:VAL:HG23	2.09	0.53
25:W:29:VAL:O	25:W:30:ASN:HB2	2.09	0.53
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.08	0.53
1:0:926:A:O2'	14:L:41:HIS:HD2	1.92	0.52
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.52
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.74	0.52
1:0:2103:A:H8	1:0:2103:A:H5''	1.74	0.52
1:0:2421:G:H1'	39:0:4276:HOH:O	2.08	0.52
2:9:3028:U:H2'	2:9:3029:C:C6	2.44	0.52
12:J:19:MET:HE2	12:J:79:PHE:HA	1.89	0.52
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.08	0.52
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.08	0.52
1:0:1835:U:C5	1:0:1840:A:N7	2.66	0.52
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.44	0.52
28:Z:10:ARG:HA	39:Z:9215:HOH:O	2.09	0.52
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.91	0.52
1:0:737:A:H2'	1:0:738:G:O4'	2.10	0.52
1:0:2265:U:H2'	1:0:2266:A:C8	2.44	0.52
1:0:2486:A:H2	3:4:177:TSE:H2P2	1.74	0.52
4:A:88:ILE:O	4:A:88:ILE:HG22	2.08	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.52
24:V:1:THR:HG23	24:V:2:VAL:N	2.18	0.52
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.89	0.52
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.52
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.52
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.73	0.52
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.38	0.52
5:B:254:GLN:NE2	39:B:9523:HOH:O	2.42	0.52
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.36	0.52
1:0:162:C:H2'	1:0:163:U:H5'	1.91	0.52
1:0:1205:U:H2'	1:0:1206:U:H5''	1.92	0.52
1:0:2896:A:H2'	39:0:6611:HOH:O	2.09	0.52
4:A:65:ARG:C	4:A:66:ARG:HG3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.75	0.52
20:R:39:THR:HB	20:R:42:GLU:HG3	1.92	0.52
1:0:1555:G:H4'	1:0:1630:A:C2	2.44	0.52
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.10	0.52
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.52
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.09	0.52
26:X:31:ILE:O	26:X:35:GLU:HG3	2.09	0.52
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.10	0.52
1:0:622:G:P	27:Y:148:GLY:HA3	2.49	0.52
1:0:2414:A:H2'	1:0:2415:A:C8	2.45	0.52
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.43	0.52
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.45	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.52
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.42	0.52
1:0:343:C:O2'	1:0:344:C:H5'	2.10	0.52
1:0:1626:A:H2'	1:0:1627:G:O4'	2.10	0.52
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.10	0.52
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.45	0.52
5:B:185:GLY:HA2	39:B:9564:HOH:O	2.10	0.52
6:C:25:PRO:HG2	39:C:9519:HOH:O	2.09	0.52
14:L:136:ALA:HB3	39:L:9470:HOH:O	2.10	0.52
25:W:88:THR:CG2	25:W:89:ASP:H	2.23	0.52
30:2:41:HIS:HD2	30:2:44:ARG:H	1.58	0.52
1:0:603:A:H5''	1:0:604:G:OP1	2.09	0.52
1:0:653:C:H2'	1:0:654:A:C8	2.44	0.52
1:0:1314:U:H2'	39:0:6396:HOH:O	2.09	0.52
2:9:3107:C:H5	39:9:3167:HOH:O	1.93	0.52
20:R:9:ASP:O	20:R:13:THR:HB	2.10	0.52
1:0:299:U:H5'	39:0:7788:HOH:O	2.09	0.51
1:0:1252:A:H2'	1:0:1253:C:O4'	2.10	0.51
1:0:1730:G:C5'	1:0:1731:C:C6	2.93	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.88	0.51
6:C:154:VAL:O	6:C:158:GLU:HG3	2.10	0.51
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.40	0.51
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.39	0.51
10:G:12:ILE:N	10:G:13:PRO:CD	2.73	0.51
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.25	0.51
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.92	0.51
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.30	0.51
23:U:5:GLU:HG2	23:U:10:GLY:O	2.10	0.51
8:E:84:MET:HE3	8:E:148:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:82:GLU:O	20:R:86:LYS:HG3	2.10	0.51
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.11	0.51
31:3:62:THR:HB	39:3:9484:HOH:O	2.09	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.40	0.51
12:J:99:GLU:HA	39:J:7377:HOH:O	2.10	0.51
16:N:147:ILE:HB	39:N:9343:HOH:O	2.10	0.51
2:9:3045:A:H4'	7:D:143:LYS:O	2.11	0.51
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.91	0.51
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.41	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.26	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.51
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.40	0.51
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.11	0.51
1:0:2591:C:H2'	1:0:2592:G:O4'	2.10	0.51
10:G:16:LYS:O	10:G:20:VAL:HG23	2.11	0.51
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.92	0.51
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.35	0.51
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.10	0.51
2:9:3044:A:O4'	7:D:76:ARG:NE	2.44	0.51
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.38	0.51
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.40	0.51
18:P:141:ILE:C	18:P:143:ALA:H	2.14	0.51
24:V:39:ALA:C	24:V:41:GLU:H	2.14	0.51
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.92	0.51
1:0:292:G:H2'	1:0:358:G:N2	2.26	0.51
1:0:558:C:C2'	1:0:559:U:C5'	2.89	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.46	0.51
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.11	0.51
1:0:2333:G:P	7:D:56:ARG:HH22	2.33	0.51
2:9:3039:U:HO2'	2:9:3042:C:H5	1.52	0.51
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.39	0.51
4:A:232:ARG:NH2	4:A:236:GLY:O	2.41	0.51
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.23	0.51
30:2:41:HIS:H	30:2:45:ASN:ND2	1.91	0.51
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.51
1:0:757:C:OP1	14:L:27:ARG:HD2	2.11	0.51
1:0:1278:A:H4'	1:0:1279:U:C4	2.46	0.51
6:C:236:THR:HA	39:C:9648:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:89:GLY:O	16:N:92:ALA:HB3	2.11	0.51
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.40	0.51
30:2:41:HIS:N	30:2:45:ASN:HD22	1.91	0.51
1:0:1242:A:C5'	12:J:82:THR:HG23	2.32	0.50
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.10	0.50
4:A:53:ALA:HB3	39:A:9597:HOH:O	2.11	0.50
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.92	0.50
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.29	0.50
20:R:29:LYS:NZ	39:R:9453:HOH:O	2.44	0.50
22:T:71:VAL:HG13	22:T:91:LEU:O	2.10	0.50
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.25	0.50
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.41	0.50
1:0:2717:C:O2'	1:0:2718:C:H5''	2.11	0.50
4:A:132:ASP:OD1	4:A:133:ARG:N	2.44	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.92	0.50
1:0:1789:G:O6	18:P:73:HIS:HE1	1.94	0.50
1:0:2486:A:C2	3:4:177:TSE:H2P2	2.46	0.50
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.41	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.11	0.50
25:W:149:LEU:HG	25:W:153:MET:HE2	1.92	0.50
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.12	0.50
1:0:1066:U:H2'	1:0:1067:A:C8	2.46	0.50
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.50
4:A:33:GLU:OE1	4:A:33:GLU:N	2.43	0.50
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.50
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.50
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.43	0.50
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.93	0.50
15:M:60:VAL:C	15:M:61:ILE:HD12	2.31	0.50
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.11	0.50
1:0:196:G:H2'	39:0:7143:HOH:O	2.11	0.50
1:0:466:A:OP1	30:2:38:LYS:HE2	2.11	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1506:U:H6	1:0:1506:U:H5'	1.77	0.50
1:0:1667:A:H2'	1:0:1668:U:C6	2.46	0.50
4:A:36:ASP:O	4:A:38:ILE:N	2.40	0.50
25:W:105:THR:HA	25:W:109:GLU:OE1	2.11	0.50
1:0:848:C:H5'	39:0:7729:HOH:O	2.11	0.50
1:0:1666:C:C2'	1:0:1667:A:H5''	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1946:C:H2'	1:0:1971:G:C8	2.46	0.50
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.50
5:B:175:LEU:O	5:B:175:LEU:HD23	2.12	0.50
5:B:321:PRO:HG3	39:B:9530:HOH:O	2.11	0.50
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.44	0.50
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.12	0.50
1:0:1205:U:H2'	1:0:1206:U:H5'	1.94	0.50
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.12	0.50
7:D:154:LYS:H	7:D:154:LYS:CD	2.22	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.12	0.50
11:H:27:LYS:H	11:H:59:HIS:CD2	2.22	0.50
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.94	0.50
11:H:158:THR:HB	11:H:159:PRO:HD3	1.94	0.50
12:J:15:ARG:CZ	12:J:43:ARG:HH11	2.25	0.50
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.94	0.50
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.92	0.50
1:0:204:A:C2'	1:0:205:U:H5'	2.42	0.50
1:0:1724:U:H5''	39:0:4307:HOH:O	2.11	0.50
1:0:1838:U:C1'	1:0:2644:C:H5'	2.38	0.50
1:0:1942:A:H3'	39:0:7795:HOH:O	2.11	0.50
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.77	0.50
5:B:62:ARG:HA	5:B:65:MET:HE2	1.94	0.50
7:D:60:GLU:HG3	7:D:60:GLU:O	2.11	0.50
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.42	0.50
22:T:47:THR:HB	22:T:100:ASP:HB3	1.94	0.50
24:V:29:ASN:O	24:V:33:VAL:HG23	2.12	0.50
26:X:43:VAL:HG12	26:X:44:ASP:N	2.27	0.50
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.94	0.50
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:447:A:OP2	22:T:1:SER:HB2	2.11	0.49
1:0:926:A:H5'	14:L:39:GLU:OE2	2.12	0.49
12:J:15:ARG:CZ	12:J:43:ARG:NH1	2.74	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.93	0.49
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.11	0.49
1:0:156:C:H5''	15:M:171:ARG:CD	2.31	0.49
1:0:1044:C:H5''	39:0:9648:HOH:O	2.12	0.49
1:0:1406:A:H4'	1:0:1407:A:H5''	1.94	0.49
5:B:72:THR:HB	39:B:9536:HOH:O	2.12	0.49
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.13	0.49
8:E:7:ILE:HG22	8:E:45:ASP:O	2.12	0.49
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.95	0.49
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.12	0.49
9:F:99:THR:O	9:F:100:ASP:HB2	2.12	0.49
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.94	0.49
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.13	0.49
14:L:148:GLU:HB2	39:L:9484:HOH:O	2.12	0.49
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.94	0.49
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.12	0.49
20:R:114:VAL:HB	20:R:145:LEU:HD12	1.94	0.49
1:O:119:A:H2'	1:O:120:A:H5''	1.94	0.49
1:O:284:C:H4'	1:O:285:A:H8	1.76	0.49
1:O:960:G:N3	1:O:960:G:H2'	2.28	0.49
1:O:1736:A:H1'	39:O:8078:HOH:O	2.13	0.49
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.94	0.49
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.77	0.49
12:J:54:VAL:O	12:J:58:GLU:HG3	2.12	0.49
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.27	0.49
32:I:75:THR:HA	32:I:112:LYS:NZ	2.27	0.49
32:I:113:HIS:N	32:I:114:PRO:CD	2.76	0.49
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.12	0.49
11:H:116:ALA:O	11:H:117:PHE:C	2.51	0.49
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.95	0.49
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.48	0.49
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.95	0.49
32:I:139:ILE:HG22	32:I:140:GLU:N	2.27	0.49
1:O:2812:A:C2	1:O:2814:A:N6	2.71	0.49
7:D:27:ILE:HG22	7:D:28:GLY:N	2.27	0.49
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.93	0.49
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.43	0.49
31:3:3:MET:O	31:3:90:PHE:HA	2.13	0.49
1:O:542:A:H2'	1:O:543:G:O4'	2.12	0.49
1:O:830:G:O2'	1:O:831:U:H5'	2.13	0.49
1:O:951:A:C2'	1:O:952:G:H5'	2.42	0.49
1:O:1135:G:H5'	39:O:6447:HOH:O	2.13	0.49
1:O:1926:G:H2'	1:O:1927:A:C8	2.47	0.49
1:O:1973:A:H5'	1:O:1973:A:C8	2.44	0.49
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.96	0.49
7:D:65:GLU:HA	39:D:6752:HOH:O	2.12	0.49
18:P:13:VAL:HG11	18:P:40:VAL:HG11	1.95	0.49
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.43	0.49
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.48	0.49
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.13	0.49
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.49
1:0:545:G:H5'	1:0:545:G:C8	2.46	0.49
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.13	0.49
5:B:16:ARG:NH2	39:B:9489:HOH:O	2.44	0.49
5:B:321:PRO:HA	39:B:9587:HOH:O	2.12	0.49
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.95	0.49
9:F:14:ASP:O	9:F:18:GLU:HG3	2.13	0.49
14:L:145:LEU:HD23	14:L:145:LEU:O	2.13	0.49
20:R:132:ARG:CZ	39:R:9497:HOH:O	2.61	0.49
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.76	0.49
30:2:20:ARG:HG3	30:2:21:VAL:H	1.77	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.27	0.49
1:0:1180:U:H2'	1:0:1181:A:C8	2.47	0.49
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.49
1:0:2103:A:H5''	1:0:2103:A:C8	2.47	0.49
39:0:6828:HOH:O	8:E:35:TYR:HB2	2.13	0.49
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.13	0.49
20:R:132:ARG:NH2	39:R:9497:HOH:O	2.46	0.49
24:V:12:THR:HG23	24:V:14:ALA:H	1.76	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.28	0.48
1:0:1422:U:H2'	1:0:1423:C:C6	2.48	0.48
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.13	0.48
14:L:57:VAL:HG12	14:L:57:VAL:O	2.13	0.48
16:N:152:GLU:C	16:N:154:LEU:H	2.16	0.48
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.13	0.48
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.48
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.95	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.13	0.48
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.96	0.48
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.43	0.48
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.94	0.48
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.13	0.48
27:Y:155:ARG:NH1	39:Y:9354:HOH:O	2.46	0.48
1:0:1189:A:H1'	1:0:1209:C:H1'	1.95	0.48
1:0:2679:G:H2'	1:0:2681:A:OP2	2.12	0.48
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.13	0.48
6:C:236:THR:H	6:C:239:ALA:HB3	1.78	0.48
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.43	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:11:VAL:O	25:W:12:ASN:HB2	2.12	0.48
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.95	0.48
1:0:1441:G:O2'	1:0:1442:A:H5'	2.14	0.48
1:0:2453:G:H5''	39:L:9438:HOH:O	2.13	0.48
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.44	0.48
1:0:2507:G:H2'	1:0:2510:C:H42	1.77	0.48
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.80	0.48
11:H:30:GLN:H	11:H:66:ARG:HH11	1.62	0.48
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.42	0.48
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.94	0.48
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.13	0.48
1:0:236:A:H8	1:0:236:A:OP1	1.97	0.48
1:0:2456:A:H2'	1:0:2457:U:C6	2.49	0.48
8:E:22:VAL:O	8:E:28:SER:HA	2.13	0.48
1:0:93:C:H5''	24:V:1:THR:CB	2.42	0.48
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.48
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.13	0.48
1:0:2100:A:H4'	6:C:64:GLY:O	2.14	0.48
2:9:3002:U:OP2	2:9:3003:A:H5'	2.13	0.48
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.48
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.78	0.48
6:C:93:LYS:O	6:C:98:ARG:NH2	2.44	0.48
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.95	0.48
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.17	0.48
1:0:793:A:H5''	18:P:83:LYS:HG2	1.96	0.48
1:0:1562:C:N4	39:0:6387:HOH:O	2.27	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.34	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.48
1:0:1592:G:O2'	1:0:1593:C:O4'	2.29	0.48
7:D:173:GLU:HG3	7:D:174:VAL:N	2.28	0.48
12:J:39:VAL:CG1	12:J:40:ASN:N	2.76	0.48
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.78	0.48
15:M:58:GLN:HG3	39:M:9413:HOH:O	2.13	0.48
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.96	0.48
1:0:249:G:O2'	1:0:250:C:H5'	2.14	0.48
1:0:870:G:OP2	4:A:3:ARG:HD3	2.14	0.48
1:0:2747:C:H4'	39:0:8438:HOH:O	2.13	0.48
1:0:2769:C:H2'	1:0:2770:G:H5'	1.93	0.48
1:0:2862:G:H4'	5:B:336:GLN:O	2.14	0.48
8:E:133:VAL:HG12	8:E:141:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:76:GLU:O	11:H:77:LEU:HD23	2.14	0.48
12:J:70:PHE:CG	12:J:70:PHE:O	2.66	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.29	0.48
4:A:123:GLY:HA3	4:A:162:GLY:CA	2.44	0.48
6:C:133:ARG:HH11	6:C:133:ARG:HG3	1.78	0.48
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.29	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.47
2:9:3054:A:O2'	2:9:3055:U:H5'	2.14	0.47
4:A:65:ARG:HG2	4:A:65:ARG:HH11	1.78	0.47
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.95	0.47
6:C:55:ARG:NH2	29:1:56:GLU:OE2	2.37	0.47
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.13	0.47
10:G:24:VAL:O	10:G:28:GLU:HB2	2.13	0.47
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.96	0.47
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.96	0.47
22:T:19:ARG:HD3	22:T:67:LEU:O	2.14	0.47
25:W:122:ARG:NH1	25:W:152:ALA:O	2.46	0.47
1:0:1666:C:C2'	1:0:1667:A:C5'	2.93	0.47
1:0:2415:A:O2'	16:N:29:SER:HB3	2.14	0.47
6:C:246:ARG:NH1	39:C:9570:HOH:O	2.46	0.47
14:L:92:ASP:HA	14:L:121:ILE:HB	1.94	0.47
22:T:69:LYS:O	22:T:71:VAL:HG23	2.15	0.47
24:V:12:THR:HG23	24:V:14:ALA:N	2.28	0.47
28:Z:39:CYS:HB3	28:Z:42:CYS:SG	2.53	0.47
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.47
1:0:432:G:O2'	1:0:433:C:H5'	2.14	0.47
1:0:1164:U:OP1	32:I:74:PRO:HA	2.14	0.47
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.96	0.47
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.34	0.47
1:0:1751:G:C2'	1:0:1752:G:H5''	2.41	0.47
4:A:206:ARG:HH11	4:A:206:ARG:HG3	1.80	0.47
5:B:171:VAL:HG23	5:B:172:SER:N	2.30	0.47
7:D:170:TYR:O	7:D:171:ASP:CB	2.61	0.47
11:H:45:VAL:HA	11:H:167:PRO:O	2.14	0.47
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.50	0.47
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.95	0.47
32:I:87:THR:HG22	32:I:88:GLY:N	2.29	0.47
1:0:92:G:H4'	24:V:44:GLY:HA3	1.97	0.47
1:0:816:G:H5'	1:0:1598:A:H4'	1.96	0.47
1:0:945:U:H2'	1:0:946:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	0.47
1:0:1218:U:H2'	1:0:1219:U:C6	2.49	0.47
1:0:2421:G:H4'	39:0:5318:HOH:O	2.13	0.47
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.43	0.47
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.12	0.47
12:J:130:VAL:HG12	12:J:131:THR:N	2.29	0.47
14:L:143:THR:CG2	14:L:144:ASP:N	2.77	0.47
16:N:154:LEU:O	16:N:155:GLU:CB	2.62	0.47
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.26	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.50	0.47
1:0:666:A:H2'	1:0:667:C:O4'	2.15	0.47
1:0:1168:C:H5''	32:I:87:THR:CG2	2.43	0.47
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.49	0.47
1:0:2072:G:C6	1:0:2533:C:H1'	2.50	0.47
2:9:3011:A:P	19:Q:19:ARG:HH21	2.37	0.47
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.79	0.47
16:N:154:LEU:HG	16:N:155:GLU:H	1.79	0.47
1:0:125:U:H2'	39:0:4337:HOH:O	2.15	0.47
1:0:263:U:O2	15:M:42:ARG:HD2	2.15	0.47
1:0:271:C:H41	1:0:378:A:H2	1.62	0.47
1:0:1192:A:H3'	1:0:1193:A:H5'	1.97	0.47
1:0:1745:G:H22	1:0:2033:G:H5'	1.79	0.47
1:0:2837:U:H2'	39:0:7315:HOH:O	2.15	0.47
39:0:5270:HOH:O	16:N:21:HIS:HD2	1.98	0.47
4:A:123:GLY:HA2	4:A:159:VAL:O	2.14	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.15	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.45	0.47
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.42	0.47
10:G:12:ILE:HD12	39:G:692:HOH:O	2.14	0.47
11:H:28:ILE:HG23	39:H:9545:HOH:O	2.15	0.47
12:J:45:VAL:HG22	12:J:46:ILE:N	2.30	0.47
13:K:55:VAL:CG1	13:K:56:SER:N	2.77	0.47
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.15	0.47
23:U:47:ARG:HG3	39:U:4381:HOH:O	2.14	0.47
25:W:48:VAL:O	25:W:48:VAL:CG1	2.61	0.47
25:W:72:PRO:HB2	25:W:74:GLU:O	2.14	0.47
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.29	0.47
1:0:669:G:O2'	1:0:670:G:H5'	2.15	0.47
1:0:2032:U:H2'	1:0:2033:G:H5''	1.96	0.47
1:0:2102:G:H5''	1:0:2538:A:C2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:85:ARG:HB2	5:B:99:GLU:HG2	1.96	0.47
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.95	0.47
6:C:218:VAL:HG12	39:C:9622:HOH:O	2.15	0.47
15:M:164:THR:CG2	15:M:165:GLY:N	2.77	0.47
