Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:06 AM GMT

PDB ID	:	2OTJ
Title	:	13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors	:	Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on	:	2007-02-08
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

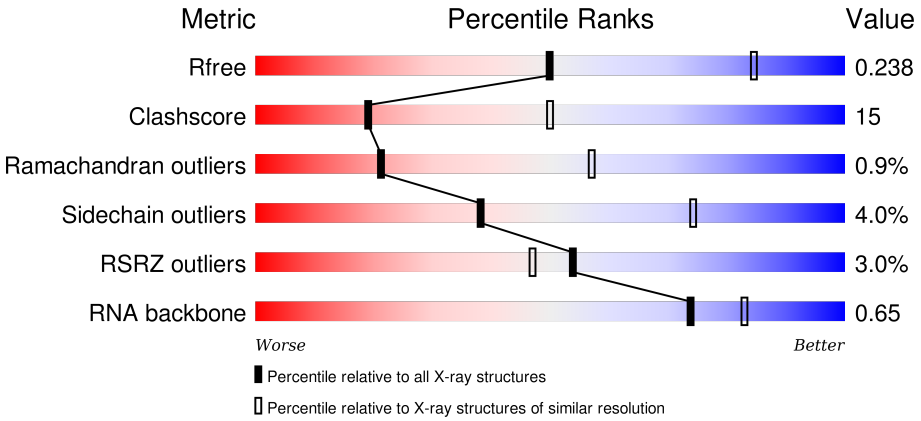
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	49% 39% 6% 6%
2	9	122	2% 38% 48% 13% •
3	A	240	3% 68% 27% • •
4	B	338	62% 34% •

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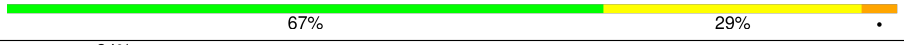
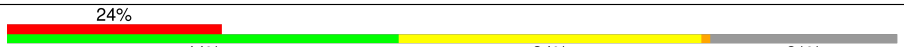
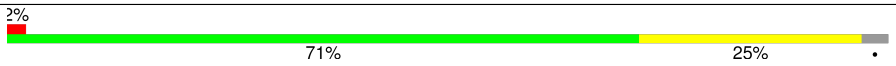
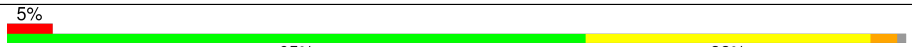
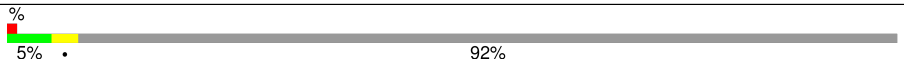
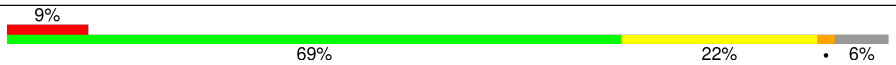
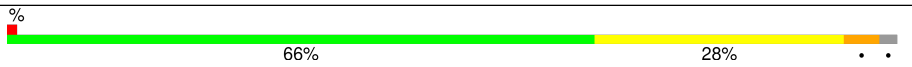
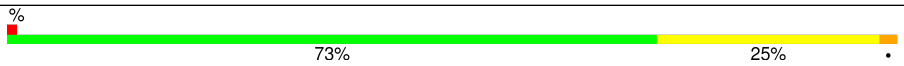
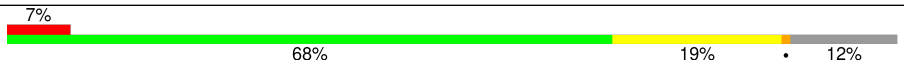
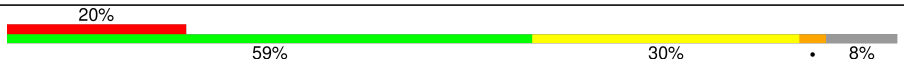
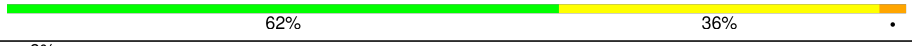
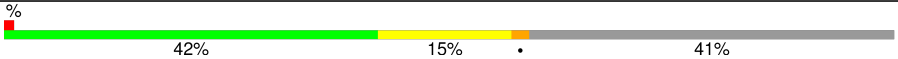
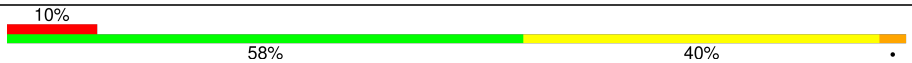
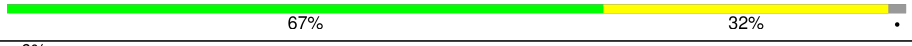
Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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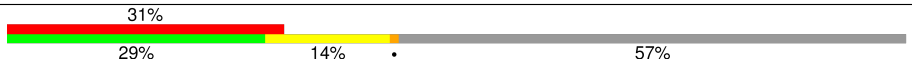
Mol	Chain	Length	Quality of chain
30	3	92	
31	I	161	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	13T	0	9000	-	-	X	X
33	MG	0	8013	-	-	-	X
33	MG	0	8062	-	-	-	X
33	MG	0	8102	-	-	-	X
33	MG	0	8114	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8515	-	-	-	X
35	NA	0	8520	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8531	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8539	-	-	-	X
35	NA	0	8540	-	-	-	X
35	NA	0	8542	-	-	X	-
35	NA	0	8543	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8579	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	J	8801	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99043 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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	237	1753	1072	352	324	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	337	2625	1616	493	511	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			579	346	116	112	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

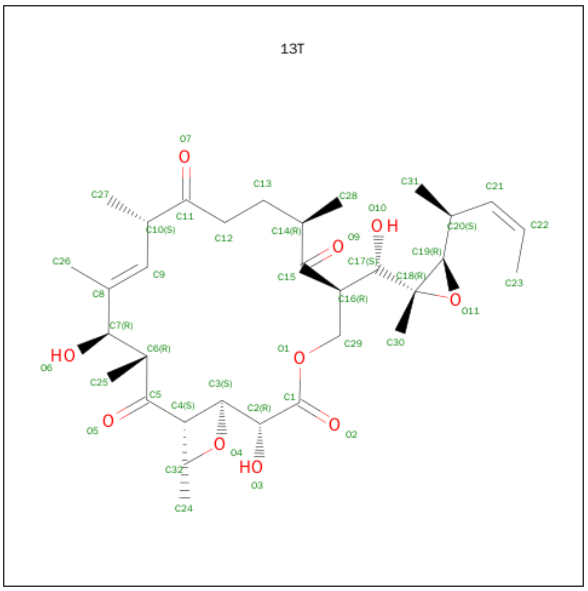
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is 13-DEOXYTEDANOLIDE (three-letter code: 13T) (formula: $C_{32}H_{50}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C O 42 32 10	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	74	Total Na 74 74	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	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	9	Total Cl 9 9	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	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	2	Total Cl 2 2	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

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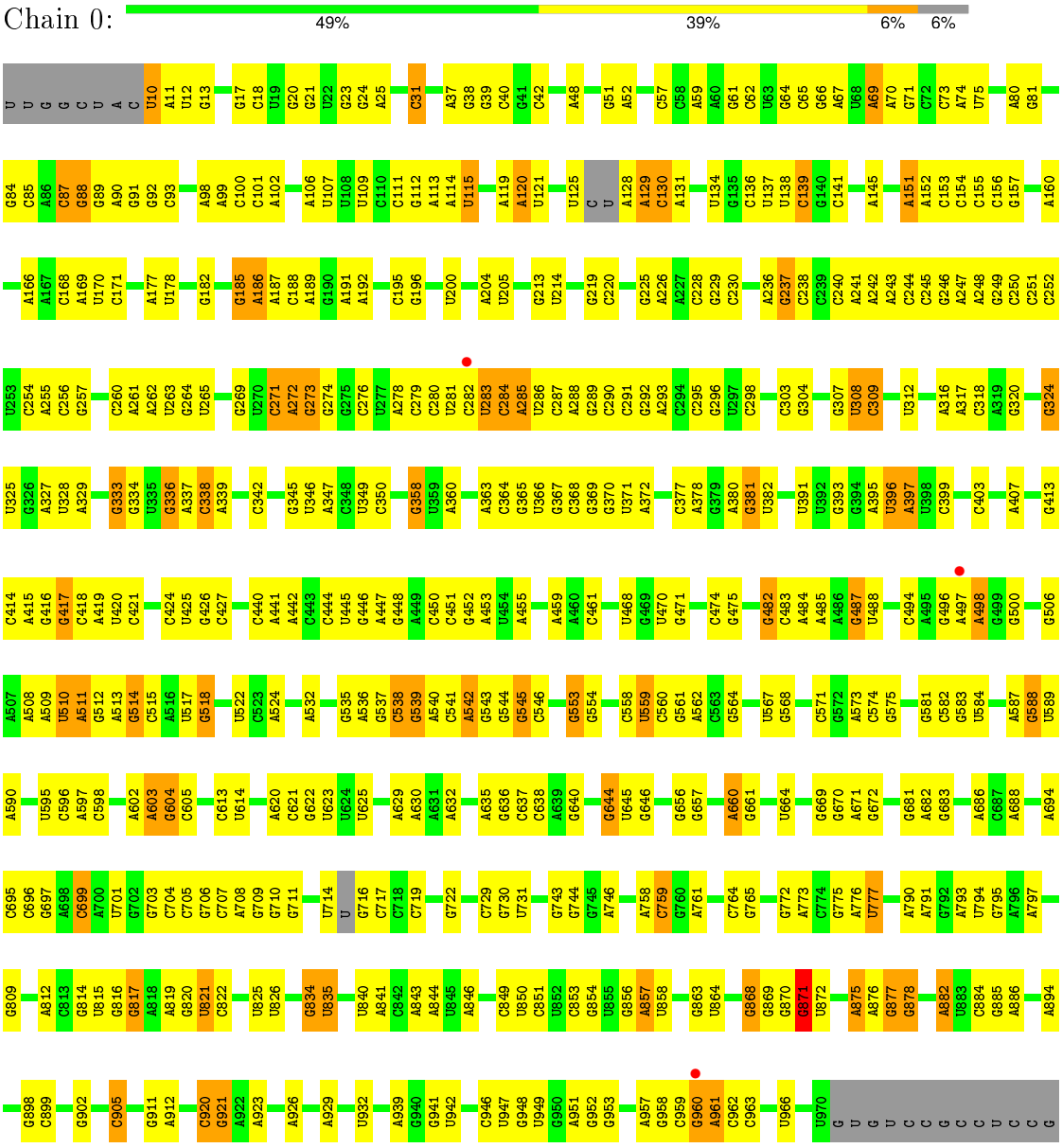
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	44	Total O 44 44	0	0
38	P	56	Total O 56 56	0	0
38	Q	51	Total O 51 51	0	0
38	R	80	Total O 80 80	0	0
38	S	36	Total O 36 36	0	0
38	T	33	Total O 33 33	0	0
38	U	26	Total O 26 26	0	0
38	V	11	Total O 11 11	0	0
38	W	67	Total O 67 67	0	0
38	X	21	Total O 21 21	0	0
38	Y	96	Total O 96 96	0	0
38	Z	31	Total O 31 31	0	0
38	1	56	Total O 56 56	0	0
38	2	45	Total O 45 45	0	0
38	3	66	Total O 66 66	0	0
38	I	8	Total O 8 8	0	0