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.96	0.47
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.50	0.47
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.50	0.47
1:0:1878:G:C1'	39:0:6632:HOH:O	2.57	0.47
1:0:2428:G:N7	31:3:60:LYS:NZ	2.62	0.47
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.47
5:B:260:HIS:HE1	39:B:9519:HOH:O	1.98	0.47
5:B:307:ARG:HD2	39:B:9583:HOH:O	2.15	0.47
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.47
25:W:88:THR:CG2	25:W:89:ASP:N	2.74	0.47
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.47	0.47
31:3:69:TYR:O	31:3:77:ALA:HA	2.14	0.47
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.14	0.47
1:0:1878:G:O2'	1:0:1879:U:C5	2.65	0.47
1:0:2032:U:H2'	1:0:2033:G:H5'	1.96	0.47
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.97	0.47
2:9:3042:C:O2	7:D:76:ARG:NH1	2.47	0.47
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.97	0.47
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.96	0.47
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.45	0.47
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.14	0.47
22:T:75:GLU:O	22:T:76:ASP:HB2	2.15	0.47
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.15	0.47
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.19	0.47
30:2:48:ASP:O	30:2:49:GLU:HB2	2.15	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.46
1:0:1714:C:O2'	1:0:1715:C:H5'	2.15	0.46
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.80	0.46
8:E:81:GLU:HG2	8:E:134:SER:CB	2.44	0.46
11:H:66:ARG:HD3	39:H:9545:HOH:O	2.14	0.46
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.64	0.46
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.60	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.97	0.46
25:W:108:ARG:HE	25:W:114:PRO:CG	2.28	0.46
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.46	0.46
1:0:1902:G:H2'	1:0:1903:U:O4'	2.15	0.46
1:0:2361:A:H2'	1:0:2362:A:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2508:C:H2'	39:0:7236:HOH:O	2.15	0.46
1:0:2769:C:H2'	1:0:2770:G:O4'	2.16	0.46
7:D:172:VAL:CG1	7:D:173:GLU:H	2.27	0.46
8:E:15:GLN:NE2	8:E:40:VAL:O	2.48	0.46
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.50	0.46
1:0:248:A:H5'	1:0:249:G:OP2	2.16	0.46
1:0:396:U:H1'	39:0:8148:HOH:O	2.15	0.46
1:0:969:G:H1	1:0:999:C:N4	2.12	0.46
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.46
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.14	0.46
39:0:4789:HOH:O	30:2:38:LYS:HE3	2.15	0.46
4:A:97:ALA:C	4:A:131:HIS:HE2	2.17	0.46
5:B:190:MET:CE	5:B:194:PHE:CD1	2.99	0.46
5:B:274:GLU:HA	5:B:292:GLY:O	2.16	0.46
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.97	0.46
1:0:958:G:H2'	1:0:959:C:C6	2.50	0.46
1:0:1369:A:H4'	20:R:64:SER:OG	2.16	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.80	0.46
9:F:38:LYS:HZ3	15:M:3:SER:HA	1.79	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.46
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.31	0.46
1:0:2768:A:O2'	1:0:2769:C:H5'	2.15	0.46
1:0:2820:A:H2'	1:0:2821:C:C6	2.51	0.46
2:9:3024:U:H3'	2:9:3025:G:H5'	1.96	0.46
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.51	0.46
5:B:215:VAL:HB	5:B:234:ARG:NH1	2.29	0.46
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.30	0.46
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.98	0.46
32:I:128:VAL:C	32:I:130:GLY:H	2.19	0.46
1:0:171:C:OP2	15:M:84:LYS:HG3	2.15	0.46
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.46
1:0:677:C:H4'	6:C:246:ARG:NH2	2.31	0.46
1:0:1205:U:C2'	1:0:1206:U:H5''	2.46	0.46
1:0:1625:U:H4'	39:0:5210:HOH:O	2.15	0.46
1:0:2032:U:C2'	1:0:2033:G:H5''	2.46	0.46
1:0:2344:G:H2'	1:0:2344:G:N3	2.30	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.16	0.46
4:A:93:THR:C	4:A:94:LEU:HD23	2.36	0.46
5:B:87:TYR:O	5:B:138:GLY:N	2.32	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:98:GLN:O	15:M:102:GLU:HG3	2.16	0.46
23:U:9:CYS:O	23:U:52:THR:HG23	2.15	0.46
1:0:263:U:C2	9:F:59:ILE:HD12	2.51	0.46
1:0:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
1:0:710:G:H5'	17:O:25:VAL:CG1	2.46	0.46
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.46
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.48	0.46
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.98	0.46
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.46
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.98	0.46
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.98	0.46
1:0:1739:G:O2'	1:0:1740:U:H5'	2.15	0.46
1:0:2238:A:O2'	1:0:2239:C:H5'	2.15	0.46
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.46
1:0:2453:G:H4'	14:L:50:GLY:C	2.36	0.46
2:9:3051:A:H5'	16:N:160:SER:CB	2.42	0.46
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.97	0.46
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.18	0.46
22:T:89:ARG:HG3	22:T:89:ARG:O	2.16	0.46
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.16	0.46
4:A:122:SER:O	4:A:124:VAL:HG13	2.15	0.46
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.49	0.46
5:B:205:VAL:O	5:B:307:ARG:NE	2.42	0.46
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.98	0.46
8:E:80:TRP:O	8:E:134:SER:HA	2.15	0.46
14:L:21:ARG:N	39:L:9428:HOH:O	2.49	0.46
20:R:106:GLY:HA2	20:R:109:MET:CE	2.46	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.51	0.46
1:0:1342:C:C2'	1:0:1343:C:H5'	2.46	0.46
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.16	0.46
14:L:73:VAL:HG23	14:L:74:THR:N	2.25	0.46
24:V:49:LEU:O	24:V:53:ILE:HG13	2.16	0.46
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.98	0.46
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.81	0.46
1:0:1118:A:C8	1:0:1119:G:H5''	2.50	0.45
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.98	0.45
1:0:2894:C:O2'	1:0:2895:C:H5'	2.15	0.45
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.51	0.45
12:J:63:ILE:HG22	12:J:64:GLY:N	2.31	0.45
13:K:80:ILE:HG23	39:K:7064:HOH:O	2.16	0.45
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:155:C:OP2	15:M:188:ARG:HD3	2.16	0.45
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.45
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.45
1:0:1406:A:H4'	1:0:1407:A:C5'	2.46	0.45
1:0:2767:C:OP1	5:B:318:ASN:ND2	2.49	0.45
1:0:2820:A:OP1	5:B:98:THR:HG22	2.17	0.45
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.45
39:9:5071:HOH:O	16:N:23:ARG:HD3	2.16	0.45
4:A:55:VAL:HG12	4:A:67:LEU:HD22	1.98	0.45
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.46	0.45
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.33	0.45
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.82	0.45
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.98	0.45
23:U:49:LEU:HG	39:U:3805:HOH:O	2.17	0.45
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.51	0.45
1:0:329:A:OP2	6:C:206:ASN:HB2	2.16	0.45
1:0:333:G:O2'	1:0:334:G:H5'	2.17	0.45
1:0:656:G:OP2	17:O:37:ARG:HD2	2.16	0.45
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.51	0.45
12:J:142:ASN:O	12:J:144:THR:N	2.50	0.45
13:K:14:LYS:HG3	13:K:32:ILE:O	2.16	0.45
15:M:74:LYS:HG2	15:M:75:ARG:N	2.30	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.67	0.45
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.45
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.45
1:0:1947:G:H2'	1:0:1948:G:C8	2.50	0.45
1:0:2326:U:H4'	1:0:2412:G:C4'	2.47	0.45
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.16	0.45
2:9:3012:C:H5'	2:9:3070:U:O4'	2.16	0.45
2:9:3091:C:H2'	2:9:3092:G:O4'	2.17	0.45
6:C:236:THR:HG22	6:C:239:ALA:HB2	1.97	0.45
9:F:117:GLU:C	9:F:119:ARG:H	2.19	0.45
10:G:64:ASN:N	10:G:64:ASN:ND2	2.64	0.45
30:2:49:GLU:HB2	39:2:131:HOH:O	2.16	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.13	0.45
1:0:949:U:C4'	19:Q:95:GLU:HA	2.44	0.45
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.99	0.45
4:A:179:MET:HG2	4:A:186:TRP:CB	2.47	0.45
8:E:77:THR:OG1	8:E:78:GLU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:81:GLU:HA	8:E:133:VAL:O	2.16	0.45
11:H:146:VAL:HG22	39:H:9542:HOH:O	2.16	0.45
26:X:80:GLU:HB3	39:X:5564:HOH:O	2.16	0.45
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.80	0.45
28:Z:36:ASP:HB3	28:Z:45:ASP:CB	2.35	0.45
1:0:2472:C:O2'	1:0:2634:G:H4'	2.17	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.52	0.45
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.43	0.45
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.81	0.45
8:E:119:HIS:HE1	8:E:147:ASP:OD2	1.98	0.45
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.52	0.45
15:M:65:VAL:HG21	15:M:105:ALA:HB2	1.99	0.45
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.47	0.45
1:0:602:A:O2'	1:0:605:C:H4'	2.16	0.45
1:0:903:U:O4	14:L:18:HIS:HB2	2.17	0.45
1:0:1314:U:H5''	1:0:1316:G:O4'	2.16	0.45
1:0:1733:A:H4'	5:B:212:GLN:HA	1.99	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
39:0:3164:HOH:O	25:W:119:HIS:HE1	2.00	0.45
39:0:5823:HOH:O	25:W:122:ARG:NH2	2.49	0.45
7:D:56:ARG:N	39:D:6752:HOH:O	2.49	0.45
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.97	0.45
11:H:169:GLY:C	11:H:170:ASN:HD22	2.20	0.45
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.31	0.45
25:W:149:LEU:HG	25:W:153:MET:HE1	1.97	0.45
1:0:526:U:H2'	1:0:527:U:C6	2.52	0.45
1:0:871:G:H5''	1:0:871:G:H8	1.74	0.45
1:0:1333:U:H2'	1:0:1334:C:H6	1.81	0.45
1:0:2104:C:O2	1:0:2485:A:N1	2.49	0.45
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.31	0.45
4:A:186:TRP:CG	4:A:187:PRO:HA	2.52	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.36	0.45
7:D:13:MET:HA	7:D:137:PRO:HG2	1.98	0.45
11:H:29:ALA:CB	11:H:66:ARG:HH12	2.24	0.45
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.45
16:N:147:ILE:HD12	39:N:9343:HOH:O	2.17	0.45
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.47	0.45
1:0:907:A:H2'	1:0:908:A:H8	1.82	0.45
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.17	0.45
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.52	0.45
39:0:7982:HOH:O	15:M:91:ILE:HG23	2.17	0.45
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.47	0.45
6:C:78:ARG:HD3	39:C:9535:HOH:O	2.16	0.45
14:L:125:PHE:CE2	14:L:140:VAL:HG22	2.51	0.45
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.99	0.45
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.46	0.45
23:U:20:MET:CG	23:U:28:THR:HG23	2.47	0.45
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.60	0.45
28:Z:36:ASP:CB	28:Z:45:ASP:HB3	2.36	0.45
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.17	0.45
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.47	0.45
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.34	0.45
11:H:54:THR:O	11:H:55:VAL:HG13	2.17	0.45
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.99	0.45
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.52	0.45
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.44
1:0:475:G:H5'	6:C:73:LEU:HD23	1.98	0.44
1:0:907:A:H2'	1:0:908:A:C8	2.50	0.44
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.44
1:0:2114:C:OP1	4:A:1:GLY:HA2	2.17	0.44
1:0:2712:G:H5'	39:K:4183:HOH:O	2.17	0.44
4:A:223:ARG:CZ	39:A:9563:HOH:O	2.65	0.44
4:A:223:ARG:NE	39:A:9563:HOH:O	2.49	0.44
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.52	0.44
21:S:23:LYS:HE2	39:S:9489:HOH:O	2.16	0.44
1:0:612:U:H2'	1:0:613:C:C6	2.52	0.44
1:0:1462:C:H2'	1:0:1463:A:H8	1.81	0.44
1:0:2016:U:H2'	1:0:2017:U:O4'	2.17	0.44
1:0:2362:A:H2'	1:0:2363:G:C8	2.53	0.44
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.44
3:4:76:PPU:N	3:4:176:DA:H2''	2.32	0.44
7:D:69:ILE:HG22	7:D:69:ILE:O	2.17	0.44
21:S:57:THR:HG22	21:S:58:MET:N	2.32	0.44
26:X:34:ARG:NH1	26:X:48:VAL:O	2.50	0.44
1:0:282:C:H1'	1:0:368:C:H42	1.78	0.44
1:0:1119:G:C8	12:J:52:GLN:NE2	2.82	0.44
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.17	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.32	0.44
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:150:THR:HA	6:C:203:ALA:O	2.18	0.44
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.48	0.44
10:G:12:ILE:HB	39:G:4714:HOH:O	2.17	0.44
12:J:63:ILE:CG2	12:J:64:GLY:N	2.80	0.44
16:N:37:ARG:HD3	16:N:37:ARG:HA	1.65	0.44
24:V:42:ASN:O	24:V:44:GLY:N	2.51	0.44
30:2:20:ARG:HG3	30:2:21:VAL:N	2.33	0.44
32:I:112:LYS:C	32:I:114:PRO:HD2	2.37	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.18	0.44
1:0:204:A:H2'	1:0:205:U:H5'	1.98	0.44
1:0:564:G:H1'	39:0:6813:HOH:O	2.17	0.44
1:0:1535:G:H2'	1:0:1536:C:C6	2.53	0.44
1:0:2379:G:N3	1:0:2418:G:H2'	2.32	0.44
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.80	0.44
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.46	0.44
5:B:14:GLY:HA2	5:B:15:PRO:C	2.37	0.44
8:E:7:ILE:HD11	8:E:11:VAL:C	2.38	0.44
11:H:1:LYS:HA	11:H:2:PRO:HD3	1.88	0.44
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.14	0.44
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.99	0.44
22:T:48:VAL:HG21	22:T:96:VAL:HG13	1.99	0.44
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.99	0.44
1:0:87:C:C2	30:2:30:ASP:OD2	2.71	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
1:0:447:A:O2'	1:0:448:G:H5'	2.18	0.44
1:0:1163:G:H5'	32:I:115:ASP:O	2.18	0.44
1:0:1794:G:N2	1:0:1796:A:H3'	2.33	0.44
1:0:2408:A:H4'	31:3:15:ASN:O	2.18	0.44
1:0:2676:C:H6	1:0:2676:C:H5''	1.82	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
7:D:36:ASN:HA	39:D:7500:HOH:O	2.17	0.44
12:J:52:GLN:HG3	12:J:53:ILE:N	2.33	0.44
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.50	0.44
13:K:20:CYS:HB2	13:K:29:LEU:HG	2.00	0.44
15:M:61:ILE:HD12	15:M:61:ILE:N	2.31	0.44
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.44
18:P:13:VAL:HG11	18:P:40:VAL:HG12	1.99	0.44
25:W:3:ALA:O	25:W:54:PHE:HA	2.17	0.44
31:3:70:ARG:HB3	39:3:9502:HOH:O	2.17	0.44
1:0:656:G:H5'	17:O:3:THR:CG2	2.48	0.44
1:0:1086:A:C6	25:W:11:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1730:G:H5'	1:0:1731:C:H5	1.82	0.44
1:0:1730:G:H5''	1:0:1731:C:H6	1.83	0.44
1:0:2251:G:H2'	1:0:2252:A:C8	2.53	0.44
39:0:4960:HOH:O	4:A:11:ARG:CZ	2.66	0.44
5:B:16:ARG:NE	39:B:9489:HOH:O	2.41	0.44
5:B:41:PHE:CG	5:B:79:MET:HE2	2.53	0.44
5:B:58:PRO:HA	5:B:63:GLU:CD	2.38	0.44
7:D:40:ILE:HG13	7:D:41:LEU:N	2.33	0.44
9:F:107:ASP:O	9:F:111:ILE:HG13	2.17	0.44
14:L:149:ARG:O	14:L:150:GLN:HB2	2.17	0.44
20:R:84:ALA:O	20:R:88:PHE:HD1	2.01	0.44
22:T:77:VAL:HG11	22:T:91:LEU:HD11	2.00	0.44
1:0:308:U:H5'	22:T:97:ARG:NH2	2.32	0.44
1:0:319:A:H4'	1:0:338:C:C5	2.53	0.44
1:0:656:G:H5'	17:O:3:THR:HG22	2.00	0.44
1:0:797:A:C5'	28:Z:10:ARG:N	2.81	0.44
1:0:921:G:H4'	1:0:924:G:N1	2.33	0.44
1:0:945:U:H2'	1:0:946:C:H6	1.83	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.44
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.44
1:0:1741:U:H3'	39:0:3365:HOH:O	2.17	0.44
1:0:2039:A:H4'	1:0:2760:C:O2'	2.18	0.44
1:0:2549:C:H1'	5:B:248:ARG:NH2	2.32	0.44
39:0:6243:HOH:O	13:K:87:ARG:CZ	2.65	0.44
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.44
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.99	0.44
7:D:167:GLU:C	7:D:169:THR:H	2.21	0.44
32:I:131:THR:O	32:I:135:LEU:HG	2.18	0.44
1:0:1435:U:H5'	39:0:3202:HOH:O	2.16	0.44
4:A:130:THR:HG22	4:A:131:HIS:O	2.18	0.44
5:B:312:ARG:HG2	5:B:313:PRO:N	2.32	0.44
6:C:197:SER:HB3	39:C:9574:HOH:O	2.17	0.44
6:C:242:GLU:HB2	39:C:9582:HOH:O	2.17	0.44
7:D:99:ASP:N	7:D:103:ASN:O	2.45	0.44
8:E:36:PRO:HD3	12:J:127:ILE:CD1	2.40	0.44
20:R:69:LYS:HB2	20:R:72:VAL:HG23	1.99	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.46	0.44
32:I:78:LEU:CD1	32:I:112:LYS:HZ2	2.28	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.18	0.44
1:0:697:G:H4'	1:0:730:G:O3'	2.18	0.44
1:0:1311:G:O6	6:C:173:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1940:C:H4'	39:0:7795:HOH:O	2.18	0.44
1:0:2101:A:H2'	6:C:63:SER:OG	2.18	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.35	0.44
1:0:2907:C:H2'	1:0:2908:A:O4'	2.17	0.44
5:B:81:ALA:O	5:B:186:GLY:HA3	2.18	0.44
7:D:10:PHE:CD1	7:D:11:HIS:N	2.86	0.44
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.18	0.44
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.48	0.44
13:K:115:ARG:O	13:K:118:ALA:HB3	2.18	0.44
20:R:113:HIS:HE1	20:R:144:GLU:OE1	2.00	0.44
1:0:362:G:H2'	1:0:363:A:C8	2.53	0.43
1:0:475:G:H5''	6:C:73:LEU:HD23	2.00	0.43
1:0:710:G:H5'	17:O:25:VAL:HG13	2.00	0.43
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.18	0.43
1:0:2505:G:C2'	1:0:2506:A:H5'	2.48	0.43
1:0:2568:A:C2'	1:0:2569:A:H5'	2.48	0.43
1:0:2663:U:H2'	39:0:8443:HOH:O	2.16	0.43
11:H:76:GLU:C	11:H:77:LEU:HD23	2.38	0.43
15:M:82:ARG:HA	39:M:9337:HOH:O	2.16	0.43
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.99	0.43
16:N:167:ASP:C	16:N:168:LEU:HG	2.38	0.43
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.53	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.51	0.43
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.81	0.43
1:0:1878:G:HO2'	1:0:1879:U:H5	1.61	0.43
1:0:2346:C:H4'	7:D:52:THR:CG2	2.49	0.43
1:0:2445:U:H2'	1:0:2446:G:C8	2.53	0.43
1:0:2686:C:O2	13:K:1:MET:N	2.50	0.43
1:0:2825:C:H4'	1:0:2826:G:O5'	2.19	0.43
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.48	0.43
9:F:28:ALA:CB	9:F:99:THR:HG23	2.48	0.43
11:H:136:ALA:HB3	11:H:146:VAL:HG21	2.00	0.43
14:L:144:ASP:O	14:L:147:GLU:HB2	2.16	0.43
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.33	0.43
16:N:71:TRP:HB2	39:N:9336:HOH:O	2.17	0.43
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.48	0.43
20:R:39:THR:CG2	20:R:107:GLU:O	2.65	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.00	0.43
1:0:1163:G:H2'	1:0:1164:U:C5	2.53	0.43
1:0:2784:A:H1'	8:E:60:SER:OG	2.18	0.43
2:9:3003:A:H2'	39:9:2430:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:133:ARG:NH1	39:C:9610:HOH:O	2.51	0.43
6:C:140:VAL:HB	39:C:9648:HOH:O	2.18	0.43
7:D:78:GLU:O	7:D:82:GLU:HG3	2.18	0.43
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.54	0.43
14:L:35:ARG:C	14:L:35:ARG:HD3	2.39	0.43
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.18	0.43
18:P:16:VAL:CG1	18:P:17:GLY:N	2.81	0.43
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.48	0.43
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.53	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.18	0.43
1:0:1350:U:H2'	1:0:1351:G:O4'	2.19	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.99	0.43
1:0:2912:C:H2'	1:0:2913:A:O4'	2.19	0.43
6:C:219:ASN:O	6:C:222:ASP:HB2	2.18	0.43
9:F:58:GLU:HG3	9:F:61:MET:CE	2.48	0.43
16:N:127:LEU:HD13	39:N:9353:HOH:O	2.17	0.43
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.83	0.43
25:W:34:LEU:HD12	25:W:107:LEU:HD11	1.99	0.43
1:0:185:G:O3'	1:0:186:A:H4'	2.19	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.05	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.01	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
4:A:82:VAL:HG13	4:A:93:THR:HB	1.98	0.43
5:B:264:GLU:HG2	5:B:267:LYS:HD3	2.00	0.43
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.53	0.43
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.93	0.43
9:F:26:THR:HG21	9:F:102:GLY:C	2.39	0.43
9:F:99:THR:O	9:F:99:THR:HG23	2.19	0.43
11:H:29:ALA:C	11:H:30:GLN:HG3	2.39	0.43
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.34	0.43
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.39	0.43
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.48	0.43
26:X:66:THR:HG22	26:X:67:PRO:O	2.18	0.43
26:X:66:THR:HG23	26:X:67:PRO:HD2	2.01	0.43
29:1:28:HIS:HD2	29:1:31:LYS:H	1.65	0.43
32:I:99:ASP:O	32:I:100:LEU:HD23	2.19	0.43
1:0:12:U:C2'	1:0:13:G:H5'	2.47	0.43
1:0:1086:A:N6	25:W:11:VAL:HG11	2.34	0.43
1:0:1098:A:H2'	1:0:1099:G:O4'	2.19	0.43
1:0:1299:G:N2	39:0:5226:HOH:O	2.52	0.43
1:0:1972:U:H2'	1:0:1973:A:C5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2067:A:H2'	1:0:2068:G:O4'	2.18	0.43
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	2.00	0.43
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.43
6:C:153:VAL:O	6:C:157:LEU:HG	2.18	0.43
7:D:96:SER:C	7:D:98:PHE:H	2.21	0.43
1:0:255:A:H2'	1:0:256:C:C6	2.54	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.43
1:0:1311:G:O2'	1:0:1312:G:H5'	2.19	0.43
1:0:2768:A:H2'	1:0:2769:C:O4'	2.18	0.43
4:A:179:MET:HG2	4:A:186:TRP:CG	2.54	0.43
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.36	0.43
7:D:128:LEU:C	7:D:128:LEU:HD23	2.38	0.43
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.43
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.18	0.43
1:0:56:G:H5''	24:V:50:ARG:NH1	2.34	0.43
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.43
1:0:2642:G:H2'	1:0:2643:G:O4'	2.19	0.43
2:9:3114:G:H2'	2:9:3115:C:C6	2.54	0.43
4:A:103:VAL:O	4:A:105:VAL:HG23	2.18	0.43
9:F:60:VAL:O	9:F:60:VAL:CG1	2.66	0.43
9:F:102:GLY:O	9:F:103:GLU:HB2	2.19	0.43
12:J:46:ILE:HA	39:J:1123:HOH:O	2.19	0.43
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.54	0.43
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.53	0.43
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.19	0.43
1:0:449:A:C8	6:C:43:LYS:HG2	2.54	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
1:0:1165:G:H1'	1:0:1174:A:H1'	2.01	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:2541:U:H3'	1:0:2541:U:H6	1.84	0.43
4:A:75:GLY:HA2	28:Z:64:PHE:HA	2.01	0.43
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.01	0.43
8:E:108:LEU:HB3	39:E:1306:HOH:O	2.17	0.43
16:N:67:ALA:O	16:N:69:TYR:N	2.52	0.43
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.01	0.43
1:0:138:U:OP2	1:0:139:C:H5	2.01	0.43
1:0:424:C:H2'	1:0:425:U:C6	2.53	0.43
1:0:426:G:H2'	1:0:427:C:O4'	2.19	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.54	0.43
1:0:1269:G:H2'	1:0:1270:U:C6	2.54	0.43
1:0:1299:G:H5'	39:0:4638:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2011:A:H4'	1:0:2012:U:O5'	2.19	0.43
1:0:2456:A:H5'	39:0:6224:HOH:O	2.18	0.43
1:0:2667:G:H1'	1:0:2914:A:N3	2.34	0.43
1:0:2717:C:H2'	1:0:2718:C:C5'	2.36	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.17	0.43
2:9:3054:A:H2	39:9:3535:HOH:O	2.02	0.43
2:9:3076:G:H3'	2:9:3077:A:C5'	2.30	0.43
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.48	0.43
16:N:72:GLU:O	16:N:72:GLU:HG2	2.17	0.43
20:R:61:GLN:NE2	39:R:9453:HOH:O	2.52	0.43
1:0:1072:G:OP2	27:Y:154:ARG:NH2	2.52	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.42
1:0:1624:A:H4'	1:0:1625:U:H5'	2.00	0.42
1:0:2748:G:H4'	1:0:2749:U:H5'	2.01	0.42
4:A:173:GLY:O	4:A:176:HIS:HB3	2.19	0.42
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.19	0.42
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.49	0.42
15:M:71:SER:HB2	15:M:92:THR:HG22	2.01	0.42
18:P:14:LEU:HD13	18:P:51:ALA:HB2	2.01	0.42
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.34	0.42
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.34	0.42
1:0:441:A:H8	1:0:441:A:O5'	2.02	0.42
1:0:1182:C:H1'	1:0:1192:A:C8	2.44	0.42
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.42
1:0:1250:C:O2'	1:0:1251:C:H5'	2.18	0.42
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.82	0.42
1:0:2019:A:H5'	39:0:5088:HOH:O	2.19	0.42
1:0:2568:A:H2'	1:0:2569:A:H5'	2.01	0.42
4:A:94:LEU:HD23	4:A:94:LEU:N	2.34	0.42
8:E:69:ILE:HA	8:E:72:MET:CE	2.49	0.42
15:M:159:VAL:HG13	15:M:160:PHE:N	2.34	0.42
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.97	0.42
31:3:6:ARG:HA	31:3:20:HIS:O	2.19	0.42
32:I:103:ASP:HA	32:I:106:LYS:HD2	2.01	0.42
1:0:130:C:H2'	39:0:3747:HOH:O	2.19	0.42
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.42
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.42
1:0:1139:U:H2'	1:0:1140:C:C6	2.54	0.42
1:0:1921:A:O2'	1:0:1922:A:H5'	2.19	0.42
1:0:2106:C:H2'	1:0:2107:U:C6	2.54	0.42
1:0:2296:C:H2'	1:0:2297:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2346:C:H6	1:0:2346:C:O5'	2.01	0.42
1:0:2526:C:O2'	1:0:2527:U:H5'	2.19	0.42
1:0:2672:C:H4'	5:B:163:GLU:OE1	2.20	0.42
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.45	0.42
4:A:36:ASP:O	4:A:36:ASP:CG	2.57	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.72	0.42
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.49	0.42
16:N:8:VAL:CG1	16:N:14:ARG:HE	2.32	0.42
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.42
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.48	0.42
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.84	0.42
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.20	0.42
28:Z:40:PRO:C	28:Z:42:CYS:H	2.22	0.42
1:0:23:G:C6	1:0:24:G:N1	2.87	0.42
1:0:396:U:OP2	31:3:38:ARG:HD2	2.18	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
1:0:2324:G:N2	1:0:2377:U:H1'	2.35	0.42
1:0:2388:C:H5'	19:Q:83:THR:O	2.19	0.42
5:B:294:TYR:HE2	39:B:9580:HOH:O	2.02	0.42
6:C:77:ALA:O	6:C:78:ARG:HG3	2.20	0.42
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.55	0.42
16:N:182:GLY:O	16:N:183:ASP:C	2.56	0.42
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.83	0.42
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.35	0.42
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.50	0.42
28:Z:39:CYS:SG	28:Z:41:ASN:N	2.93	0.42
30:2:18:ASN:HD21	30:2:40:ARG:N	2.04	0.42
1:0:401:C:O2'	15:M:92:THR:HB	2.20	0.42
1:0:407:A:H5'	39:0:6539:HOH:O	2.20	0.42
1:0:517:U:H1'	39:0:8049:HOH:O	2.19	0.42
1:0:709:G:O2'	17:O:25:VAL:CG1	2.66	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:1181:A:N1	1:0:1192:A:O2'	2.49	0.42
1:0:1592:G:H2'	1:0:1593:C:C6	2.55	0.42
1:0:2072:G:H3'	1:0:2073:G:C5'	2.49	0.42
1:0:2090:G:H2'	1:0:2091:G:C8	2.54	0.42
1:0:2435:U:H1'	39:0:5962:HOH:O	2.19	0.42
1:0:2672:C:O2'	1:0:2673:U:H5'	2.19	0.42
5:B:314:ALA:HB3	5:B:317:PRO:HG3	2.01	0.42
7:D:25:MET:HE1	7:D:37:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:84:LEU:HA	7:D:87:ALA:HB3	2.01	0.42
12:J:107:ASN:C	12:J:107:ASN:HD22	2.23	0.42
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.82	0.42
14:L:143:THR:CG2	14:L:144:ASP:H	2.27	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
1:0:1717:A:H5''	18:P:54:LYS:HB2	2.00	0.42
1:0:1797:A:H2'	1:0:1799:G:O5'	2.20	0.42
1:0:2456:A:H2'	1:0:2457:U:H6	1.85	0.42
2:9:3057:A:C8	7:D:141:VAL:HG21	2.55	0.42
4:A:17:ARG:HD2	39:A:9534:HOH:O	2.19	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
11:H:47:ILE:HG21	39:H:9542:HOH:O	2.19	0.42
19:Q:53:HIS:CE1	19:Q:55:ARG:HB2	2.54	0.42
1:0:500:G:H21	20:R:98:ASN:HD21	1.67	0.42
1:0:500:G:O2'	20:R:94:ASN:ND2	2.53	0.42
1:0:1268:C:O2'	1:0:1269:G:H5'	2.19	0.42
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.81	0.42
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.42
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.42
15:M:47:ASP:CG	15:M:48:LYS:N	2.73	0.42
15:M:74:LYS:CG	15:M:75:ARG:N	2.82	0.42
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.19	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.19	0.42
1:0:612:U:H2'	1:0:613:C:H6	1.84	0.42
1:0:1185:U:H4'	32:I:123:ASN:HB3	2.02	0.42
1:0:2241:C:O2'	1:0:2242:U:H5'	2.19	0.42
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.80	0.42
2:9:3049:G:C2'	2:9:3050:G:H5'	2.50	0.42
12:J:88:PRO:O	12:J:94:GLY:HA3	2.20	0.42
13:K:49:LEU:HD12	13:K:80:ILE:HG21	2.01	0.42
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.19	0.42
17:O:73:ASP:HA	17:O:92:VAL:O	2.20	0.42
18:P:104:LYS:HE2	18:P:138:GLU:OE2	2.20	0.42
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.99	0.42
27:Y:115:ARG:NE	39:Y:9352:HOH:O	2.52	0.42
1:0:189:A:OP1	15:M:171:ARG:NH2	2.52	0.42
1:0:819:A:H5''	39:Z:9219:HOH:O	2.20	0.42
1:0:1168:C:H5''	32:I:87:THR:HG23	2.02	0.42
1:0:1291:A:H2	39:0:5826:HOH:O	2.03	0.42
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.19	0.42
1:0:2072:G:H4'	39:0:4368:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.19	0.42
1:0:2748:G:H8	39:0:7977:HOH:O	2.03	0.42
1:0:2868:C:H2'	1:0:2869:G:O4'	2.20	0.42
3:4:176:DA:H5''	3:4:175:C:H3'	2.02	0.42
6:C:61:PHE:HB3	39:C:9642:HOH:O	2.20	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
15:M:46:LEU:HD22	15:M:50:ARG:HG3	2.01	0.42
1:0:136:C:H2'	1:0:137:U:O4'	2.19	0.42
1:0:625:U:H5'	39:0:3772:HOH:O	2.20	0.42
1:0:656:G:H1'	39:C:9658:HOH:O	2.20	0.42
1:0:932:U:H2'	1:0:933:C:C6	2.55	0.42
1:0:2072:G:H3'	1:0:2073:G:H5''	2.02	0.42
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.19	0.42
1:0:2857:C:H2'	1:0:2858:U:C6	2.55	0.42
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.35	0.42
5:B:41:PHE:HA	5:B:79:MET:CE	2.50	0.42
6:C:30:LEU:HD23	6:C:30:LEU:HA	1.89	0.42
7:D:137:PRO:O	7:D:139:TYR:N	2.52	0.42
8:E:1:PRO:HG2	8:E:59:MET:SD	2.60	0.42
11:H:2:PRO:HD2	11:H:5:MET:SD	2.59	0.42
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.01	0.42
1:0:960:G:N3	1:0:960:G:C2'	2.83	0.41
1:0:1095:U:O2	25:W:120:PRO:HG2	2.20	0.41
1:0:1836:A:H1'	29:1:1:THR:O	2.19	0.41
1:0:2541:U:C2	1:0:2620:U:O4	2.73	0.41
1:0:2782:G:O6	1:0:2790:C:H5''	2.20	0.41
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.45	0.41
7:D:18:ILE:HG12	7:D:134:LEU:HD23	2.02	0.41
12:J:45:VAL:CG2	12:J:129:PHE:CD1	3.03	0.41
16:N:167:ASP:O	16:N:168:LEU:HG	2.20	0.41
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.34	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.55	0.41
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.41
1:0:1886:A:H5'	39:Z:9227:HOH:O	2.19	0.41
1:0:2775:A:C6	1:0:2799:A:C8	3.08	0.41
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.20	0.41
7:D:67:ASP:O	7:D:69:ILE:HG13	2.20	0.41
7:D:172:VAL:CG1	7:D:173:GLU:N	2.82	0.41
9:F:46:GLU:CD	9:F:100:ASP:HA	2.40	0.41
11:H:9:ILE:HD12	11:H:54:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:22:ASP:O	13:K:110:LYS:HE3	2.20	0.41
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.46	0.41
20:R:107:GLU:HG3	39:R:9488:HOH:O	2.20	0.41
22:T:51:LEU:HD11	22:T:97:ARG:HB2	2.02	0.41
25:W:85:ALA:HB2	25:W:91:ASP:O	2.20	0.41
31:3:65:THR:HG22	31:3:67:LEU:CG	2.49	0.41
1:0:590:A:H2'	1:0:591:A:H5'	2.02	0.41
1:0:820:G:H5'	1:0:821:U:H5'	2.01	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.35	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.56	0.41
1:0:2436:U:H5'	31:3:68:LYS:HE2	2.02	0.41
4:A:33:GLU:CD	4:A:33:GLU:N	2.67	0.41
5:B:271:ASP:HB3	5:B:296:LEU:HD12	2.01	0.41
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.35	0.41
7:D:65:GLU:HG3	39:D:6752:HOH:O	2.20	0.41
11:H:154:TYR:CD1	11:H:154:TYR:C	2.94	0.41
13:K:118:ALA:HA	13:K:125:ALA:HB2	2.01	0.41
14:L:104:ASP:HB2	39:L:9459:HOH:O	2.19	0.41
22:T:62:VAL:HB	39:T:3851:HOH:O	2.20	0.41
25:W:38:THR:HG22	25:W:39:ASP:H	1.85	0.41
25:W:146:ILE:HG22	25:W:147:ASP:N	2.35	0.41
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.73	0.41
27:Y:122:ARG:NH2	39:Y:9334:HOH:O	2.53	0.41
28:Z:39:CYS:O	28:Z:42:CYS:O	2.38	0.41
30:2:40:ARG:HD2	30:2:47:THR:HG22	2.02	0.41
32:I:72:VAL:HG13	32:I:73:PRO:HD2	2.02	0.41
1:0:1201:C:C2'	1:0:1202:A:H5'	2.45	0.41
39:0:7475:HOH:O	19:Q:9:GLY:HA2	2.19	0.41
5:B:24:PRO:HG3	5:B:204:GLY:HA2	2.01	0.41
6:C:200:PRO:HB3	6:C:212:VAL:HG23	2.03	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
12:J:47:THR:CG2	12:J:48:GLY:N	2.83	0.41
13:K:23:ASN:HD21	13:K:107:THR:HB	1.85	0.41
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.55	0.41
16:N:110:THR:HB	16:N:113:SER:HG	1.83	0.41
18:P:105:LEU:HD21	18:P:137:LEU:HD21	2.01	0.41
22:T:23:VAL:HG23	22:T:41:ARG:HG3	2.02	0.41
25:W:125:HIS:HE1	39:W:3071:HOH:O	2.02	0.41
32:I:92:PRO:C	32:I:94:GLU:N	2.71	0.41
1:0:87:C:H2'	30:2:28:LYS:O	2.21	0.41
1:0:364:C:H2'	1:0:365:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:952:G:N3	1:0:2302:A:H2'	2.36	0.41
1:0:1244:U:H2'	12:J:47:THR:HG21	2.03	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.55	0.41
1:0:2698:G:H2'	1:0:2699:A:C8	2.55	0.41
1:0:2911:C:O2'	1:0:2912:C:H5'	2.21	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
5:B:91:PRO:O	12:J:144:THR:HG21	2.21	0.41
9:F:39:SER:HB3	9:F:45:ALA:HB2	2.02	0.41
11:H:51:VAL:CG1	11:H:53:GLU:O	2.69	0.41
12:J:4:ALA:O	12:J:5:GLU:HB2	2.20	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.41	0.41
20:R:82:GLU:OE1	20:R:86:LYS:HE3	2.20	0.41
30:2:18:ASN:HD22	30:2:18:ASN:HA	1.60	0.41
1:0:185:G:C4'	1:0:186:A:H4'	2.51	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.21	0.41
1:0:968:G:H1'	11:H:32:LYS:HD2	2.02	0.41
1:0:1014:A:H2'	1:0:1015:C:H5'	2.02	0.41
1:0:1760:G:H5'	1:0:1818:C:O2'	2.20	0.41
1:0:1966:U:H2'	1:0:1967:U:H2'	2.02	0.41
7:D:25:MET:CE	7:D:41:LEU:HG	2.37	0.41
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.55	0.41
11:H:73:LEU:HD21	11:H:146:VAL:HA	2.03	0.41
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.49	0.41
14:L:77:ALA:C	14:L:79:ASP:H	2.24	0.41
15:M:86:GLN:O	15:M:88:VAL:HG23	2.20	0.41
17:O:44:ASN:OD1	17:O:67:SER:HB2	2.21	0.41
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.19	0.41
1:0:37:A:H2'	1:0:38:G:C8	2.56	0.41
1:0:195:C:H5''	39:0:5935:HOH:O	2.21	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.41
1:0:1406:A:H5'	1:0:1407:A:C8	2.56	0.41
1:0:1884:G:O6	4:A:190:ARG:HD2	2.20	0.41
1:0:2323:G:H5'	39:0:7492:HOH:O	2.21	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.20	0.41
1:0:2842:G:H2'	1:0:2843:A:H5'	2.02	0.41
39:0:5823:HOH:O	25:W:119:HIS:CG	2.73	0.41
4:A:203:GLY:HA2	39:A:9538:HOH:O	2.20	0.41
12:J:19:MET:CE	12:J:132:LEU:HD21	2.47	0.41
16:N:119:GLN:O	16:N:123:ILE:HG13	2.21	0.41
16:N:181:ASP:O	16:N:184:ILE:HG22	2.21	0.41
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.20	0.41
1:0:559:U:H2'	1:0:560:C:O4'	2.21	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.36	0.41
1:0:1120:U:H5''	1:0:1120:U:C6	2.56	0.41
1:0:1218:U:H2'	1:0:1219:U:H6	1.86	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:2715:G:O2'	5:B:262:ARG:HD2	2.20	0.41
4:A:26:ASP:OD1	4:A:26:ASP:O	2.38	0.41
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.47	0.41
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.85	0.41
7:D:25:MET:CE	7:D:40:ILE:HD11	2.51	0.41
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.54	0.41
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.18	0.41
17:O:32:ARG:NH2	17:O:35:LYS:NZ	2.66	0.41
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.50	0.41
25:W:26:ILE:O	25:W:26:ILE:HG13	2.21	0.41
30:2:44:ARG:HD3	30:2:44:ARG:HA	1.83	0.41
30:2:46:ASP:OD1	30:2:47:THR:O	2.37	0.41
1:0:247:A:H2'	39:0:4490:HOH:O	2.20	0.41
1:0:338:C:H4'	6:C:174:ILE:HD12	2.01	0.41
1:0:359:U:H3'	39:0:6292:HOH:O	2.20	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.54	0.41
1:0:1163:G:H1	1:0:1184:C:N4	2.18	0.41
1:0:1203:G:O2'	1:0:1204:C:H5'	2.20	0.41
1:0:1342:C:O2'	1:0:1343:C:H5'	2.20	0.41
1:0:1516:C:H2'	1:0:1517:U:C6	2.56	0.41
1:0:1641:A:C2'	1:0:1642:A:H5'	2.49	0.41
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.41
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.03	0.41
1:0:2316:G:OP1	1:0:2317:C:H1'	2.21	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
4:A:135:VAL:HG13	4:A:135:VAL:O	2.20	0.41
5:B:62:ARG:CA	5:B:65:MET:HE3	2.50	0.41
11:H:79:GLU:C	11:H:80:GLU:HG3	2.41	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.95	0.41
14:L:67:ARG:HH11	14:L:67:ARG:HG2	1.85	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.92	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:19:THR:HG22	23:U:20:MET:N	2.36	0.41
25:W:82:GLU:O	25:W:86:GLU:HG3	2.21	0.41
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.20	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
1:0:1160:G:HO2'	1:0:1190:G:H8	1.66	0.41
1:0:1527:A:H1'	1:0:1528:A:C8	2.56	0.41
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.54	0.41
2:9:3052:A:O2'	2:9:3053:G:H5'	2.21	0.41
7:D:91:ALA:HB2	7:D:106:PHE:CD2	2.56	0.41
16:N:48:VAL:HG11	16:N:55:ASP:HB3	2.00	0.41
23:U:4:ARG:HG2	23:U:4:ARG:HH11	1.85	0.41
1:0:635:A:H2'	1:0:636:G:H5''	2.02	0.40
1:0:894:A:N1	6:C:87:ARG:NH2	2.68	0.40
1:0:1187:U:H2'	1:0:1189:A:OP2	2.21	0.40
1:0:1213:C:O2'	1:0:1214:G:H5'	2.22	0.40
1:0:1544:U:O2'	1:0:1545:C:H5'	2.21	0.40
1:0:2091:G:O3'	5:B:235:ARG:HD3	2.22	0.40
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.21	0.40
4:A:36:ASP:O	4:A:36:ASP:OD1	2.40	0.40
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.86	0.40
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.56	0.40
8:E:100:ASP:HB2	39:E:2789:HOH:O	2.22	0.40
11:H:63:GLU:O	11:H:67:LEU:HB2	2.22	0.40
13:K:81:ARG:CD	13:K:87:ARG:NH1	2.83	0.40
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.47	0.40
22:T:78:THR:HG22	22:T:88:PRO:HA	2.03	0.40
22:T:85:GLU:CG	22:T:86:GLU:N	2.84	0.40
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.38	0.40
28:Z:39:CYS:HA	28:Z:40:PRO:HD3	1.99	0.40
32:I:100:LEU:O	32:I:139:ILE:HG23	2.21	0.40
1:0:407:A:H8	39:0:5008:HOH:O	2.04	0.40
1:0:604:G:H2'	39:0:8275:HOH:O	2.20	0.40
1:0:1076:G:C2	1:0:1084:C:C2	3.09	0.40
1:0:1318:A:H4'	1:0:1343:C:H4'	2.03	0.40
1:0:1525:G:H5'	1:0:1526:A:OP2	2.21	0.40
1:0:1862:C:H1'	39:0:7683:HOH:O	2.21	0.40
1:0:2296:C:H2'	1:0:2297:U:C6	2.56	0.40
1:0:2365:G:H4'	19:Q:45:PRO:O	2.21	0.40
1:0:2386:U:H2'	1:0:2387:U:O4'	2.20	0.40
2:9:3042:C:H5'	2:9:3043:G:OP2	2.22	0.40
4:A:194:MET:CE	4:A:199:HIS:HB2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.40
7:D:19:GLU:O	7:D:76:ARG:HG2	2.21	0.40
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.40
8:E:101:GLU:HB2	8:E:116:THR:O	2.21	0.40
9:F:101:ALA:HA	39:F:5413:HOH:O	2.21	0.40
11:H:83:TYR:CD1	11:H:83:TYR:C	2.94	0.40
11:H:88:ARG:H	11:H:88:ARG:HG2	1.73	0.40
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.56	0.40
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.86	0.40
24:V:60:GLN:O	24:V:65:ASP:N	2.54	0.40
1:0:1669:A:H2'	1:0:1670:G:C8	2.57	0.40
1:0:2112:A:H2'	1:0:2113:G:C8	2.57	0.40
5:B:8:LYS:HG3	5:B:220:VAL:HG12	2.04	0.40
5:B:183:GLU:O	5:B:184:ASP:C	2.60	0.40
7:D:50:VAL:HG23	7:D:72:LYS:O	2.21	0.40
8:E:108:LEU:CD1	8:E:164:ASP:HB2	2.50	0.40
11:H:167:PRO:O	11:H:168:ALA:HB2	2.21	0.40
18:P:18:LYS:O	18:P:21:VAL:HG13	2.21	0.40
25:W:5:VAL:O	25:W:52:VAL:HG23	2.21	0.40
1:0:282:C:O2'	1:0:283:U:C5'	2.68	0.40
1:0:613:C:H2'	1:0:614:U:H6	1.87	0.40
1:0:644:G:H5'	1:0:644:G:N3	2.37	0.40
1:0:821:U:H2'	1:0:822:C:H6	1.86	0.40
1:0:1060:C:H5'	1:0:1060:C:H6	1.87	0.40
1:0:1576:G:H2'	1:0:1577:U:O4'	2.22	0.40
1:0:1873:G:H2'	1:0:1874:U:H5'	2.03	0.40
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.21	0.40
39:O:7993:HOH:O	31:3:61:PRO:HG2	2.20	0.40
2:9:3057:A:H2'	2:9:3058:G:O4'	2.21	0.40
5:B:264:GLU:HG2	5:B:267:LYS:NZ	2.36	0.40
15:M:74:LYS:HA	39:M:9374:HOH:O	2.21	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.54	0.40
16:N:67:ALA:C	16:N:69:TYR:H	2.24	0.40
21:S:53:ASN:ND2	39:S:9479:HOH:O	2.53	0.40
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.57	0.40
1:0:802:G:H2'	1:0:803:C:C6	2.56	0.40
1:0:1019:C:O2	19:Q:94:GLN:NE2	2.52	0.40
1:0:1701:A:P	39:O:4934:HOH:O	2.79	0.40
1:0:2568:A:H2'	1:0:2569:A:O4'	2.22	0.40
2:9:3080:A:C2	2:9:3103:A:C4	3.09	0.40
5:B:60:SER:HA	5:B:61:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:118:LEU:O	9:F:119:ARG:HB3	2.21	0.40
31:3:7:PHE:HE2	31:3:22:VAL:HG21	1.87	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%)	214 (91%)	16 (7%)	5 (2%)	7 5
5	B	335/338 (99%)	313 (93%)	17 (5%)	5 (2%)	10 10
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100 100
7	D	134/177 (76%)	106 (79%)	16 (12%)	12 (9%)	1 0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100 100
9	F	117/120 (98%)	104 (89%)	12 (10%)	1 (1%)	17 20
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	12 12
12	J	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	7 5
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	19 23
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	22 26
15	M	192/195 (98%)	181 (94%)	10 (5%)	1 (0%)	29 35
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	3 1
17	O	113/116 (97%)	108 (96%)	5 (4%)	0	100 100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100 100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100 100
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	8
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	9	9
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	15
32	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	4	3
All	All	3705/4431 (84%)	3420 (92%)	237 (6%)	48 (1%)	12	12