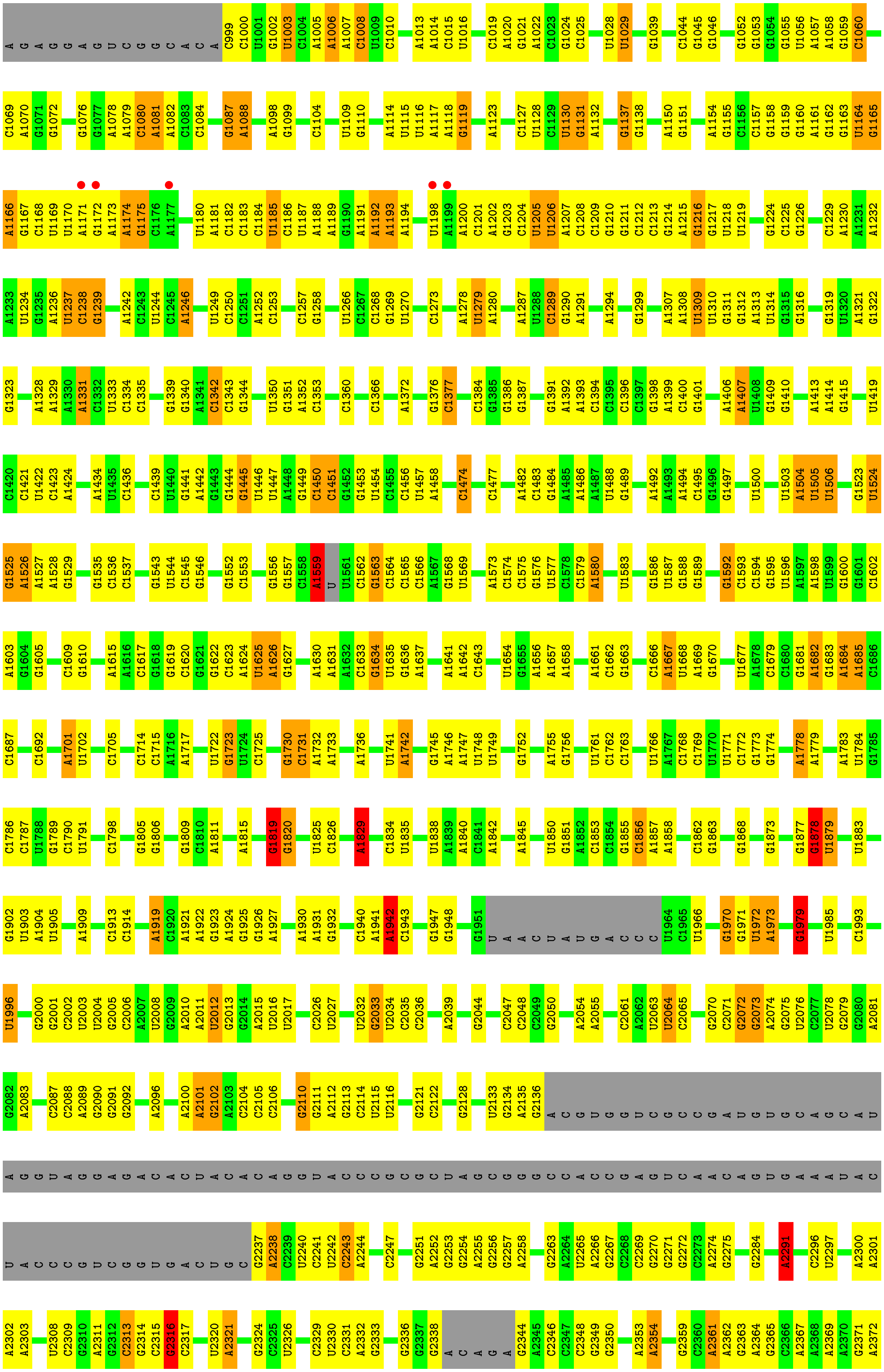
3 Residue-property plots (i)

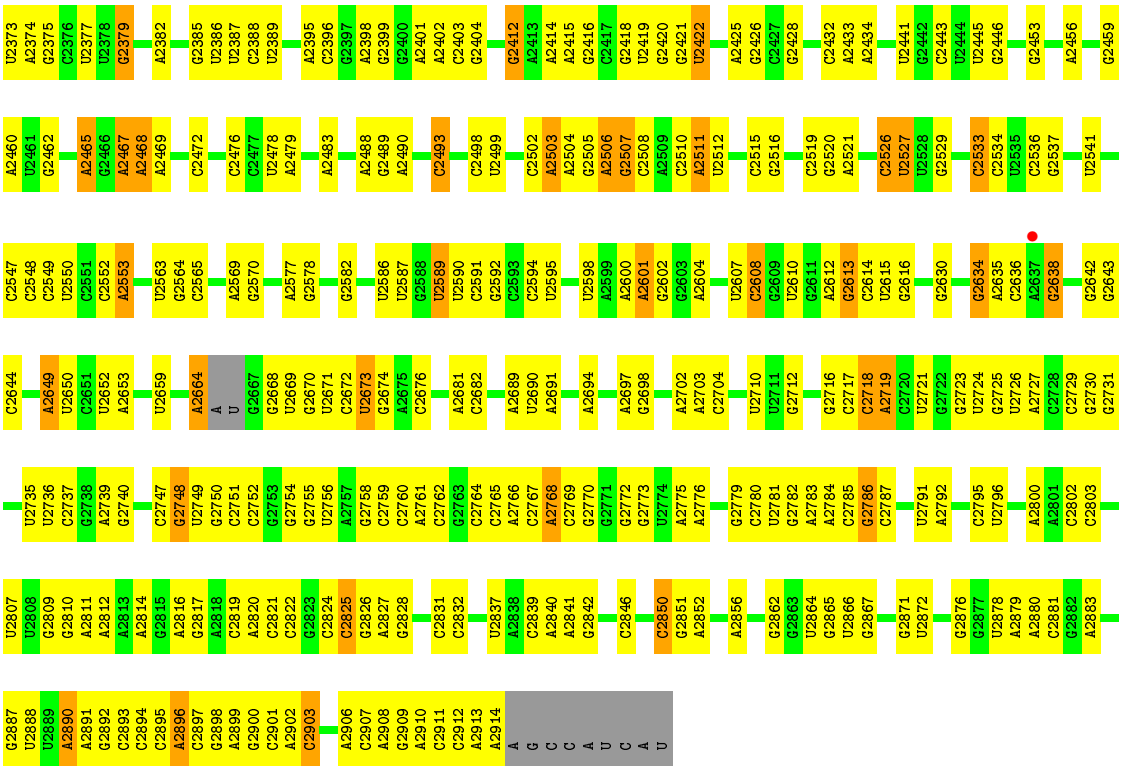
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 23S ribosomal RNA

Chain 0:

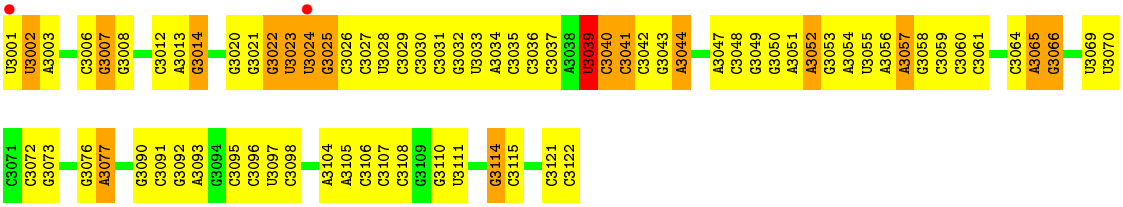






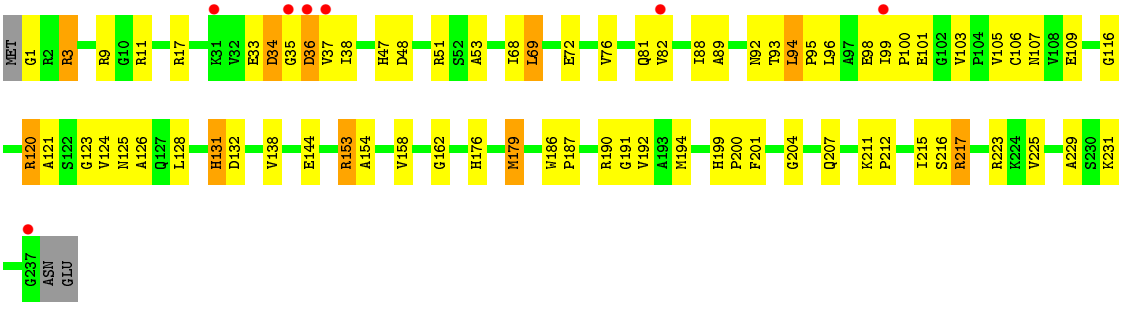
• Molecule 2: 5S ribosomal RNA

Chain 9:



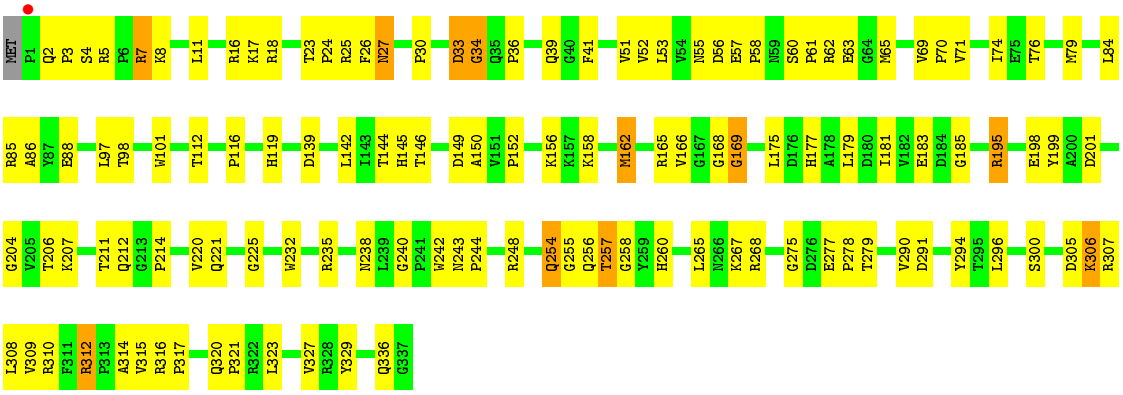
• Molecule 3: 50S ribosomal protein L2P

Chain A:



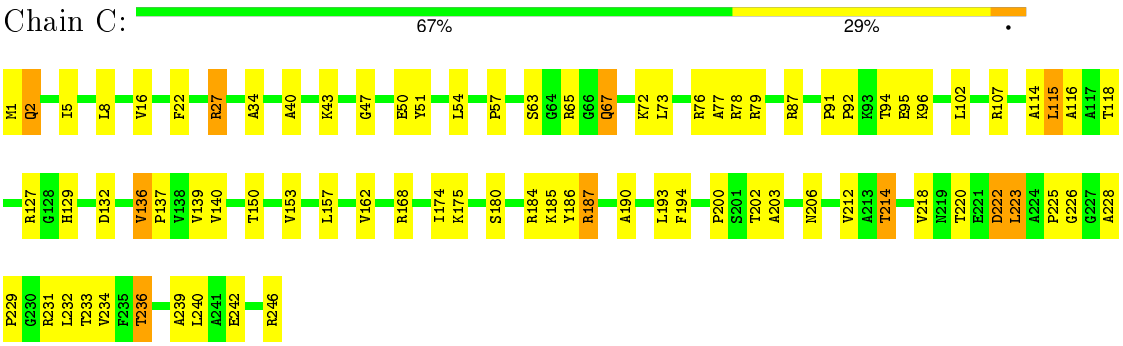
• Molecule 4: 50S ribosomal protein L3P

Chain B:



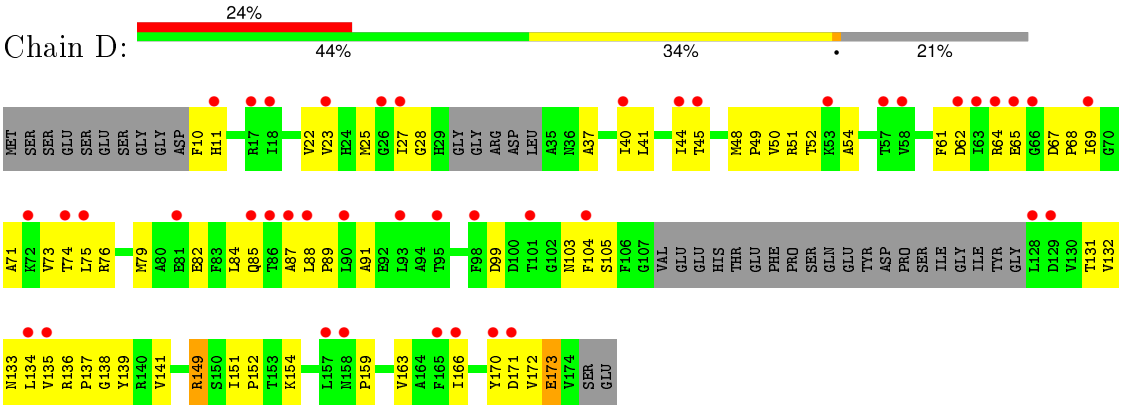
• Molecule 5: 50S ribosomal protein L4P

Chain C:



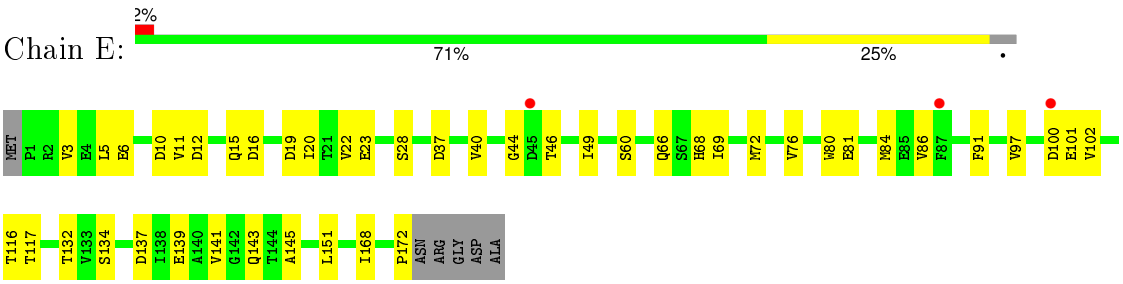
• Molecule 6: 50S ribosomal protein L5P

Chain D:



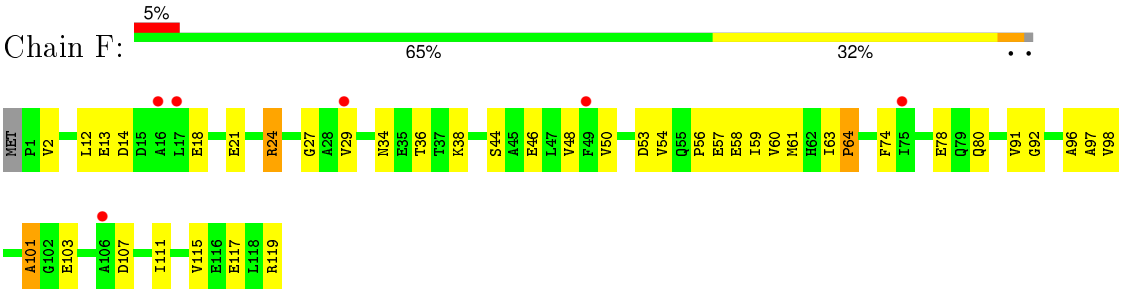
• Molecule 7: 50S ribosomal protein L6P

Chain E:



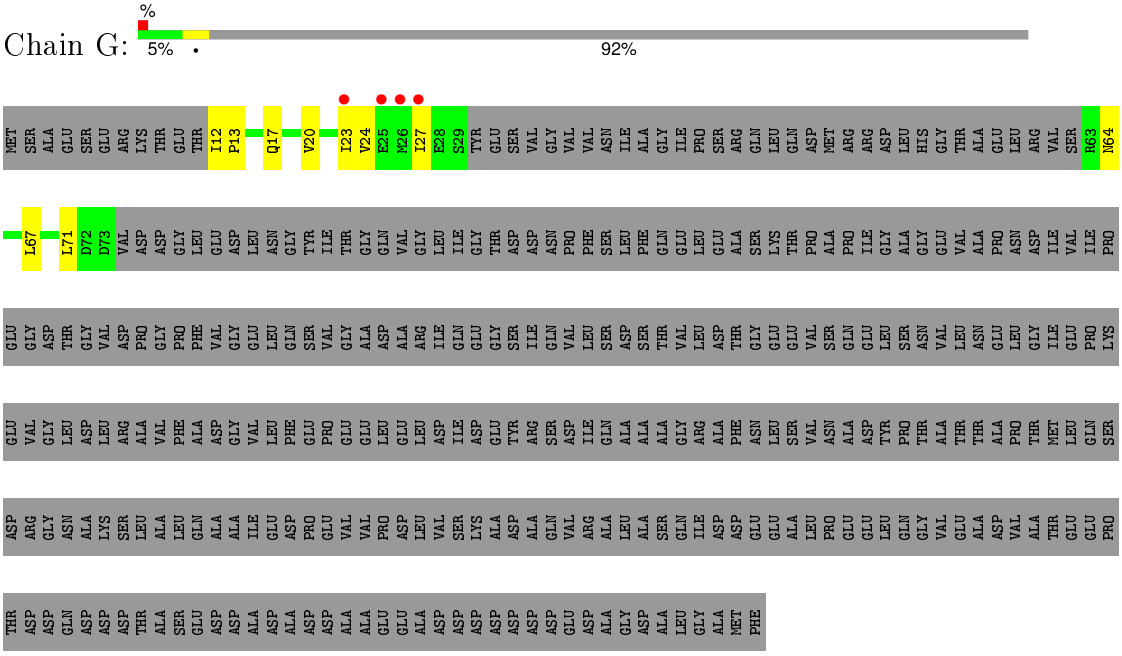
• Molecule 8: 50S ribosomal protein L7Ae

Chain F:



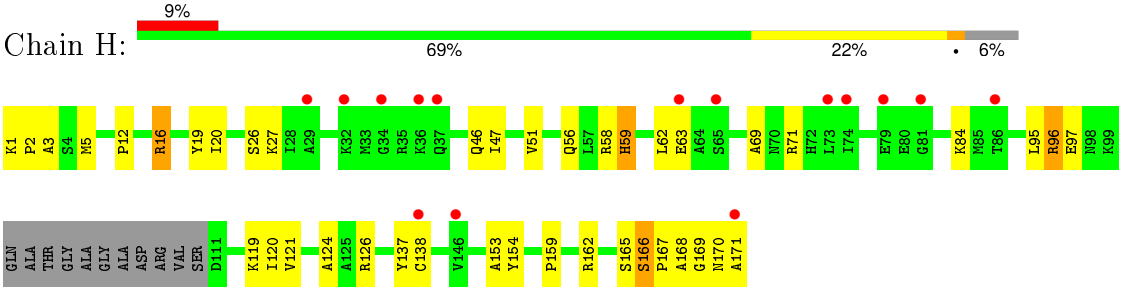
- Molecule 9: 50S ribosomal protein L10E

Chain G:



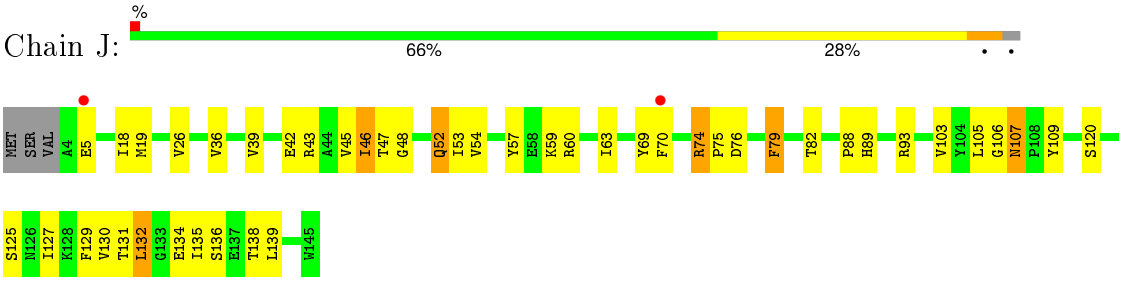
- Molecule 10: 50S ribosomal protein L10e