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	27	ILE
7	D	60	GLU
7	D	137	PRO
11	H	166	SER
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	42	CYS
28	Z	81	ARG
5	B	34	GLY
5	B	169	GLY
7	D	16	PRO
7	D	138	GLY
7	D	171	ASP
9	F	101	ALA
11	H	168	ALA
12	J	143	LYS
15	M	83	SER
22	T	53	GLY
28	Z	20	ARG

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Mol	Chain	Res	Type
4	A	34	ASP
5	B	139	ASP
5	B	185	GLY
7	D	28	GLY
7	D	56	ARG
7	D	61	PHE
7	D	97	GLN
16	N	68	GLU
16	N	164	ASP
24	V	43	PRO
4	A	132	ASP
5	B	184	ASP
12	J	65	ASN
16	N	167	ASP
31	3	56	PRO
32	I	76	ALA
12	J	5	GLU
13	K	126	SER
7	D	147	ALA
16	N	155	GLU
22	T	44	ALA
28	Z	21	VAL
4	A	112	PRO
4	A	236	GLY
7	D	69	ILE
32	I	73	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%)	168 (94%)	11 (6%)	18 25
5	B	282/283 (100%)	265 (94%)	17 (6%)	19 26
6	C	193/193 (100%)	174 (90%)	19 (10%)	8 9
7	D	117/148 (79%)	110 (94%)	7 (6%)	19 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	152/156 (97%)	146 (96%)	6 (4%)	32	46
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	86
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	41	57
12	J	118/121 (98%)	110 (93%)	8 (7%)	16	21
13	K	106/106 (100%)	100 (94%)	6 (6%)	20	28
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	50
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	54
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	51
17	O	93/94 (99%)	90 (97%)	3 (3%)	39	54
18	P	113/117 (97%)	111 (98%)	2 (2%)	59	75
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	47
20	R	117/122 (96%)	115 (98%)	2 (2%)	60	76
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	81
22	T	105/106 (99%)	100 (95%)	5 (5%)	25	36
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	72
25	W	130/130 (100%)	125 (96%)	5 (4%)	33	47
26	X	66/74 (89%)	59 (89%)	7 (11%)	6	7
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	17
28	Z	60/68 (88%)	57 (95%)	3 (5%)	24	34
29	1	46/47 (98%)	45 (98%)	1 (2%)	52	69
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	66
31	3	79/79 (100%)	77 (98%)	2 (2%)	47	65
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2955 (96%)	138 (4%)	27	39

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP
4	A	33	GLU

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Mol	Chain	Res	Type
4	A	36	ASP
4	A	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	112	THR
5	B	113	LEU
5	B	162	MET
5	B	163	GLU
5	B	190	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	277	GLU
5	B	279	THR
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	78	ARG
6	C	94	THR
6	C	101	ASP
6	C	115	LEU
6	C	136	VAL
6	C	162	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

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Mol	Chain	Res	Type
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
7	D	137	PRO
8	E	15	GLN
8	E	102	VAL
8	E	131	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
11	H	84	LYS
11	H	154	TYR
11	H	159	PRO
11	H	170	ASN
12	J	46	ILE
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	49	LEU
13	K	84	ASP
13	K	98	VAL
13	K	100	GLU
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG

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Mol	Chain	Res	Type
15	M	116	ASN
16	N	26	LEU
16	N	49	THR
16	N	65	ASP
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	43	VAL
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	132	ARG
21	S	71	ASP
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	142	ASP
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	27	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR

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Mol	Chain	Res	Type
27	Y	204	ARG
27	Y	235	GLU
28	Z	22	SER
28	Z	44	GLU
28	Z	78	THR
29	1	47	ASP
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 (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	199	HIS
5	B	27	ASN
5	B	94	GLN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
6	C	163	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN

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Mol	Chain	Res	Type
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
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
20	R	113	HIS
20	R	117	HIS
21	S	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS

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Mol	Chain	Res	Type
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	119	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	30	GLN
31	3	48	ASN
32	I	113	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	2 (1%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	251 (8%)	38 (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	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A

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Mol	Chain	Res	Type
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
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	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
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A

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Mol	Chain	Res	Type
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	702	G
1	0	735	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G

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Mol	Chain	Res	Type
1	0	1130	U
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	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A

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Mol	Chain	Res	Type
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	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
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	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2134	G
1	0	2238	A
1	0	2243	C

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Mol	Chain	Res	Type
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	2476	C
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
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	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
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	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U

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Mol	Chain	Res	Type
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	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
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	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	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G

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Mol	Chain	Res	Type
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	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2320	U
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3055	U
2	9	3065	A

5.4 Non-standard residues in protein, DNA, RNA chains

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	PSU	0	2621	1	18,21,22	1.57	2 (11%)	22,30,33	1.24	3 (13%)
3	PPU	4	76	3,1	32,40,41	1.21	1 (3%)	33,57,60	0.97	3 (9%)
1	OMU	0	2587	1	19,22,23	0.26	0	26,31,34	0.38	0
1	1MA	0	628	1,35	16,25,26	1.32	3 (18%)	18,37,40	1.12	2 (11%)
1	OMG	0	2588	3,1	18,26,27	0.97	2 (11%)	19,38,41	0.78	1 (5%)
1	UR3	0	2619	1	19,22,23	0.38	0	26,32,35	0.63	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	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	PPU	4	76	3,1	-	1/21/43/44	0/4/4/4
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
1	OMG	0	2588	3,1	-	0/5/27/28	0/3/3/3
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)
3	4	76	PPU	OC-CM	-5.64	1.25	1.42
1	0	2621	PSU	C2-N1	5.05	1.43	1.36
1	0	628	1MA	C2-N3	3.48	1.33	1.29
1	0	2621	PSU	C6-C5	3.13	1.39	1.35
1	0	628	1MA	C6-N6	2.55	1.34	1.27
1	0	2588	OMG	C8-N7	-2.30	1.31	1.35
1	0	2588	OMG	C5-C6	-2.28	1.42	1.47
1	0	628	1MA	C8-N7	-2.03	1.31	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.44	120.60	118.20
1	0	2621	PSU	C6-N1-C2	-2.86	119.76	122.68
1	0	628	1MA	N1-C2-N3	2.78	129.26	126.02
3	4	76	PPU	C-CA-N	-2.65	99.16	109.40
1	0	628	1MA	C5-C6-N1	2.53	117.67	113.90
1	0	2621	PSU	O2-C2-N1	2.50	125.55	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2619	UR3	C4-N3-C2	2.43	126.86	124.56
3	4	76	PPU	CM-OC-CZ	2.30	122.51	117.51
1	0	2588	OMG	O6-C6-C5	2.23	128.74	124.37
3	4	76	PPU	C3'-N3'-C	-2.00	120.20	123.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	76	PPU	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	76	PPU	1	0
1	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 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