Chain H:



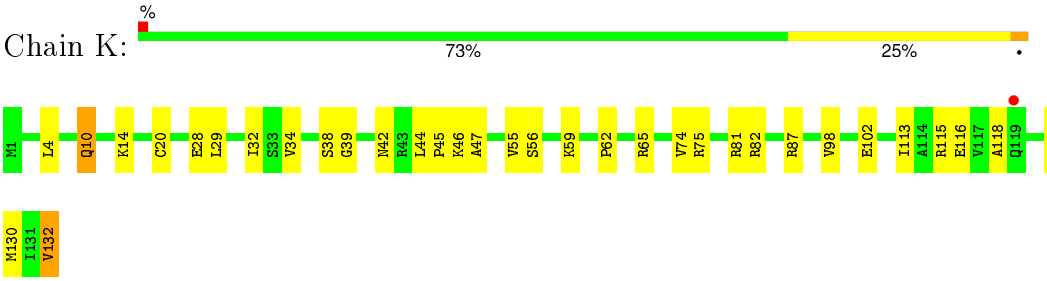
- Molecule 11: 50S ribosomal protein L13P

Chain J:



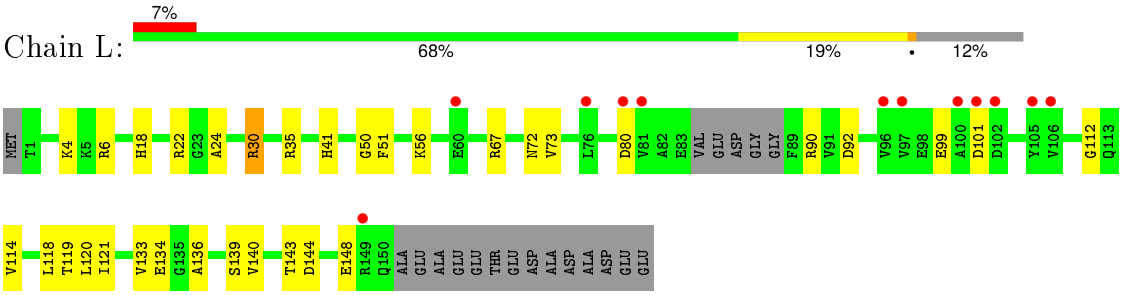
• Molecule 12: 50S ribosomal protein L14P

Chain K:



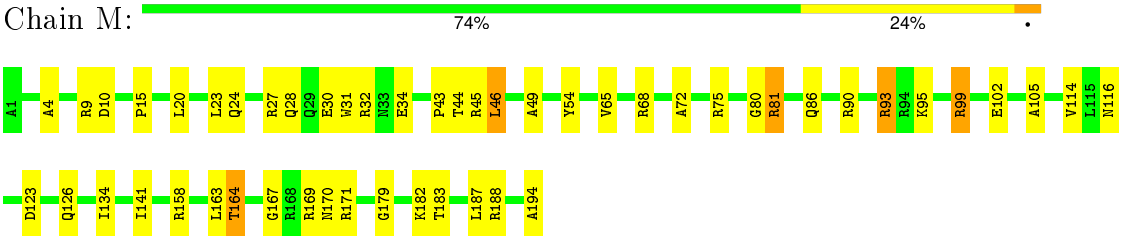
• Molecule 13: 50S ribosomal protein L15P

Chain L:



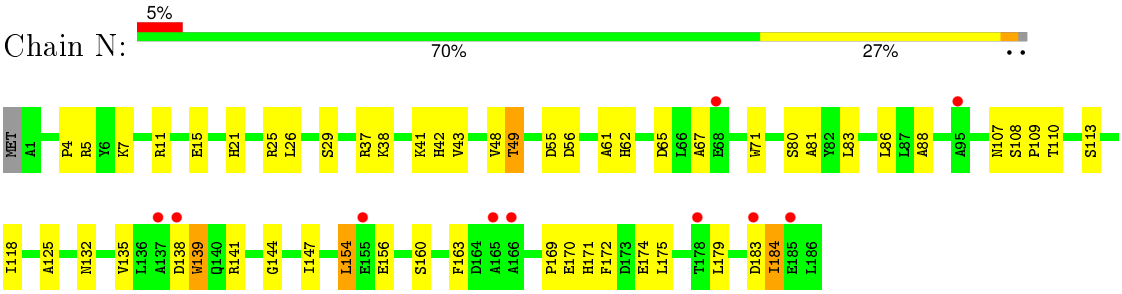
• Molecule 14: 50S ribosomal protein L15e

Chain M:



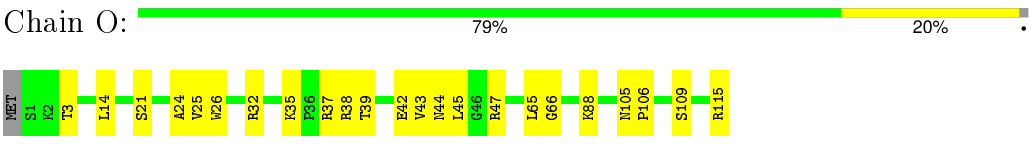
• Molecule 15: 50S ribosomal protein L18P

Chain N:



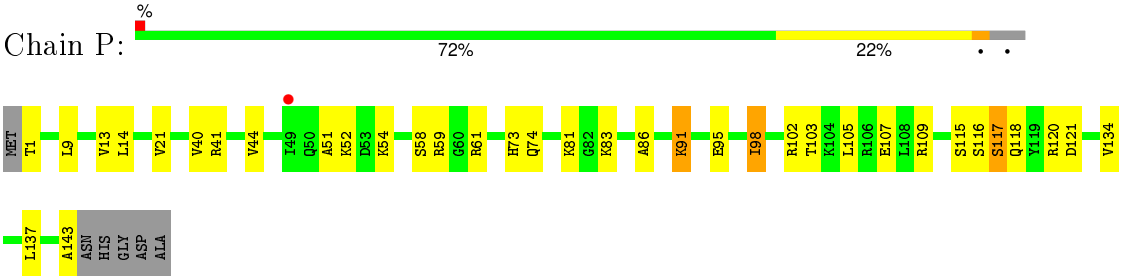
• Molecule 16: 50S ribosomal protein L18e

Chain O:



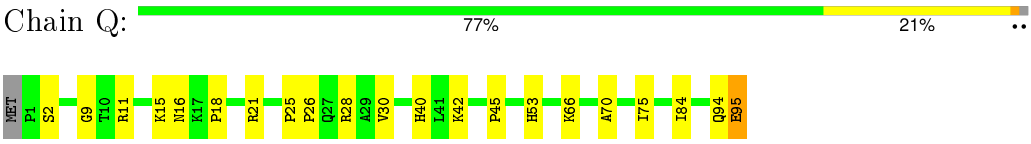
• Molecule 17: 50S ribosomal protein L19e

Chain P:



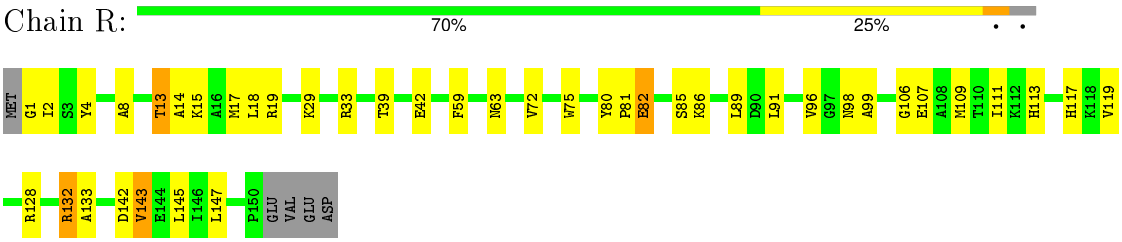
• Molecule 18: 50S ribosomal protein L21e

Chain Q:



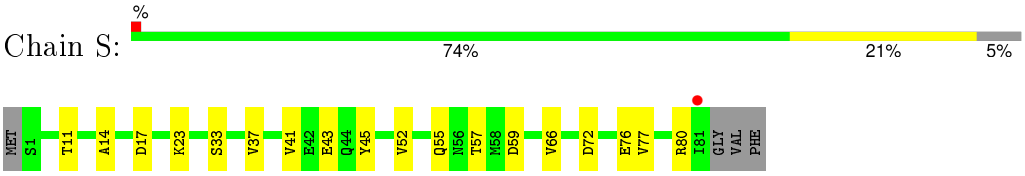
• Molecule 19: 50S ribosomal protein L22P

Chain R:



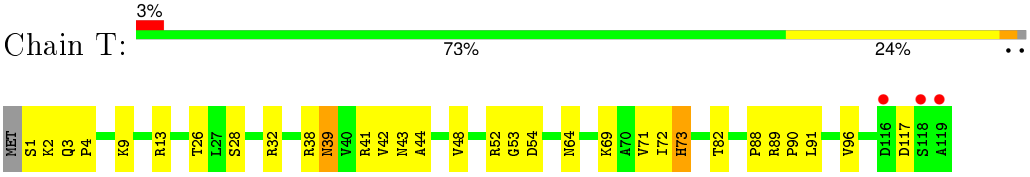
• Molecule 20: 50S ribosomal protein L23P

Chain S:



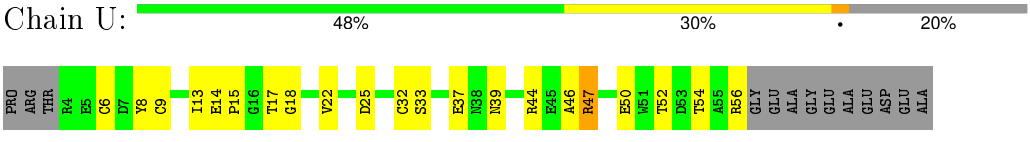
• Molecule 21: 50S ribosomal protein L24P

Chain T:



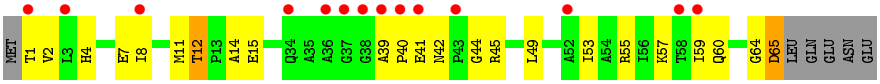
• Molecule 22: 50S ribosomal protein L24e

Chain U:



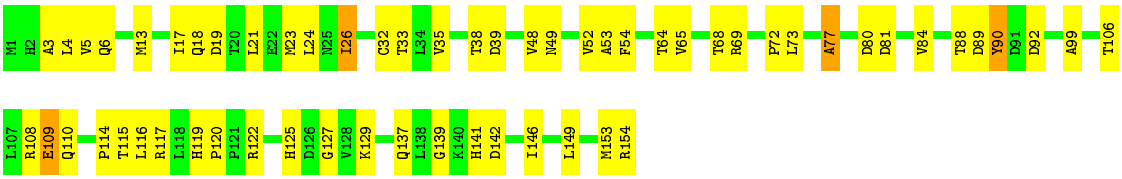
• Molecule 23: 50S ribosomal protein L29P