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%)	-0.08	93 (3%) 45 52	24, 46, 90, 150	0
2	9	122/122 (100%)	0.17	5 (4%) 37 44	42, 65, 90, 149	0
3	4	5/7 (71%)	-0.41	0 100 100	40, 47, 49, 54	0
4	A	237/240 (98%)	0.54	19 (8%) 12 16	28, 50, 83, 105	0
5	B	337/338 (99%)	0.35	12 (3%) 42 49	29, 52, 78, 90	0
6	C	246/246 (100%)	0.14	5 (2%) 65 71	26, 47, 69, 81	0
7	D	140/177 (79%)	2.42	70 (50%) 0 0	59, 93, 123, 132	0
8	E	172/178 (96%)	0.98	33 (19%) 1 1	44, 66, 84, 89	0
9	F	119/120 (99%)	1.27	35 (29%) 0 0	46, 72, 98, 109	0
10	G	29/348 (8%)	2.85	19 (65%) 0 0	71, 91, 100, 102	0
11	H	160/171 (93%)	0.70	23 (14%) 2 3	41, 59, 92, 98	0
12	J	142/145 (97%)	0.24	4 (2%) 53 60	37, 50, 70, 89	0
13	K	132/132 (100%)	0.03	3 (2%) 60 67	34, 46, 68, 78	0
14	L	145/165 (87%)	0.96	29 (20%) 1 1	26, 64, 108, 121	0
15	M	194/195 (99%)	0.64	17 (8%) 10 13	31, 45, 76, 85	0
16	N	186/187 (99%)	1.12	39 (20%) 1 1	44, 62, 110, 116	0
17	O	115/116 (99%)	0.29	3 (2%) 56 63	39, 55, 69, 77	0
18	P	143/149 (95%)	0.16	1 (0%) 87 91	37, 51, 65, 74	0
19	Q	95/96 (98%)	0.29	4 (4%) 36 43	38, 47, 64, 73	0
20	R	150/155 (96%)	0.04	3 (2%) 65 71	31, 44, 64, 74	0
21	S	81/85 (95%)	0.43	5 (6%) 20 26	41, 56, 77, 93	0
22	T	119/120 (99%)	0.71	11 (9%) 9 12	42, 55, 81, 110	0
23	U	53/66 (80%)	0.32	1 (1%) 66 73	41, 51, 72, 79	0
24	V	65/71 (91%)	2.22	21 (32%) 0 0	54, 75, 113, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.23	4 (2%) 56 63	40, 52, 71, 81	0
26	X	82/92 (89%)	0.86	11 (13%) 3 4	43, 55, 83, 100	0
27	Y	142/241 (58%)	0.35	11 (7%) 13 17	30, 45, 65, 87	0
28	Z	73/83 (87%)	1.97	26 (35%) 0 0	48, 78, 93, 101	0
29	1	56/57 (98%)	-0.29	0 100 100	27, 33, 41, 47	0
30	2	46/50 (92%)	1.03	8 (17%) 1 1	35, 59, 82, 94	0
31	3	92/92 (100%)	0.34	4 (4%) 35 42	35, 55, 69, 83	0
32	I	70/162 (43%)	6.69	65 (92%) 0 0	111, 123, 141, 141	0
All	All	6651/7482 (88%)	0.40	584 (8%) 10 13	24, 51, 97, 150	0

All (584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	25.2
24	V	1	THR	16.1
32	I	79	ILE	14.7
32	I	133	THR	13.9
24	V	39	ALA	13.5
7	D	63	ILE	13.5
32	I	96	PHE	13.1
32	I	76	ALA	12.8
32	I	75	THR	12.8
32	I	118	SER	11.9
32	I	116	LEU	11.6
7	D	57	THR	11.6
32	I	109	ALA	11.5
16	N	166	ALA	11.5
32	I	105	VAL	11.0
28	Z	11	SER	10.9
32	I	137	VAL	10.9
32	I	111	GLN	10.1
28	Z	22	SER	10.0
24	V	40	PRO	9.8
26	X	88	GLU	9.7
22	T	119	ALA	9.7
32	I	85	PHE	9.2
32	I	108	ILE	9.1
32	I	117	LEU	9.0
32	I	102	VAL	9.0

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Mol	Chain	Res	Type	RSRZ
2	9	3001	U	8.9
32	I	113	HIS	8.8
32	I	121	LEU	8.5
32	I	93	GLN	8.3
32	I	114	PRO	8.3
7	D	61	PHE	8.3
30	2	49	GLU	8.1
32	I	77	GLU	8.0
24	V	38	GLY	7.8
32	I	125	ALA	7.7
15	M	74	LYS	7.7
32	I	107	GLN	7.7
32	I	91	GLU	7.7
32	I	78	LEU	7.6
32	I	126	LYS	7.5
32	I	129	VAL	7.4
32	I	87	THR	7.4
32	I	136	GLY	7.3
4	A	37	VAL	7.2
15	M	79	ALA	7.2
32	I	132	CYS	7.2
10	G	26	MET	7.2
28	Z	21	VAL	7.1
28	Z	19	GLY	7.1
24	V	37	GLY	7.1
7	D	69	ILE	7.0
32	I	88	GLY	7.0
32	I	89	SER	7.0
32	I	81	ASP	6.9
32	I	104	GLN	6.9
32	I	74	PRO	6.8
10	G	23	ILE	6.7
28	Z	25	ARG	6.7
7	D	90	LEU	6.7
15	M	70	GLY	6.6
32	I	97	VAL	6.5
28	Z	20	ARG	6.4
32	I	83	ALA	6.3
22	T	118	SER	6.3
28	Z	24	ARG	6.2
14	L	97	VAL	6.0
32	I	122	THR	6.0

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Mol	Chain	Res	Type	RSRZ
7	D	44	ILE	5.9
21	S	81	ILE	5.9
1	0	497	A	5.9
32	I	103	ASP	5.8
8	E	45	ASP	5.8
1	0	1951	G	5.8
7	D	64	ARG	5.7
15	M	80	GLY	5.7
1	0	282	C	5.7
7	D	170	TYR	5.7
24	V	36	ALA	5.6
28	Z	18	TYR	5.5
1	0	1199	A	5.4
7	D	73	VAL	5.4
28	Z	34	ASN	5.4
7	D	26	GLY	5.4
2	9	3024	U	5.2
7	D	88	LEU	5.2
30	2	35	ARG	5.2
7	D	40	ILE	5.2
26	X	80	GLU	5.2
32	I	86	GLU	5.1
1	0	1173	A	5.1
7	D	134	LEU	5.1
22	T	116	ASP	5.1
7	D	92	GLU	5.1
7	D	62	ASP	5.0
7	D	104	PHE	5.0
24	V	41	GLU	5.0
1	0	960	G	5.0
32	I	112	LYS	4.9
32	I	138	THR	4.9
24	V	43	PRO	4.9
10	G	24	VAL	4.9
28	Z	31	SER	4.9
1	0	1163	G	4.9
14	L	102	ASP	4.9
28	Z	32	GLU	4.9
1	0	1172	G	4.9
9	F	119	ARG	4.9
28	Z	29	ILE	4.8
8	E	86	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
9	F	16	ALA	4.8
12	J	4	ALA	4.8
32	I	123	ASN	4.8
10	G	27	ILE	4.8
14	L	75	LEU	4.8
12	J	70	PHE	4.7
2	9	3023	U	4.7
14	L	105	TYR	4.7
16	N	155	GLU	4.7
32	I	94	GLU	4.7
1	0	2645	U	4.7
28	Z	23	ARG	4.7
7	D	93	LEU	4.6
7	D	166	ILE	4.6
7	D	85	GLN	4.6
16	N	165	ALA	4.6
7	D	23	VAL	4.6
1	0	272	A	4.6
14	L	93	VAL	4.6
8	E	87	PHE	4.6
1	0	1177	A	4.6
1	0	1525	G	4.6
7	D	11	HIS	4.5
1	0	970	U	4.5
27	Y	235	GLU	4.5
1	0	2237	G	4.5
26	X	71	ARG	4.5
1	0	2769	C	4.4
1	0	999	C	4.4
6	C	61	PHE	4.4
30	2	39	ARG	4.4
7	D	106	PHE	4.3
7	D	130	VAL	4.3
7	D	27	ILE	4.3
28	Z	10	ARG	4.3
16	N	175	LEU	4.3
4	A	237	GLY	4.3
32	I	106	LYS	4.2
2	9	3002	U	4.2
32	I	115	ASP	4.2
11	H	37	GLN	4.2
1	0	1169	U	4.2

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Mol	Chain	Res	Type	RSRZ
28	Z	33	MET	4.2
15	M	78	LYS	4.2
28	Z	12	GLY	4.2
14	L	60	GLU	4.2
7	D	89	PRO	4.2
14	L	100	ALA	4.2
1	0	280	C	4.1
32	I	72	VAL	4.1
15	M	86	GLN	4.1
4	A	35	GLY	4.1
14	L	145	LEU	4.1
1	0	1965	C	4.1
1	0	2004	U	4.1
10	G	66	LEU	4.1
1	0	1198	U	4.1
32	I	119	TYR	4.1
9	F	22	VAL	4.0
7	D	172	VAL	4.0
32	I	134	SER	4.0
10	G	67	LEU	4.0
32	I	98	ALA	4.0
1	0	2238	A	4.0
9	F	17	LEU	4.0
14	L	80	ASP	4.0
14	L	91	VAL	3.9
14	L	106	VAL	3.9
32	I	99	ASP	3.9
28	Z	14	PHE	3.9
32	I	73	PRO	3.9
26	X	10	VAL	3.9
11	H	74	ILE	3.9
10	G	69	ARG	3.9
1	0	735	C	3.9
16	N	68	GLU	3.8
1	0	1200	A	3.8
16	N	95	ALA	3.8
7	D	41	LEU	3.8
15	M	75	ARG	3.8
1	0	1171	A	3.8
9	F	98	VAL	3.8
24	V	8	ILE	3.8
4	A	133	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
11	H	171	ALA	3.8
10	G	71	LEU	3.8
7	D	18	ILE	3.8
9	F	106	ALA	3.8
1	0	10	U	3.8
9	F	117	GLU	3.7
10	G	25	GLU	3.7
7	D	81	GLU	3.7
2	9	3122	C	3.7
9	F	110	ASP	3.7
28	Z	45	ASP	3.7
4	A	36	ASP	3.7
1	0	514	G	3.7
4	A	85	SER	3.7
1	0	285	A	3.7
16	N	184	ILE	3.7
26	X	85	VAL	3.6
23	U	47	ARG	3.6
8	E	10	ASP	3.6
32	I	95	ASP	3.6
7	D	51	ARG	3.6
1	0	288	A	3.6
7	D	68	PRO	3.6
8	E	43	ASP	3.6
7	D	56	ARG	3.6
11	H	146	VAL	3.6
15	M	77	HIS	3.6
10	G	73	ASP	3.6
16	N	163	PHE	3.6
11	H	73	LEU	3.6
14	L	76	LEU	3.6
1	0	2508	C	3.5
1	0	1202	A	3.5
9	F	28	ALA	3.5
25	W	86	GLU	3.5
1	0	1168	C	3.5
30	2	44	ARG	3.5
1	0	1165	G	3.5
15	M	88	VAL	3.5
24	V	63	GLU	3.5
1	0	1180	U	3.5
9	F	118	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	0	358	G	3.5
1	0	1181	A	3.4
32	I	92	PRO	3.4
30	2	27	LEU	3.4
15	M	76	ARG	3.4
32	I	80	LYS	3.4
7	D	10	PHE	3.4
7	D	128	LEU	3.4
8	E	118	ILE	3.4
7	D	66	GLY	3.4
11	H	35	ARG	3.4
10	G	22	ALA	3.4
26	X	7	GLU	3.4
32	I	110	GLU	3.4
32	I	120	ASP	3.4
15	M	83	SER	3.4
27	Y	95	THR	3.4
32	I	90	GLY	3.3
15	M	84	LYS	3.3
7	D	91	ALA	3.3
13	K	118	ALA	3.3
9	F	12	LEU	3.3
9	F	49	PHE	3.3
16	N	152	GLU	3.3
1	0	1948	G	3.3
8	E	42	VAL	3.3
16	N	159	TYR	3.3
27	Y	216	ARG	3.3
14	L	99	GLU	3.3
7	D	135	VAL	3.3
7	D	173	GLU	3.3
31	3	92	GLU	3.3
8	E	154	ILE	3.3
16	N	134	ASP	3.3
31	3	62	THR	3.2
7	D	154	LYS	3.2
16	N	147	ILE	3.2
28	Z	26	VAL	3.2
28	Z	30	GLU	3.2
21	S	20	PHE	3.2
5	B	57	GLU	3.2
7	D	45	THR	3.2