Chain V:



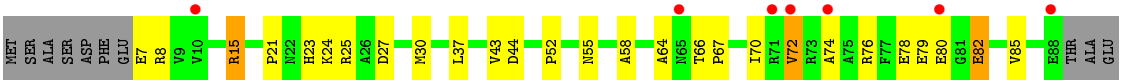
- Molecule 24: 50S ribosomal protein L30P

Chain W:



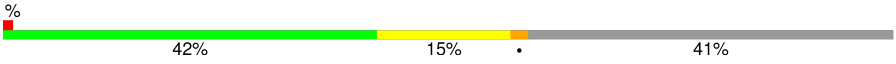
- Molecule 25: 50S ribosomal protein L31e

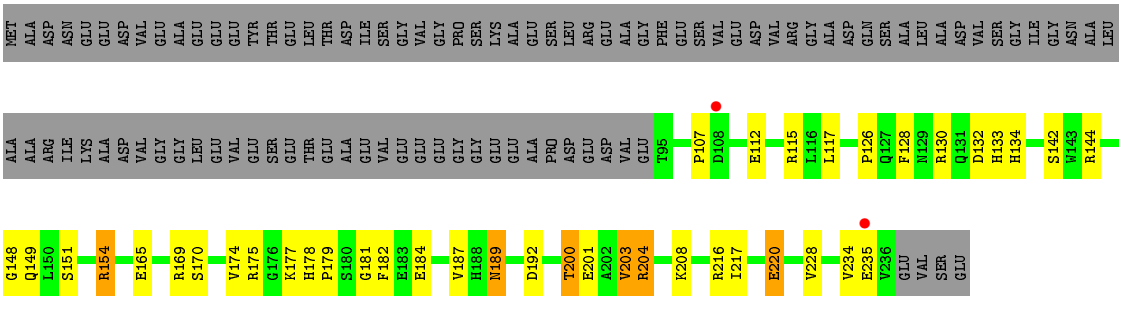
Chain X:



- Molecule 26: 50S ribosomal protein L32e

Chain Y:



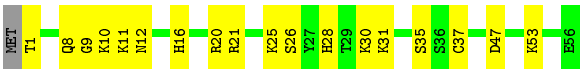


- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:

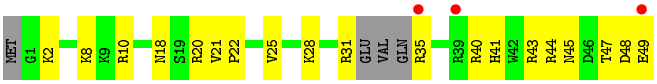
- Molecule 28: 50S ribosomal protein L37e

Chain 1:



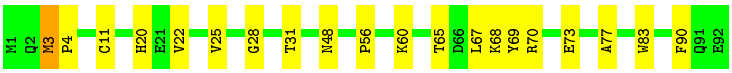
- Molecule 29: 50S ribosomal protein L39e

Chain 2:



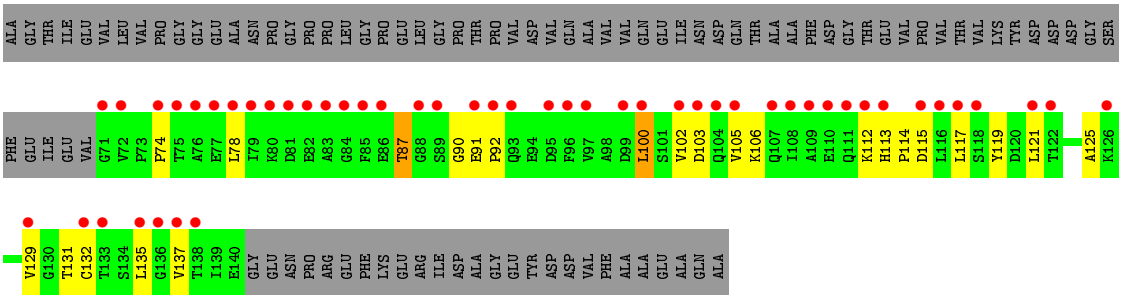
• Molecule 30: 50S ribosomal protein L44E

Chain 3:



• Molecule 31: 50S ribosomal protein L11P

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 91.7 (85.48-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.238 0.209 , 0.238	Depositor DCC
R_{free} test set	3898 reflections (1.06%)	DCC
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 422682 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	99043	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, OMG, CL, NA, K, UR3, CD, OMU, 13T, 1MA, 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	0.39	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.69	1/4528 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.34	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.58	0/1498
7	E	0.34	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.33	0/241	0.49	0/324
10	H	0.38	0/1287	0.65	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.35	0/1130	0.64	0/1509
14	M	0.37	0/1584	0.63	0/2119
15	N	0.31	0/1474	0.65	1/1999 (0.1%)
16	O	0.36	0/874	0.61	1/1181 (0.1%)
17	P	0.35	0/1147	0.55	0/1528
18	Q	0.37	0/749	0.68	0/1005
19	R	0.36	0/1172	0.64	0/1578
20	S	0.35	0/648	0.59	0/875
21	T	0.34	0/958	0.63	0/1289
22	U	0.36	0/417	0.56	0/562
23	V	0.35	0/502	0.56	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.59	0/895
26	Y	0.36	0/1146	0.63	0/1536
27	Z	0.39	0/590	0.64	0/787
28	1	0.40	0/438	0.63	0/578
29	2	0.37	0/401	0.56	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.35	0/526	0.57	0/716
All	All	0.38	0/98693	0.67	17/147577 (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	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.37	130.11	109.50
2	9	3039	U	N1-C1'-C2'	6.50	122.45	114.00
1	0	2316	G	C5'-C4'-C3'	-6.49	105.61	116.00
1	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
1	0	1942	A	C5'-C4'-C3'	6.20	125.92	116.00
15	N	163	PHE	N-CA-C	-5.68	95.66	111.00
16	O	66	GLY	N-CA-C	5.59	127.06	113.10
1	0	871	G	C5'-C4'-O4'	-5.54	102.45	109.10
1	0	1504	A	N9-C1'-C2'	5.52	121.17	114.00
1	0	1819	G	C5'-C4'-C3'	5.40	124.64	116.00
1	0	1829	A	N9-C1'-C2'	-5.39	106.07	112.00
1	0	2313	C	C5'-C4'-O4'	5.31	115.47	109.10
1	0	2291	A	N9-C1'-C2'	5.15	120.70	114.00
1	0	1559	A	C2'-C3'-O3'	5.15	121.94	113.70
1	0	2313	C	O4'-C4'-C3'	-5.07	98.93	104.00
1	0	1878	G	N9-C1'-C2'	-5.04	106.46	112.00
1	0	777	U	O4'-C1'-N1	5.03	112.23	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1131	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	1309	U	Sidechain
1	0	131	A	Sidechain
1	0	1376	G	Sidechain
1	0	1445	G	Sidechain
1	0	1458	A	Sidechain
1	0	1635	U	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	1993	C	Sidechain
1	0	220	C	Sidechain
1	0	2308	U	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	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	391	U	Sidechain
1	0	396	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
2	9	3039	U	Sidechain
2	9	3090	G	Sidechain
24	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1337	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	78	0
4	B	2625	0	2533	112	0
5	C	1859	0	1816	74	0
6	D	1094	0	1085	56	0
7	E	1357	0	1266	38	0
8	F	890	0	843	32	0
9	G	240	0	231	9	0
10	H	1266	0	1268	39	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	40	0
13	L	1118	0	1076	28	0
14	M	1560	0	1568	45	0
15	N	1445	0	1401	45	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	41	0
20	S	641	0	605	14	0
21	T	950	0	923	25	0
22	U	410	0	364	21	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	25	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	21	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	74	0	0	2	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	2	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	2	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0
38	A	112	0	0	8	0
38	B	142	0	0	21	0
38	C	170	0	0	16	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H8	1:0:871:G:H5'	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5"	1.37	1.07
1:0:1474:C:H6	1:0:1474:C:H5'	1.16	1.06
2:9:3006:C:H5"	15:N:37:ARG:NH1	1.70	1.06
2:9:3056:A:H2'	2:9:3057:A:H5"	1.34	1.05
1:0:1242:A:H5'	11:J:82:THR:HG23	1.34	1.04
1:0:541:C:H2'	1:0:542:A:H5"	1.41	1.03
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.41	1.02
1:0:542:A:H5'	1:0:542:A:H8	1.25	1.01
1:0:1559:A:H1'	38:0:5876:HOH:O	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:C2'	1:0:2718:C:H5"	1.91	1.01
1:0:381:G:H5"	38:0:4329:HOH:O	1.61	1.00
1:0:1474:C:C6	1:0:1474:C:H5'	1.99	0.98
1:0:1701:A:H4'	1:0:1702:U:H5"	1.44	0.98
1:0:1666:C:O2'	1:0:1667:A:H5"	1.64	0.98
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.45	0.98
1:0:156:C:H5"	14:M:171:ARG:HD3	1.41	0.97
1:0:1118:A:H62	1:0:1244:U:H3	1.09	0.97
1:0:2717:C:H2'	1:0:2718:C:H5"	1.46	0.96
1:0:2460:A:H5'	32:0:9000:13T:C23	1.96	0.96
2:9:3092:G:H2'	2:9:3093:A:C8	2.01	0.96
2:9:3076:G:H3'	2:9:3077:A:H5"	1.43	0.95
5:C:236:THR:HG22	5:C:239:ALA:H	1.28	0.95
1:0:871:G:H8	1:0:871:G:C5'	1.80	0.95
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.49	0.94
1:0:1205:U:H2'	1:0:1206:U:H5"	1.50	0.94
1:0:2460:A:H5'	32:0:9000:13T:H233	1.46	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.34	0.93
29:2:41:HIS:H	29:2:45:ASN:HD22	1.16	0.93
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.49	0.93
1:0:289:G:H22	1:0:363:A:H2	0.97	0.93
1:0:1172:G:H5"	38:0:7252:HOH:O	1.69	0.93
1:0:877:G:H5'	1:0:878:G:OP1	1.69	0.93
1:0:282:C:H1'	1:0:368:C:N4	1.84	0.93
1:0:2710:U:H1'	38:0:7605:HOH:O	1.68	0.92
1:0:545:G:H8	1:0:545:G:H5'	1.34	0.92
1:0:1372:A:H3'	38:0:7182:HOH:O	1.69	0.92
12:K:10:GLN:H	12:K:10:GLN:HE21	0.93	0.92
1:0:2506:A:HO2'	1:0:2507:G:H8	0.93	0.92
1:0:506:G:H22	1:0:509:A:C5'	1.82	0.91
1:0:1118:A:H3'	1:0:1118:A:C8	2.05	0.91
1:0:1118:A:H3'	1:0:1118:A:H8	1.33	0.91
1:0:2812:A:H2	1:0:2814:A:H62	1.06	0.91
1:0:541:C:C2'	1:0:542:A:H5"	1.99	0.91
1:0:870:G:H2'	1:0:871:G:H5"	1.50	0.90
1:0:1184:C:H1'	38:0:7452:HOH:O	1.70	0.90
1:0:1603:A:H5'	1:0:1605:G:O4'	1.72	0.90
1:0:93:C:H5"	23:V:1:THR:HB	1.51	0.90
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.54	0.89
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.53	0.89
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2529:G:H3'	38:0:7177:HOH:O	1.70	0.89
1:0:289:G:N2	1:0:363:A:H2	1.70	0.89
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.55	0.88
1:0:317:A:H4'	38:0:3775:HOH:O	1.73	0.88
17:P:115:SER:H	17:P:118:GLN:HE21	1.20	0.88
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.56	0.88
1:0:1209:C:H2'	1:0:1210:G:H8	1.39	0.87
1:0:2508:C:H2'	38:0:6748:HOH:O	1.72	0.87
1:0:1165:G:H4'	1:0:1174:A:O2'	1.74	0.87
1:0:506:G:H22	1:0:509:A:H5"	1.37	0.87
2:9:3049:G:H5"	38:N:8842:HOH:O	1.73	0.87
1:0:1641:A:H2'	1:0:1642:A:H5'	1.55	0.86
1:0:1116:U:H3	1:0:1246:A:H62	1.21	0.86
1:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
1:0:1701:A:H5'	38:0:6285:HOH:O	1.77	0.84
12:K:10:GLN:N	12:K:10:GLN:HE21	1.76	0.84
1:0:2769:C:C2'	1:0:2770:G:H5'	2.08	0.84
12:K:10:GLN:H	12:K:10:GLN:NE2	1.76	0.84
1:0:182:G:H5'	38:0:5159:HOH:O	1.78	0.83
1:0:2291:A:C8	1:0:2309:C:H5'	2.13	0.83
1:0:21:G:H5'	19:R:2:ILE:HA	1.61	0.83
15:N:113:SER:HB2	38:N:8855:HOH:O	1.78	0.83
1:0:272:A:H3'	38:0:7515:HOH:O	1.79	0.83
1:0:272:A:H5'	1:0:273:G:OP2	1.79	0.83
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.61	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.76	0.83
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.25	0.83
1:0:282:C:O2'	1:0:283:U:H5'	1.79	0.83
2:9:3056:A:C2'	2:9:3057:A:H5"	2.09	0.83
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.59	0.82
4:B:307:ARG:HG3	4:B:307:ARG:HH11	1.42	0.82
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.61	0.82
1:0:559:U:H5'	1:0:559:U:H6	1.44	0.82
1:0:69:A:H5'	1:0:69:A:C8	2.14	0.82
24:W:88:THR:HB	38:W:6679:HOH:O	1.79	0.82
1:0:797:A:H4'	27:Z:10:ARG:N	1.94	0.82
1:0:1183:C:H2'	38:0:6249:HOH:O	1.79	0.81
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.62	0.81
1:0:1187:U:HO2'	1:0:1189:A:H2	1.26	0.81
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.23	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:5223:HOH:O	12:K:39:GLY:HA2	1.81	0.81
1:0:236:A:H4'	1:0:237:G:H5'	1.63	0.81
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.62	0.81
1:0:2717:C:O2'	1:0:2718:C:H5"	1.80	0.81
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.62	0.80
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.29	0.80
1:0:515:C:H5"	38:0:5657:HOH:O	1.81	0.80
3:A:199:HIS:HD2	3:A:201:PHE:H	1.27	0.80
1:0:558:C:O2'	1:0:559:U:H5"	1.81	0.80
1:0:1160:G:H5'	1:0:1161:A:H5'	0.88	0.80
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.64	0.80
1:0:541:C:H2'	1:0:542:A:C5'	2.12	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.79
1:0:1835:U:H5	1:0:1840:A:N7	1.79	0.79
1:0:1206:U:H5'	1:0:1206:U:H6	1.47	0.79
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.63	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.61	0.79
1:0:292:G:H2'	1:0:358:G:N2	1.97	0.79
1:0:2716:G:H5"	4:B:206:THR:HG21	1.63	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.63	0.79