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Mol	Chain	Res	Type	RSRZ
9	F	25	ASP	3.2
22	T	117	ASP	3.2
1	0	2748	G	3.2
7	D	75	LEU	3.2
1	0	1170	U	3.1
9	F	19	ALA	3.1
1	0	284	C	3.1
1	0	2511	A	3.1
24	V	20	LEU	3.1
1	0	969	G	3.1
28	Z	59	TYR	3.1
8	E	128	GLY	3.1
7	D	53	LYS	3.1
1	0	372	A	3.1
15	M	73	ARG	3.1
9	F	111	ILE	3.1
24	V	59	ILE	3.1
8	E	6	GLU	3.1
1	0	1950	G	3.1
7	D	25	MET	3.1
1	0	1000	C	3.1
12	J	5	GLU	3.1
24	V	33	VAL	3.0
17	O	23	GLY	3.0
9	F	15	ASP	3.0
19	Q	76	VAL	3.0
32	I	100	LEU	3.0
9	F	100	ASP	3.0
16	N	160	SER	3.0
7	D	95	THR	3.0
8	E	108	LEU	3.0
14	L	148	GLU	3.0
14	L	62	ALA	3.0
1	0	1192	A	3.0
9	F	108	VAL	3.0
13	K	132	VAL	3.0
26	X	72	VAL	3.0
16	N	177	GLU	3.0
1	0	2344	G	3.0
15	M	81	ARG	3.0
24	V	14	ALA	3.0
24	V	32	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
16	N	172	PHE	3.0
16	N	181	ASP	3.0
28	Z	36	ASP	3.0
16	N	148	ALA	3.0
14	L	121	ILE	3.0
9	F	99	THR	3.0
1	0	1196	C	2.9
24	V	2	VAL	2.9
14	L	79	ASP	2.9
16	N	161	GLY	2.9
4	A	99	ILE	2.9
1	0	1178	G	2.9
8	E	100	ASP	2.9
16	N	156	GLU	2.9
1	0	281	U	2.9
1	0	1164	U	2.9
8	E	94	GLN	2.9
1	0	295	C	2.9
16	N	94	GLU	2.9
14	L	81	VAL	2.9
32	I	135	LEU	2.9
5	B	2	GLN	2.9
7	D	107	GLY	2.9
8	E	161	VAL	2.9
7	D	67	ASP	2.9
16	N	183	ASP	2.9
17	O	22	GLY	2.8
1	0	1179	C	2.8
8	E	76	VAL	2.8
7	D	71	ALA	2.8
10	G	12	ILE	2.8
1	0	1966	U	2.8
11	H	138	CYS	2.8
8	E	4	GLU	2.8
10	G	70	ALA	2.8
32	I	124	ALA	2.8
22	T	112	LEU	2.8
14	L	104	ASP	2.8
4	A	236	GLY	2.8
7	D	167	GLU	2.8
7	D	58	VAL	2.8
9	F	75	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
11	H	47	ILE	2.7
6	C	132	ASP	2.7
7	D	157	LEU	2.7
16	N	178	THR	2.7
1	0	370	G	2.7
10	G	21	ASP	2.7
1	0	1625	U	2.7
8	E	88	TYR	2.7
11	H	79	GLU	2.7
7	D	129	ASP	2.7
9	F	11	ASP	2.7
1	0	1174	A	2.7
15	M	82	ARG	2.7
20	R	104	PHE	2.7
16	N	139	TRP	2.7
16	N	180	LEU	2.7
4	A	31	LYS	2.7
16	N	149	GLU	2.7
1	0	1929	G	2.7
1	0	1189	A	2.7
9	F	29	VAL	2.7
1	0	1208	C	2.7
7	D	70	GLY	2.7
8	E	127	ASP	2.7
11	H	83	TYR	2.7
8	E	169	THR	2.7
27	Y	236	VAL	2.7
15	M	87	GLY	2.7
16	N	185	GLU	2.6
16	N	179	LEU	2.6
22	T	36	GLY	2.6
27	Y	234	VAL	2.6
5	B	1	PRO	2.6
8	E	126	ILE	2.6
7	D	86	THR	2.6
14	L	120	LEU	2.6
22	T	35	TYR	2.6
27	Y	96	GLU	2.6
11	H	166	SER	2.6
15	M	72	ALA	2.6
5	B	104	GLU	2.6
9	F	107	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
10	G	72	ASP	2.6
14	L	95	ASP	2.6
27	Y	108	ASP	2.6
9	F	21	GLU	2.6
7	D	171	ASP	2.6
11	H	34	GLY	2.6
16	N	138	ASP	2.6
1	0	1981	A	2.6
25	W	91	ASP	2.6
16	N	158	LEU	2.5
27	Y	187	VAL	2.5
8	E	121	ASP	2.5
27	Y	98	GLN	2.5
1	0	1476	A	2.5
4	A	38	ILE	2.5
10	G	68	GLU	2.5
5	B	119	HIS	2.5
8	E	98	GLU	2.5
22	T	82	THR	2.5
8	E	1	PRO	2.5
7	D	87	ALA	2.5
1	0	279	C	2.5
11	H	82	ASP	2.5
8	E	160	ARG	2.5
1	0	1186	C	2.5
31	3	56	PRO	2.5
16	N	154	LEU	2.5
8	E	11	VAL	2.4
30	2	20	ARG	2.4
20	R	150	PRO	2.4
11	H	78	GLY	2.4
1	0	289	G	2.4
1	0	1190	G	2.4
32	I	82	GLU	2.4
4	A	97	ALA	2.4
26	X	41	PHE	2.4
31	3	41	GLU	2.4
32	I	127	GLU	2.4
1	0	716	G	2.4
16	N	87	LEU	2.4
4	A	145	MET	2.4
10	G	65	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	1184	C	2.4
1	0	1527	A	2.4
20	R	7	GLU	2.4
7	D	52	THR	2.4
8	E	7	ILE	2.4
21	S	45	TYR	2.4
7	D	43	GLU	2.4
1	0	2345	A	2.4
10	G	63	ARG	2.4
11	H	143	ALA	2.4
24	V	52	ALA	2.4
1	0	1195	G	2.4
17	O	1	SER	2.4
28	Z	28	GLU	2.4
4	A	88	ILE	2.4
26	X	73	ARG	2.4
14	L	142	LEU	2.4
16	N	62	HIS	2.4
7	D	80	ALA	2.4
7	D	165	PHE	2.4
1	0	283	U	2.3
14	L	130	ARG	2.3
7	D	65	GLU	2.3
7	D	84	LEU	2.3
7	D	94	ALA	2.3
16	N	106	LEU	2.3
1	0	441	A	2.3
1	0	1526	A	2.3
1	0	1967	U	2.3
7	D	98	PHE	2.3
1	0	1162	G	2.3
5	B	117	GLU	2.3
28	Z	35	GLU	2.3
8	E	167	TYR	2.3
6	C	139	VAL	2.3
8	E	156	ASP	2.3
8	E	129	GLU	2.3
1	0	298	C	2.3
1	0	138	U	2.3
4	A	128	LEU	2.3
11	H	154	TYR	2.3
12	J	7	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
21	S	2	TRP	2.3
1	0	1197	G	2.3
1	0	1206	U	2.3
5	B	181	ILE	2.3
5	B	183	GLU	2.3
14	L	61	ALA	2.3
13	K	119	GLN	2.3
1	0	293	A	2.3
10	G	15	TRP	2.3
4	A	135	VAL	2.3
8	E	159	VAL	2.3
22	T	42	VAL	2.3
5	B	108	GLU	2.3
1	0	365	G	2.3
5	B	134	ALA	2.3
7	D	38	GLU	2.3
4	A	58	VAL	2.3
4	A	82	VAL	2.3
1	0	296	G	2.3
25	W	4	LEU	2.2
9	F	103	GLU	2.2
22	T	115	GLU	2.2
9	F	45	ALA	2.2
16	N	137	ALA	2.2
1	0	362	G	2.2
5	B	186	GLY	2.2
14	L	147	GLU	2.2
22	T	59	GLU	2.2
1	0	2890	A	2.2
26	X	77	PHE	2.2
8	E	99	GLY	2.2
16	N	67	ALA	2.2
26	X	9	VAL	2.2
1	0	1188	A	2.2
7	D	74	THR	2.2
9	F	26	THR	2.2
21	S	19	ASP	2.2
11	H	70	ASN	2.2
11	H	162	ARG	2.2
24	V	9	ARG	2.2
9	F	44	SER	2.2
19	Q	95	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	1166	A	2.2
9	F	23	ALA	2.2
8	E	89	SER	2.2
5	B	33	ASP	2.2
11	H	111	ASP	2.2
24	V	10	ASP	2.2
28	Z	37	HIS	2.2
30	2	48	ASP	2.2
9	F	72	VAL	2.1
14	L	96	VAL	2.1
27	Y	196	VAL	2.1
7	D	160	ALA	2.1
8	E	122	THR	2.1
16	N	81	ALA	2.1
25	W	93	ILE	2.1
19	Q	18	PRO	2.1
9	F	24	ARG	2.1
7	D	29	HIS	2.1
14	L	44	GLU	2.1
9	F	101	ALA	2.1
4	A	68	ILE	2.1
19	Q	84	ILE	2.1
4	A	134	ASN	2.1
24	V	45	ARG	2.1
9	F	18	GLU	2.1
18	P	18	LYS	2.1
1	0	1161	A	2.1
9	F	109	GLU	2.1
1	0	130	C	2.1
30	2	26	MET	2.1
16	N	153	GLN	2.1
9	F	69	GLU	2.1
24	V	46	ILE	2.1
6	C	245	GLU	2.1
11	H	139	ASN	2.1
32	I	128	VAL	2.1
32	I	84	GLY	2.1
1	0	369	G	2.0
14	L	101	ASP	2.0
11	H	66	ARG	2.0
28	Z	13	ARG	2.0
7	D	150	SER	2.0