12:K:98:VAL:HG13	12:K:102:GLU:HA	1.64	0.79
1:0:2054:A:N3	19:R:128:ARG:NH2	2.30	0.79
1:0:1615:A:H5'	38:0:4195:HOH:O	1.83	0.79
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.18	0.79
1:0:1667:A:C8	1:0:1667:A:H5'	2.18	0.79
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.79
1:0:1119:G:N2	1:0:1246:A:C2	2.51	0.79
20:S:57:THR:HG22	20:S:59:ASP:H	1.48	0.79
27:Z:46:ARG:HD3	27:Z:59:TYR:HB2	1.64	0.79
1:0:1002:G:C2'	1:0:1003:U:H5"	2.13	0.78
1:0:1741:U:H5'	1:0:1742:A:OP1	1.83	0.78
1:0:1441:G:H1'	38:0:7748:HOH:O	1.82	0.78
32:0:9000:13T:H2	32:0:9000:13T:H262	1.65	0.78
1:0:514:G:H4'	38:0:5657:HOH:O	1.83	0.78
1:0:1919:A:H4'	38:0:4858:HOH:O	1.83	0.78
1:0:1878:G:H1'	38:0:6128:HOH:O	1.83	0.78
1:0:1666:C:C2'	1:0:1667:A:H5"	2.14	0.78
1:0:2908:A:H2'	1:0:2909:G:O4'	1.83	0.78
1:0:871:G:C8	1:0:871:G:C5'	2.59	0.77
1:0:681:G:N3	1:0:681:G:H5'	1.99	0.77
1:0:1474:C:C5'	1:0:1474:C:H6	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:G:C5'	19:R:2:ILE:HA	2.13	0.77
1:0:130:C:H2'	38:0:3162:HOH:O	1.84	0.77
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.66	0.77
1:0:2426:G:H1'	38:0:6098:HOH:O	1.85	0.77
1:0:1679:C:H5'	38:0:9320:HOH:O	1.85	0.77
1:0:542:A:H5'	1:0:542:A:C8	2.15	0.77
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.66	0.77
5:C:127:ARG:NH2	5:C:225:PRO:HG2	2.00	0.77
32:0:9000:13T:H21	32:0:9000:13T:C30	2.14	0.76
32:0:9000:13T:C2	32:0:9000:13T:H262	2.14	0.76
1:0:1205:U:H2'	1:0:1206:U:C5'	2.15	0.76
1:0:2769:C:H2'	1:0:2770:G:H5'	1.68	0.76
6:D:154:LYS:HD2	6:D:154:LYS:H	1.50	0.76
1:0:12:U:H2'	1:0:13:G:H5'	1.67	0.76
1:0:1603:A:H5"	1:0:1605:G:H5'	1.67	0.75
1:0:1701:A:H4'	1:0:1702:U:C5'	2.15	0.75
1:0:1058:A:H2'	1:0:1060:C:H5"	1.67	0.75
1:0:2851:G:O2'	1:0:2852:A:H5'	1.87	0.75
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.66	0.75
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.68	0.74
1:0:2502:C:C2'	1:0:2503:A:H5'	2.16	0.74
1:0:558:C:C2'	1:0:559:U:H5"	2.17	0.74
1:0:2010:A:H2'	38:0:5968:HOH:O	1.86	0.74
1:0:2570:G:H5"	38:0:4917:HOH:O	1.86	0.74
1:0:2766:A:H5'	38:B:8824:HOH:O	1.87	0.74
1:0:1205:U:C2'	1:0:1206:U:H5"	2.18	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.31	0.74
1:0:2768:A:O2'	1:0:2769:C:H5'	1.86	0.74
1:0:2005:G:H3'	1:0:2005:G:OP2	1.87	0.74
24:W:84:VAL:HG12	38:W:6679:HOH:O	1.88	0.74
1:0:396:U:H1'	38:0:7612:HOH:O	1.88	0.74
1:0:899:C:H5'	38:0:3205:HOH:O	1.86	0.74
1:0:949:U:H4'	18:Q:95:GLU:HA	1.68	0.74
1:0:69:A:H5'	1:0:69:A:H8	1.52	0.74
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.70	0.74
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.86	0.73
1:0:797:A:C4'	27:Z:10:ARG:N	2.51	0.73
1:0:711:G:H1'	38:0:7092:HOH:O	1.87	0.73
1:0:1926:G:H2'	1:0:1927:A:H8	1.53	0.73
2:9:3014:G:H8	2:9:3014:G:H5'	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2578:G:H5'	1:0:2578:G:H8	1.53	0.73
1:0:961:A:H4'	38:0:6766:HOH:O	1.89	0.73
1:0:2468:A:H61	30:3:48:ASN:HD21	1.35	0.73
3:A:35:GLY:O	3:A:36:ASP:HB3	1.87	0.73
1:0:2748:G:H1'	38:0:7883:HOH:O	1.87	0.73
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.71	0.73
3:A:51:ARG:HB2	38:A:8897:HOH:O	1.89	0.73
22:U:14:GLU:O	22:U:17:THR:HB	1.88	0.73
11:J:127:ILE:HG22	36:J:8801:CL:CL	2.25	0.73
1:0:288:A:H61	1:0:364:C:H42	1.36	0.73
1:0:544:G:H2'	1:0:545:G:H5"	1.70	0.72
5:C:233:THR:HG22	5:C:234:VAL:H	1.54	0.72
1:0:545:G:C8	1:0:545:G:H5'	2.22	0.72
1:0:587:A:H5"	38:0:7279:HOH:O	1.89	0.72
1:0:2781:U:C2'	1:0:2782:G:H5'	2.19	0.72
1:0:1926:G:H2'	1:0:1927:A:C8	2.24	0.72
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.07	0.72
1:0:2781:U:H2'	1:0:2782:G:H5'	1.70	0.72
1:0:1634:G:H3'	38:0:3901:HOH:O	1.89	0.72
1:0:870:G:C2'	1:0:871:G:H5"	2.17	0.72
1:0:1350:U:H4'	38:0:5124:HOH:O	1.88	0.72
1:0:1080:C:H4'	1:0:1081:A:OP1	1.89	0.72
1:0:2505:G:O2'	1:0:2506:A:H5'	1.89	0.71
1:0:2507:G:H2'	1:0:2510:C:H42	1.55	0.71
1:0:1593:C:H5'	17:P:116:SER:O	1.89	0.71
1:0:2243:C:H5"	38:0:3753:HOH:O	1.88	0.71
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.71	0.71
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.55	0.71
38:0:3759:HOH:O	21:T:9:LYS:HD3	1.88	0.71
1:0:1189:A:H1'	1:0:1209:C:O4'	1.91	0.71
1:0:1189:A:H1'	1:0:1209:C:C1'	2.19	0.71
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.73	0.71
1:0:2878:U:H2'	1:0:2879:A:O4'	1.90	0.71
1:0:2420:G:O2'	1:0:2421:G:H5'	1.90	0.71
1:0:2862:G:H4'	4:B:336:GLN:O	1.91	0.71
1:0:2827:A:H2'	1:0:2828:G:O4'	1.90	0.71
16:O:32:ARG:HE	16:O:35:LYS:HD2	1.56	0.71
2:9:3039:U:H3'	2:9:3040:C:H5"	1.73	0.71
1:0:156:C:H5"	14:M:171:ARG:CD	2.19	0.71
1:0:308:U:H5'	1:0:309:C:OP1	1.90	0.71
1:0:271:C:H41	1:0:378:A:H2	1.36	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:C5'	2.21	0.70
5:C:236:THR:HG22	5:C:239:ALA:N	2.04	0.70
13:L:133:VAL:HA	38:L:8872:HOH:O	1.90	0.70
1:0:2364:A:H5"	18:Q:15:LYS:HD3	1.73	0.70
1:0:1342:C:C2'	1:0:1343:C:H5'	2.20	0.70
19:R:81:PRO:O	19:R:85:SER:HB2	1.91	0.70
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.72	0.70
1:0:214:U:H5'	38:0:6147:HOH:O	1.91	0.70
1:0:2526:C:O2'	1:0:2527:U:H5'	1.91	0.70
1:0:544:G:C2'	1:0:545:G:H5"	2.22	0.70
8:F:58:GLU:HA	8:F:61:MET:HE2	1.74	0.70
3:A:191:GLY:HA2	3:A:194:MET:CE	2.22	0.69
17:P:115:SER:H	17:P:118:GLN:NE2	1.90	0.69
1:0:962:C:H1'	15:N:5:ARG:NH1	2.07	0.69
1:0:2748:G:H2'	38:0:7526:HOH:O	1.91	0.69
24:W:72:PRO:HG2	24:W:77:ALA:HB3	1.74	0.69
17:P:143:ALA:HA	38:P:5521:HOH:O	1.93	0.69
1:0:2748:G:H5'	38:0:7526:HOH:O	1.92	0.69
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.74	0.69
1:0:338:C:H4'	5:C:174:ILE:CD1	2.21	0.69
1:0:960:G:H4'	38:0:7420:HOH:O	1.92	0.69
1:0:1299:G:O6	13:L:6:ARG:HD3	1.92	0.69
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.74	0.69
24:W:80:ASP:O	24:W:84:VAL:HG23	1.92	0.69
6:D:103:ASN:ND2	6:D:134:LEU:H	1.90	0.69
1:0:559:U:H5'	1:0:559:U:C6	2.27	0.69
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.75	0.69
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.73	0.69
24:W:88:THR:HG22	24:W:89:ASP:H	1.58	0.69
1:0:2004:U:H4'	38:0:5313:HOH:O	1.93	0.69
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.08	0.69
1:0:558:C:H2'	1:0:559:U:C5'	2.23	0.69
4:B:238:ASN:HD22	4:B:240:GLY:H	1.41	0.69
1:0:1189:A:H3'	38:0:7666:HOH:O	1.93	0.68
1:0:560:C:H42	1:0:597:A:H61	1.39	0.68
1:0:1242:A:H5'	11:J:82:THR:CG2	2.18	0.68
32:0:9000:13T:H301	32:0:9000:13T:H21	1.74	0.68
1:0:657:G:OP1	5:C:27:ARG:NH2	2.26	0.68
2:9:3054:A:O2'	2:9:3055:U:H5'	1.94	0.68
10:H:166:SER:HB2	10:H:167:PRO:CD	2.21	0.68
1:0:1641:A:C2'	1:0:1642:A:H5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:8813:CL:CL	38:0:4691:HOH:O	2.48	0.68
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.94	0.68
1:0:821:U:H2'	1:0:822:C:H6	1.57	0.68
1:0:1183:C:H42	1:0:1184:C:H41	1.42	0.68
3:A:199:HIS:CD2	3:A:201:PHE:H	2.10	0.68
1:0:2635:A:O2'	1:0:2636:C:H5'	1.94	0.68
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.75	0.68
1:0:1244:U:OP1	11:J:18:ILE:HD13	1.93	0.68
1:0:2459:G:H2'	32:0:9000:13T:C23	2.24	0.68
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.76	0.68
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.22	0.68
1:0:2812:A:C2	1:0:2814:A:N6	2.55	0.68
1:0:603:A:H5"	1:0:604:G:OP1	1.93	0.68
24:W:125:HIS:HD2	24:W:127:GLY:H	1.40	0.68
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.68
14:M:134:ILE:HG23	14:M:141:ILE:HD13	1.76	0.68
1:0:138:U:H5"	1:0:139:C:OP2	1.95	0.67
1:0:500:G:H21	19:R:98:ASN:HD21	1.41	0.67
1:0:2374:A:H2'	1:0:2375:G:C8	2.29	0.67
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.67
29:2:35:ARG:HB2	38:2:2691:HOH:O	1.95	0.67
1:0:1189:A:O2'	1:0:1208:C:H2'	1.95	0.67
1:0:1213:C:O2'	1:0:1214:G:H5'	1.94	0.67
1:0:1118:A:N6	1:0:1244:U:H3	1.87	0.67
1:0:506:G:H22	1:0:509:A:H5'	1.57	0.67
23:V:57:LYS:HA	23:V:60:GLN:HE21	1.60	0.67
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.29	0.67
1:0:2533:C:C6	1:0:2533:C:H5'	2.28	0.67
11:J:107:ASN:HD22	11:J:109:TYR:H	1.42	0.67
1:0:706:G:HO2'	1:0:707:C:H6	1.43	0.67
1:0:2717:C:OP1	4:B:207:LYS:HG3	1.95	0.67
11:J:76:ASP:HA	38:J:8868:HOH:O	1.94	0.67
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.77	0.67
1:0:1973:A:H5'	1:0:1973:A:H8	1.59	0.67
1:0:280:C:H2'	1:0:281:U:O4'	1.95	0.66
4:B:267:LYS:HD3	38:B:8824:HOH:O	1.95	0.66
1:0:2563:U:H2'	1:0:2565:C:O5'	1.96	0.66
1:0:2100:A:H5'	38:C:8662:HOH:O	1.93	0.66
1:0:2256:G:H2'	1:0:2257:G:C5'	2.25	0.66
27:Z:10:ARG:HA	38:Z:8715:HOH:O	1.96	0.66
11:J:74:ARG:HB3	11:J:74:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:485:A:N3	1:0:487:G:H5"	2.10	0.66
1:0:2256:G:H2'	1:0:2257:G:H5'	1.78	0.66
5:C:1:MET:HG2	5:C:2:GLN:H	1.61	0.66
1:0:2489:G:H1'	38:0:7268:HOH:O	1.95	0.66
1:0:284:C:H4'	1:0:285:A:O5'	1.96	0.66
30:3:73:GLU:HB3	38:3:8854:HOH:O	1.94	0.66
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.24	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.72	0.66
1:0:1209:C:H2'	1:0:1210:G:C8	2.26	0.66
1:0:2521:A:OP2	10:H:3:ALA:HB3	1.96	0.66
1:0:1524:U:OP1	1:0:1524:U:H4'	1.94	0.66
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.96	0.66
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.78	0.66
1:0:694:A:H2'	1:0:695:C:H5'	1.77	0.66