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Mol	Chain	Res	Type	RSRZ
27	Y	193	LEU	2.0
1	0	371	U	2.0
1	0	1175	G	2.0
1	0	1279	U	2.0
6	C	1	MET	2.0
11	H	80	GLU	2.0
16	N	128	ASP	2.0
7	D	72	LYS	2.0
7	D	158	ASN	2.0
11	H	50	ILE	2.0
14	L	122	ALA	2.0
16	N	92	ALA	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	OMG	0	2588	24/25	0.97	0.12	30,33,37,38	0
1	OMU	0	2587	21/22	0.98	0.11	30,36,38,38	0
1	1MA	0	628	23/24	0.98	0.15	32,34,36,38	0
1	UR3	0	2619	21/22	0.98	0.13	33,36,40,41	0
1	PSU	0	2621	20/21	0.98	0.12	31,34,41,42	0
3	PPU	4	76	37/38	0.98	0.12	36,42,57,61	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(\AA^2)	Q<0.9
33	MG	0	8082	1/1	0.31	0.29	85,85,85,85	0
35	NA	0	9169	1/1	0.36	0.56	115,115,115,115	0
38	CD	Z	9203	1/1	0.44	0.18	92,92,92,92	0
37	SR	0	9547	1/1	0.58	0.40	191,191,191,191	0
33	MG	0	8094	1/1	0.60	0.44	85,85,85,85	0
33	MG	0	8014	1/1	0.64	0.37	84,84,84,84	0
35	NA	0	9129	1/1	0.67	0.21	81,81,81,81	0
35	NA	0	9174	1/1	0.70	0.33	70,70,70,70	0
33	MG	0	8042	1/1	0.71	0.10	56,56,56,56	0
33	MG	0	8091	1/1	0.72	0.08	54,54,54,54	0
35	NA	0	9173	1/1	0.74	0.30	70,70,70,70	0
33	MG	0	8059	1/1	0.74	0.46	85,85,85,85	0
35	NA	0	9111	1/1	0.74	0.20	68,68,68,68	0
35	NA	0	9171	1/1	0.74	0.26	63,63,63,63	0
33	MG	0	8050	1/1	0.75	0.23	87,87,87,87	0
35	NA	9	9183	1/1	0.77	0.16	76,76,76,76	0
35	NA	0	9122	1/1	0.77	0.37	79,79,79,79	0
33	MG	0	8089	1/1	0.77	0.21	53,53,53,53	0
35	NA	0	9185	1/1	0.79	0.56	61,61,61,61	0
35	NA	S	9112	1/1	0.79	0.32	74,74,74,74	0
35	NA	J	9146	1/1	0.80	0.15	55,55,55,55	0
35	NA	0	9181	1/1	0.80	0.17	53,53,53,53	0
33	MG	0	8055	1/1	0.80	0.22	103,103,103,103	0
35	NA	0	9152	1/1	0.80	0.24	65,65,65,65	0
33	MG	0	8108	1/1	0.81	0.19	96,96,96,96	0
33	MG	0	8024	1/1	0.81	0.42	64,64,64,64	0
33	MG	0	8054	1/1	0.82	0.12	47,47,47,47	0
35	NA	0	9126	1/1	0.83	0.11	53,53,53,53	0
35	NA	0	9102	1/1	0.83	0.22	58,58,58,58	0
35	NA	0	9140	1/1	0.83	0.47	63,63,63,63	0
37	SR	0	9521	1/1	0.83	0.28	175,175,175,175	0
33	MG	0	8102	1/1	0.83	0.10	67,67,67,67	0
33	MG	0	8045	1/1	0.83	0.23	76,76,76,76	0
35	NA	0	9179	1/1	0.84	0.73	103,103,103,103	0
33	MG	0	8113	1/1	0.84	0.10	42,42,42,42	0
37	SR	0	9590	1/1	0.84	0.07	102,102,102,102	0
33	MG	0	8101	1/1	0.84	0.14	70,70,70,70	0
35	NA	0	9157	1/1	0.85	0.19	46,46,46,46	0
35	NA	0	9107	1/1	0.85	0.26	63,63,63,63	0
37	SR	0	9467	1/1	0.85	0.12	84,84,84,84	0
33	MG	0	8022	1/1	0.85	0.59	107,107,107,107	0
35	NA	0	9184	1/1	0.85	0.16	74,74,74,74	0
35	NA	0	9172	1/1	0.85	0.40	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9127	1/1	0.85	0.15	60,60,60,60	0
33	MG	0	8116	1/1	0.86	0.11	57,57,57,57	0
37	SR	0	9484	1/1	0.86	0.08	136,136,136,136	0
33	MG	0	8041	1/1	0.86	0.12	49,49,49,49	0
35	NA	0	9163	1/1	0.86	0.19	68,68,68,68	0
33	MG	0	8103	1/1	0.86	0.21	64,64,64,64	0
37	SR	0	9626	1/1	0.86	0.34	142,142,142,142	0
37	SR	C	9500	1/1	0.86	0.63	187,187,187,187	0
35	NA	0	9141	1/1	0.86	0.09	59,59,59,59	0
35	NA	0	9182	1/1	0.87	0.15	87,87,87,87	0
35	NA	0	9132	1/1	0.87	0.21	59,59,59,59	0
33	MG	0	8047	1/1	0.88	0.44	86,86,86,86	0
33	MG	9	8095	1/1	0.88	0.21	51,51,51,51	0
38	CD	O	9205	1/1	0.88	0.06	124,124,124,124	0
33	MG	0	8084	1/1	0.88	0.38	69,69,69,69	0
33	MG	0	8039	1/1	0.89	0.10	74,74,74,74	0
35	NA	0	9164	1/1	0.89	0.46	65,65,65,65	0
33	MG	0	8061	1/1	0.89	0.13	71,71,71,71	0
35	NA	0	9110	1/1	0.89	0.15	45,45,45,45	0
33	MG	0	8090	1/1	0.89	0.33	79,79,79,79	0
35	NA	0	9113	1/1	0.89	0.14	63,63,63,63	0
33	MG	0	8052	1/1	0.89	0.26	82,82,82,82	0
34	K	0	9001	1/1	0.89	0.30	81,81,81,81	0
35	NA	0	9150	1/1	0.90	0.18	47,47,47,47	0
37	SR	0	9529	1/1	0.90	0.08	103,103,103,103	0
35	NA	0	9120	1/1	0.90	0.31	67,67,67,67	0
35	NA	R	9138	1/1	0.90	0.09	66,66,66,66	0
33	MG	0	8114	1/1	0.90	0.21	63,63,63,63	0
37	SR	9	9588	1/1	0.90	0.10	131,131,131,131	0
33	MG	0	8065	1/1	0.90	0.32	86,86,86,86	0
33	MG	0	8107	1/1	0.90	0.19	62,62,62,62	0
37	SR	0	9504	1/1	0.90	0.11	100,100,100,100	0
35	NA	0	9125	1/1	0.91	0.61	88,88,88,88	0
35	NA	0	9130	1/1	0.91	0.14	48,48,48,48	0
35	NA	0	9166	1/1	0.91	0.09	61,61,61,61	0
35	NA	D	9151	1/1	0.91	0.19	66,66,66,66	0
35	NA	0	9175	1/1	0.91	0.25	53,53,53,53	0
35	NA	R	9137	1/1	0.91	0.11	39,39,39,39	0
35	NA	0	9168	1/1	0.91	0.22	67,67,67,67	0
33	MG	0	8106	1/1	0.91	0.11	43,43,43,43	0
36	CL	0	9316	1/1	0.91	0.15	73,73,73,73	0
36	CL	J	9321	1/1	0.91	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	A	8066	1/1	0.91	0.10	57,57,57,57	0
36	CL	N	9307	1/1	0.92	0.15	57,57,57,57	0
37	SR	0	9452	1/1	0.92	0.17	105,105,105,105	0
33	MG	0	8021	1/1	0.92	0.17	56,56,56,56	0
37	SR	0	9468	1/1	0.92	0.04	115,115,115,115	0
35	NA	0	9167	1/1	0.92	0.17	54,54,54,54	0
37	SR	0	9495	1/1	0.92	0.08	97,97,97,97	0
33	MG	0	8040	1/1	0.92	0.42	103,103,103,103	0
37	SR	0	9517	1/1	0.92	0.04	109,109,109,109	0
33	MG	0	8093	1/1	0.92	0.14	40,40,40,40	0
35	NA	0	9170	1/1	0.92	0.37	84,84,84,84	0
37	SR	0	9537	1/1	0.92	0.14	135,135,135,135	0
35	NA	0	9155	1/1	0.92	0.24	57,57,57,57	0
33	MG	0	8032	1/1	0.92	0.09	39,39,39,39	0
35	NA	0	9161	1/1	0.92	0.23	52,52,52,52	0
35	NA	0	9139	1/1	0.92	0.10	48,48,48,48	0
33	MG	0	8063	1/1	0.92	0.07	57,57,57,57	0
35	NA	0	9177	1/1	0.92	0.42	71,71,71,71	0
35	NA	0	9165	1/1	0.92	0.24	44,44,44,44	0
37	SR	0	9475	1/1	0.93	0.10	82,82,82,82	0
37	SR	0	9482	1/1	0.93	0.24	117,117,117,117	0
33	MG	0	8017	1/1	0.93	0.12	28,28,28,28	0
33	MG	0	8085	1/1	0.93	0.17	55,55,55,55	0
35	NA	M	9147	1/1	0.93	0.19	41,41,41,41	0
37	SR	0	9508	1/1	0.93	0.09	100,100,100,100	0
35	NA	0	9131	1/1	0.93	0.13	44,44,44,44	0
33	MG	0	8051	1/1	0.93	0.27	31,31,31,31	0
35	NA	0	9135	1/1	0.93	0.21	47,47,47,47	0
33	MG	0	8057	1/1	0.93	0.22	68,68,68,68	0
33	MG	0	8104	1/1	0.93	0.13	53,53,53,53	0
37	SR	0	9581	1/1	0.93	0.11	123,123,123,123	0
35	NA	0	9124	1/1	0.93	0.12	49,49,49,49	0
33	MG	0	8080	1/1	0.93	0.17	53,53,53,53	0
37	SR	0	9459	1/1	0.93	0.08	104,104,104,104	0
37	SR	0	9465	1/1	0.93	0.08	98,98,98,98	0
37	SR	F	9595	1/1	0.93	0.14	103,103,103,103	0
33	MG	0	8092	1/1	0.93	0.42	68,68,68,68	0
33	MG	0	8036	1/1	0.93	0.12	54,54,54,54	0
34	K	0	9002	1/1	0.94	0.15	80,80,80,80	0
37	SR	0	9539	1/1	0.94	0.40	156,156,156,156	0
35	NA	0	9118	1/1	0.94	0.23	58,58,58,58	0
35	NA	0	9158	1/1	0.94	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	MG	0	8088	1/1	0.94	0.11	44,44,44,44	0
35	NA	0	9162	1/1	0.94	0.12	47,47,47,47	0
37	SR	0	9509	1/1	0.94	0.12	88,88,88,88	0
37	SR	0	9515	1/1	0.94	0.12	95,95,95,95	0
33	MG	0	8099	1/1	0.94	0.12	68,68,68,68	0
33	MG	T	8073	1/1	0.94	0.12	47,47,47,47	0
33	MG	0	8028	1/1	0.94	0.11	37,37,37,37	0
37	SR	0	9522	1/1	0.95	0.07	109,109,109,109	0
33	MG	0	8075	1/1	0.95	0.08	40,40,40,40	0
33	MG	0	8015	1/1	0.95	0.11	31,31,31,31	0
36	CL	0	9322	1/1	0.95	0.17	59,59,59,59	0
37	SR	0	9483	1/1	0.95	0.07	77,77,77,77	0
36	CL	B	9319	1/1	0.95	0.15	55,55,55,55	0
36	CL	J	9301	1/1	0.95	0.06	55,55,55,55	0
35	NA	C	9104	1/1	0.95	0.14	28,28,28,28	0
33	MG	0	8067	1/1	0.95	0.13	40,40,40,40	0
33	MG	0	8072	1/1	0.95	0.12	68,68,68,68	0
35	NA	0	9101	1/1	0.95	0.17	45,45,45,45	0
35	NA	0	9134	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	9116	1/1	0.95	0.24	46,46,46,46	0
35	NA	Q	9148	1/1	0.96	0.13	45,45,45,45	0
33	MG	0	8098	1/1	0.96	0.07	46,46,46,46	0
35	NA	0	9159	1/1	0.96	0.15	48,48,48,48	0
37	SR	0	9489	1/1	0.96	0.09	86,86,86,86	0
37	SR	0	9490	1/1	0.96	0.08	99,99,99,99	0
35	NA	R	9186	1/1	0.96	0.21	66,66,66,66	0
33	MG	0	8020	1/1	0.96	0.19	33,33,33,33	0
36	CL	0	9311	1/1	0.96	0.09	61,61,61,61	0
36	CL	0	9314	1/1	0.96	0.06	48,48,48,48	0
33	MG	0	8117	1/1	0.96	0.08	38,38,38,38	0
35	NA	0	9178	1/1	0.96	0.36	52,52,52,52	0
36	CL	A	9309	1/1	0.96	0.11	57,57,57,57	0
33	MG	0	8076	1/1	0.96	0.15	57,57,57,57	0
33	MG	0	8058	1/1	0.96	0.25	43,43,43,43	0
37	SR	0	9534	1/1	0.96	0.16	102,102,102,102	0
33	MG	0	8046	1/1	0.96	0.08	44,44,44,44	0
33	MG	0	8083	1/1	0.96	0.08	51,51,51,51	0
36	CL	3	9304	1/1	0.96	0.07	56,56,56,56	0
37	SR	0	9560	1/1	0.96	0.05	94,94,94,94	0
37	SR	0	9405	1/1	0.96	0.13	58,58,58,58	0
33	MG	0	8056	1/1	0.96	0.18	45,45,45,45	0
33	MG	0	8074	1/1	0.96	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8096	1/1	0.96	0.09	44,44,44,44	0
37	SR	0	9466	1/1	0.96	0.05	98,98,98,98	0
33	MG	0	8097	1/1	0.96	0.14	58,58,58,58	0
35	NA	0	9156	1/1	0.96	0.22	61,61,61,61	0
35	NA	0	9108	1/1	0.96	0.13	32,32,32,32	0
33	MG	0	8003	1/1	0.97	0.10	33,33,33,33	0
35	NA	0	9106	1/1	0.97	0.23	41,41,41,41	0
33	MG	0	8112	1/1	0.97	0.04	41,41,41,41	0
33	MG	0	8060	1/1	0.97	0.13	82,82,82,82	0
33	MG	0	8037	1/1	0.97	0.05	39,39,39,39	0
33	MG	0	8115	1/1	0.97	0.11	48,48,48,48	0
35	NA	0	9136	1/1	0.97	0.11	31,31,31,31	0
33	MG	0	8004	1/1	0.97	0.09	31,31,31,31	0
35	NA	0	9114	1/1	0.97	0.12	46,46,46,46	0
33	MG	0	8026	1/1	0.97	0.15	32,32,32,32	0
35	NA	0	9149	1/1	0.97	0.11	43,43,43,43	0
35	NA	0	9117	1/1	0.97	0.11	38,38,38,38	0
36	CL	0	9317	1/1	0.97	0.06	54,54,54,54	0
37	SR	0	9505	1/1	0.97	0.10	89,89,89,89	0
33	MG	0	8027	1/1	0.97	0.25	37,37,37,37	0
33	MG	0	8013	1/1	0.97	0.43	21,21,21,21	0
33	MG	0	8043	1/1	0.97	0.06	50,50,50,50	0
33	MG	Y	8109	1/1	0.97	0.07	41,41,41,41	0
33	MG	0	8030	1/1	0.97	0.06	35,35,35,35	0
33	MG	0	8002	1/1	0.97	0.09	33,33,33,33	0
36	CL	O	9308	1/1	0.97	0.09	66,66,66,66	0
37	SR	0	9530	1/1	0.97	0.13	65,65,65,65	0
35	NA	0	9160	1/1	0.97	0.17	43,43,43,43	0
33	MG	0	8079	1/1	0.97	0.15	31,31,31,31	0
37	SR	0	9417	1/1	0.97	0.11	59,59,59,59	0
37	SR	0	9426	1/1	0.97	0.08	67,67,67,67	0
37	SR	0	9431	1/1	0.97	0.12	60,60,60,60	0
37	SR	0	9433	1/1	0.97	0.12	71,71,71,71	0
37	SR	0	9435	1/1	0.97	0.09	73,73,73,73	0
37	SR	0	9438	1/1	0.97	0.08	64,64,64,64	0
37	SR	0	9629	1/1	0.97	0.10	72,72,72,72	0
37	SR	9	9503	1/1	0.97	0.06	105,105,105,105	0
37	SR	0	9442	1/1	0.97	0.10	59,59,59,59	0
37	SR	0	9447	1/1	0.97	0.08	68,68,68,68	0
37	SR	0	9450	1/1	0.97	0.07	74,74,74,74	0
35	NA	0	9128	1/1	0.97	0.06	42,42,42,42	0
37	SR	0	9455	1/1	0.97	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	Y	9320	1/1	0.98	0.09	45,45,45,45	0
37	SR	0	9477	1/1	0.98	0.06	82,82,82,82	0
37	SR	0	9480	1/1	0.98	0.05	90,90,90,90	0
35	NA	0	9105	1/1	0.98	0.13	38,38,38,38	0
35	NA	T	9143	1/1	0.98	0.10	38,38,38,38	0
37	SR	0	9414	1/1	0.98	0.10	56,56,56,56	0
37	SR	0	9416	1/1	0.98	0.09	45,45,45,45	0
36	CL	0	9303	1/1	0.98	0.12	48,48,48,48	0
37	SR	0	9420	1/1	0.98	0.14	66,66,66,66	0
37	SR	0	9501	1/1	0.98	0.10	96,96,96,96	0
33	MG	0	8110	1/1	0.98	0.13	41,41,41,41	0
37	SR	0	9427	1/1	0.98	0.12	53,53,53,53	0
37	SR	0	9506	1/1	0.98	0.05	65,65,65,65	0
33	MG	0	8068	1/1	0.98	0.15	45,45,45,45	0
36	CL	0	9315	1/1	0.98	0.11	48,48,48,48	0
37	SR	0	9434	1/1	0.98	0.13	62,62,62,62	0
33	MG	K	8069	1/1	0.98	0.20	24,24,24,24	0
33	MG	0	8070	1/1	0.98	0.18	26,26,26,26	0
37	SR	0	9441	1/1	0.98	0.07	64,64,64,64	0
33	MG	0	8029	1/1	0.98	0.30	33,33,33,33	0
37	SR	0	9443	1/1	0.98	0.08	57,57,57,57	0
37	SR	0	9532	1/1	0.98	0.06	118,118,118,118	0
33	MG	0	8012	1/1	0.98	0.18	39,39,39,39	0
33	MG	0	8031	1/1	0.98	0.11	48,48,48,48	0
35	NA	0	9115	1/1	0.98	0.14	38,38,38,38	0
37	SR	0	9545	1/1	0.98	0.04	76,76,76,76	0
37	SR	0	9453	1/1	0.98	0.07	69,69,69,69	0
36	CL	J	9302	1/1	0.98	0.06	54,54,54,54	0
37	SR	0	9566	1/1	0.98	0.07	79,79,79,79	0
37	SR	0	9570	1/1	0.98	0.05	100,100,100,100	0
37	SR	0	9457	1/1	0.98	0.08	53,53,53,53	0
37	SR	0	9585	1/1	0.98	0.06	85,85,85,85	0
33	MG	0	8009	1/1	0.98	0.15	21,21,21,21	0
37	SR	0	9464	1/1	0.98	0.05	77,77,77,77	0
36	CL	L	9310	1/1	0.98	0.10	50,50,50,50	0
35	NA	0	9154	1/1	0.98	0.14	47,47,47,47	0
33	MG	0	8118	1/1	0.98	0.18	29,29,29,29	0
37	SR	A	9437	1/1	0.98	0.11	63,63,63,63	0
36	CL	R	9306	1/1	0.98	0.15	45,45,45,45	0
37	SR	0	9469	1/1	0.98	0.04	85,85,85,85	0
37	SR	H	9486	1/1	0.98	0.20	106,106,106,106	0
37	SR	S	9470	1/1	0.98	0.12	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	3	9439	1/1	0.98	0.05	67,67,67,67	0
37	SR	0	9473	1/1	0.98	0.03	77,77,77,77	0
37	SR	0	9474	1/1	0.98	0.11	60,60,60,60	0
37	SR	0	9488	1/1	0.99	0.12	77,77,77,77	0
33	MG	0	8038	1/1	0.99	0.26	25,25,25,25	0
35	NA	0	9123	1/1	0.99	0.10	40,40,40,40	0
33	MG	0	8025	1/1	0.99	0.38	26,26,26,26	0
37	SR	0	9498	1/1	0.99	0.05	59,59,59,59	0
37	SR	0	9440	1/1	0.99	0.03	70,70,70,70	0
33	MG	0	8001	1/1	0.99	0.22	20,20,20,20	0
37	SR	0	9406	1/1	0.99	0.16	33,33,33,33	0
37	SR	0	9407	1/1	0.99	0.13	43,43,43,43	0
37	SR	0	9444	1/1	0.99	0.05	53,53,53,53	0
37	SR	0	9445	1/1	0.99	0.09	57,57,57,57	0
37	SR	0	9446	1/1	0.99	0.09	86,86,86,86	0
37	SR	0	9408	1/1	0.99	0.16	39,39,39,39	0
37	SR	0	9448	1/1	0.99	0.06	60,60,60,60	0
37	SR	0	9449	1/1	0.99	0.06	61,61,61,61	0
37	SR	0	9410	1/1	0.99	0.14	39,39,39,39	0
37	SR	0	9451	1/1	0.99	0.11	57,57,57,57	0
37	SR	0	9411	1/1	0.99	0.16	42,42,42,42	0
37	SR	0	9412	1/1	0.99	0.12	41,41,41,41	0
37	SR	0	9454	1/1	0.99	0.06	75,75,75,75	0
37	SR	0	9413	1/1	0.99	0.12	44,44,44,44	0
37	SR	0	9456	1/1	0.99	0.07	60,60,60,60	0
33	MG	0	8005	1/1	0.99	0.12	33,33,33,33	0
37	SR	0	9415	1/1	0.99	0.10	54,54,54,54	0
37	SR	0	9461	1/1	0.99	0.04	77,77,77,77	0
37	SR	0	9568	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9462	1/1	0.99	0.12	67,67,67,67	0
36	CL	0	9305	1/1	0.99	0.06	51,51,51,51	0
33	MG	0	8008	1/1	0.99	0.17	19,19,19,19	0
36	CL	0	9312	1/1	0.99	0.11	51,51,51,51	0
37	SR	0	9601	1/1	0.99	0.04	94,94,94,94	0
37	SR	0	9421	1/1	0.99	0.09	68,68,68,68	0
37	SR	0	9422	1/1	0.99	0.12	57,57,57,57	0
37	SR	9	9481	1/1	0.99	0.04	83,83,83,83	0
37	SR	0	9423	1/1	0.99	0.08	54,54,54,54	0
37	SR	0	9425	1/1	0.99	0.11	52,52,52,52	0
37	SR	A	9436	1/1	0.99	0.05	55,55,55,55	0
36	CL	0	9313	1/1	0.99	0.10	54,54,54,54	0
37	SR	A	9497	1/1	0.99	0.10	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	B	9458	1/1	0.99	0.08	74,74,74,74	0
36	CL	M	9318	1/1	0.99	0.13	38,38,38,38	0
37	SR	0	9429	1/1	0.99	0.09	62,62,62,62	0
37	SR	0	9478	1/1	0.99	0.06	75,75,75,75	0
37	SR	R	9418	1/1	0.99	0.13	54,54,54,54	0
37	SR	0	9430	1/1	0.99	0.11	48,48,48,48	0
37	SR	1	9419	1/1	0.99	0.11	41,41,41,41	0
37	SR	1	9460	1/1	0.99	0.10	48,48,48,48	0
33	MG	0	8019	1/1	0.99	0.05	45,45,45,45	0
37	SR	0	9432	1/1	0.99	0.14	64,64,64,64	0
38	CD	U	9201	1/1	0.99	0.10	52,52,52,52	0
33	MG	0	8044	1/1	0.99	0.09	43,43,43,43	0
38	CD	3	9204	1/1	0.99	0.05	58,58,58,58	0
37	SR	0	9428	1/1	1.00	0.05	52,52,52,52	0
37	SR	0	9424	1/1	1.00	0.14	46,46,46,46	0
38	CD	1	9202	1/1	1.00	0.04	51,51,51,51	0
37	SR	L	9409	1/1	1.00	0.11	37,37,37,37	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.