19:R:99:ALA:HB1	19:R:109:MET:CE	2.26	0.66
1:0:21:G:H5"	19:R:1:GLY:O	1.97	0.65
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.61	0.65
1:0:2638:G:H1'	38:0:7742:HOH:O	1.96	0.65
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.25	0.65
2:9:3029:C:C2'	2:9:3030:C:H5'	2.26	0.65
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.79	0.65
1:0:2460:A:C5'	32:0:9000:13T:H233	2.23	0.65
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.26	0.65
5:C:140:VAL:HB	38:C:8651:HOH:O	1.94	0.65
1:0:136:C:H2'	1:0:137:U:O4'	1.97	0.65
1:0:2890:A:H1'	22:U:56:ARG:NH2	2.11	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.95	0.65
1:0:1666:C:H2'	1:0:1667:A:C5'	2.26	0.65
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.65
1:0:2414:A:H2'	1:0:2415:A:C8	2.31	0.65
1:0:447:A:O2'	1:0:448:G:H5'	1.97	0.65
1:0:1187:U:O2'	1:0:1189:A:H2	1.78	0.65
1:0:2795:C:O2'	1:0:2796:U:H5'	1.96	0.65
1:0:584:U:H3'	38:0:6101:HOH:O	1.96	0.65
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.79	0.65
1:0:407:A:H8	38:0:4466:HOH:O	1.79	0.65
2:9:3003:A:N6	2:9:3022:G:H1'	2.12	0.65
1:0:1701:A:H5"	1:0:1702:U:H3'	1.77	0.65
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.62	0.64
1:0:2320:U:H4'	1:0:2321:A:O4'	1.97	0.64
10:H:169:GLY:HA3	38:H:8591:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.62	0.64
1:0:1342:C:H2'	1:0:1343:C:H5'	1.79	0.64
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.28	0.64
1:0:2787:C:H5	38:0:4641:HOH:O	1.80	0.64
1:0:403:C:H3'	38:0:6307:HOH:O	1.97	0.64
1:0:2241:C:O2'	1:0:2242:U:H5'	1.96	0.64
1:0:281:U:O2'	1:0:282:C:H5'	1.96	0.64
6:D:99:ASP:HB3	6:D:103:ASN:H	1.62	0.64
1:0:2896:A:H5"	38:0:6105:HOH:O	1.97	0.64
1:0:441:A:H1'	1:0:442:A:N7	2.13	0.64
38:0:4678:HOH:O	4:B:300:SER:HB3	1.97	0.64
1:0:958:G:H2'	1:0:959:C:C6	2.32	0.64
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.32	0.64
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.79	0.64
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.79	0.64
2:9:3091:C:H2'	2:9:3092:G:O4'	1.97	0.64
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.27	0.64
3:A:121:ALA:O	3:A:124:VAL:HG22	1.97	0.64
1:0:2459:G:H2'	32:0:9000:13T:H233	1.80	0.64
1:0:1185:U:H2'	1:0:1186:C:C6	2.33	0.64
1:0:2769:C:O2'	1:0:2770:G:H5'	1.96	0.64
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.63	0.64
1:0:1044:C:H5	38:0:6599:HOH:O	1.81	0.64
2:9:3039:U:H1'	2:9:3044:A:H61	1.63	0.64
23:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.64
14:M:23:LEU:HD13	14:M:27:ARG:NH2	2.12	0.63
1:0:1200:A:H3'	38:0:5765:HOH:O	1.98	0.63
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.45	0.63
1:0:2769:C:H2'	1:0:2770:G:C5'	2.27	0.63
1:0:1790:C:H2'	1:0:1791:U:H6	1.63	0.63
2:9:3007:G:H5'	38:9:5071:HOH:O	1.98	0.63
5:C:236:THR:HG21	38:C:8571:HOH:O	1.98	0.63
13:L:114:VAL:HG11	38:L:8872:HOH:O	1.99	0.63
10:H:166:SER:CB	10:H:167:PRO:HD3	2.27	0.63
1:0:1165:G:H1'	1:0:1174:A:H1'	1.79	0.63
1:0:1189:A:H1'	1:0:1209:C:H1'	1.79	0.63
4:B:36:PRO:HG3	4:B:169:GLY:H	1.62	0.63
18:Q:26:PRO:O	18:Q:30:VAL:HG23	1.98	0.63
1:0:157:G:H4'	14:M:95:LYS:HE2	1.79	0.63
16:O:47:ARG:HG3	16:O:47:ARG:HH11	1.63	0.63
1:0:1185:U:H5'	38:0:7452:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1211:G:H2'	1:0:1212:C:H6	1.63	0.63
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.81	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.99	0.63
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.38	0.63
1:0:447:A:P	21:T:1:SER:HB2	2.39	0.63
13:L:148:GLU:HB2	38:L:8889:HOH:O	1.99	0.63
1:0:20:G:H21	19:R:117:HIS:HD2	1.47	0.63
4:B:71:VAL:HG21	4:B:296:LEU:HB3	1.81	0.63
1:0:289:G:O2'	1:0:290:C:H5'	1.99	0.63
1:0:1666:C:C2'	1:0:1667:A:C5'	2.77	0.62
1:0:1164:U:H3	1:0:1192:A:H2	1.46	0.62
1:0:1878:G:O2'	1:0:1879:U:C6	2.49	0.62
1:0:567:U:H5"	38:0:6400:HOH:O	1.98	0.62
2:9:3092:G:H2'	2:9:3093:A:H8	1.58	0.62
1:0:1313:A:H5'	26:Y:208:LYS:O	1.99	0.62
1:0:1666:C:H2'	1:0:1667:A:H5'	1.81	0.62
1:0:1307:A:H2'	1:0:1308:A:C8	2.34	0.62
1:0:951:A:C2'	1:0:952:G:H5'	2.29	0.62
5:C:67:GLN:HG2	38:C:8624:HOH:O	2.00	0.62
18:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
1:0:396:U:O2'	1:0:418:C:H4'	1.99	0.62
2:9:3036:C:C5	2:9:3037:C:C5	2.88	0.62
1:0:1537:C:H1'	38:0:6583:HOH:O	1.98	0.62
1:0:1667:A:H2'	1:0:1668:U:C6	2.34	0.62
1:0:292:G:H2'	1:0:358:G:H22	1.65	0.62
15:N:80:SER:HB2	38:N:8832:HOH:O	1.99	0.62
1:0:1377:C:H6	1:0:1377:C:H5'	1.64	0.62
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.80	0.62
1:0:960:G:H2'	1:0:960:G:N3	2.13	0.62
1:0:1625:U:H4'	38:0:4674:HOH:O	2.00	0.62
25:X:43:VAL:HG12	25:X:44:ASP:N	2.15	0.62
14:M:99:ARG:HH21	14:M:170:ASN:HD22	1.48	0.62
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.29	0.62
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.82	0.62
1:0:1636:G:O2'	1:0:1637:A:H5'	1.99	0.62
1:0:558:C:C2'	1:0:559:U:C5'	2.78	0.61
2:9:3014:G:C8	2:9:3014:G:H5'	2.34	0.61
23:V:39:ALA:N	23:V:40:PRO:HD2	2.14	0.61
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.82	0.61
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	16:O:3:THR:HB	1.80	0.61
35:L:8580:NA:NA	38:L:8826:HOH:O	1.71	0.61
1:0:597:A:H2'	1:0:598:C:H6	1.65	0.61
23:V:55:ARG:O	23:V:59:ILE:HG12	1.99	0.61
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.80	0.61
35:0:8542:NA:NA	38:0:5663:HOH:O	1.71	0.61
1:0:2511:A:H2'	1:0:2512:U:O4'	2.00	0.61
1:0:1603:A:C5'	1:0:1605:G:H5'	2.30	0.61
23:V:1:THR:HG23	23:V:2:VAL:H	1.65	0.61
1:0:308:U:C4	1:0:342:C:H1'	2.35	0.61
1:0:1406:A:H4'	1:0:1407:A:H5"	1.81	0.61
1:0:2445:U:H2'	1:0:2446:G:C8	2.36	0.61
1:0:1528:A:H2'	1:0:1529:G:O4'	2.00	0.61
1:0:470:U:O2'	28:1:16:HIS:HD2	1.82	0.61
38:0:7359:HOH:O	12:K:45:PRO:HB2	2.01	0.61
1:0:2338:G:H1'	6:D:105:SER:OG	1.99	0.61
1:0:1234:U:N3	4:B:244:PRO:HB3	2.15	0.61
1:0:538:C:OP2	26:Y:134:HIS:HE1	1.84	0.61
12:K:81:ARG:HD3	12:K:87:ARG:NH2	2.15	0.61
18:Q:21:ARG:HA	38:Q:6597:HOH:O	2.00	0.61
2:9:3041:C:O4'	6:D:50:VAL:HG22	2.00	0.61
24:W:13:MET:HE1	24:W:18:GLN:HA	1.82	0.61
1:0:128:A:O2'	1:0:129:A:H5'	2.01	0.61
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.82	0.61
1:0:1477:C:H5'	1:0:1868:G:C5'	2.30	0.61
2:9:3064:C:H2'	2:9:3065:A:H5'	1.83	0.61
1:0:281:U:H2'	1:0:282:C:O4'	2.01	0.61
1:0:2507:G:H2'	1:0:2510:C:N4	2.16	0.61
24:W:137:GLN:NE2	24:W:141:HIS:HE1	1.98	0.61
2:9:3064:C:C2'	2:9:3065:A:H5'	2.31	0.61
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.82	0.61
1:0:1762:C:H2'	1:0:1763:C:H6	1.65	0.61
1:0:2433:A:H2'	1:0:2434:A:C8	2.36	0.61
10:H:27:LYS:H	10:H:59:HIS:CD2	2.19	0.61
1:0:2134:G:N2	1:0:2242:U:C2	2.69	0.60
1:0:656:G:OP2	16:O:37:ARG:HD2	2.00	0.60
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.81	0.60
2:9:3006:C:H5"	15:N:37:ARG:HH12	1.62	0.60
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.60
1:0:517:U:H1'	38:0:7561:HOH:O	2.00	0.60
1:0:338:C:H4'	5:C:174:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:11:THR:H	20:S:14:ALA:HB3	1.65	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.01	0.60
32:0:9000:13T:H262	32:0:9000:13T:O3	2.01	0.60
1:0:669:G:O2'	1:0:670:G:H5'	2.01	0.60
30:3:65:THR:HG23	30:3:67:LEU:HG	1.84	0.60
1:0:2659:U:H5"	38:0:4135:HOH:O	2.00	0.60
29:2:20:ARG:HG2	29:2:21:VAL:H	1.66	0.60
1:0:1118:A:C3'	1:0:1118:A:C8	2.70	0.60
27:Z:11:SER:HB3	27:Z:23:ARG:HB2	1.83	0.60
1:0:255:A:H2'	1:0:256:C:C6	2.36	0.60
1:0:602:A:O2'	1:0:605:C:H4'	2.01	0.60
1:0:510:U:H6	38:0:7427:HOH:O	1.85	0.60
1:0:1819:G:H2'	1:0:1820:G:H4'	1.83	0.60
1:0:2359:G:H3'	38:0:5701:HOH:O	2.01	0.60
1:0:512:G:O3'	1:0:513:A:H8	1.85	0.60
14:M:187:LEU:CD2	14:M:194:ALA:HB3	2.32	0.60
3:A:48:ASP:HB3	38:A:8897:HOH:O	2.02	0.60
6:D:103:ASN:ND2	6:D:133:ASN:HA	2.17	0.59
1:0:2301:A:H5"	1:0:2302:A:H5'	1.84	0.59
1:0:255:A:H2'	1:0:256:C:H6	1.66	0.59
4:B:214:PRO:HD2	38:B:8820:HOH:O	2.02	0.59
6:D:65:GLU:HA	38:D:4069:HOH:O	2.02	0.59
27:Z:22:SER:O	27:Z:26:VAL:HG23	2.01	0.59
1:0:1202:A:H2'	1:0:1203:G:H5'	1.85	0.59
6:D:50:VAL:O	6:D:71:ALA:HA	2.02	0.59
1:0:1525:G:H5'	1:0:1526:A:OP2	2.02	0.59
1:0:450:C:OP1	5:C:184:ARG:NH2	2.34	0.59
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.66	0.59
32:0:9000:13T:H3	30:3:56:PRO:HB2	1.83	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.02	0.59
2:9:3039:U:H3'	2:9:3040:C:C5'	2.32	0.59
4:B:86:ALA:HA	38:B:8876:HOH:O	2.01	0.59
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.83	0.59
19:R:111:ILE:HG23	19:R:145:LEU:HD11	1.83	0.59
27:Z:42:CYS:SG	27:Z:43:GLY:N	2.75	0.59
14:M:114:VAL:HG23	36:M:8818:CL:CL	2.39	0.59
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.33	0.59
1:0:1504:A:H5'	38:0:4423:HOH:O	2.02	0.59
1:0:1060:C:H6	1:0:1060:C:H5'	1.65	0.59
11:J:45:VAL:HG21	11:J:129:PHE:CD1	2.38	0.59
1:0:966:U:H5'	38:0:3861:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2807:U:P	4:B:27:ASN:HD21	2.24	0.59
1:0:1163:G:H2'	1:0:1164:U:C5	2.37	0.59
23:V:12:THR:HG23	23:V:14:ALA:H	1.68	0.59
1:0:249:G:O2'	1:0:250:C:H5'	2.03	0.59
1:0:1183:C:N3	1:0:1184:C:C5	2.71	0.59
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.85	0.59
23:V:49:LEU:O	23:V:53:ILE:HG13	2.01	0.59
7:E:100:ASP:HB2	38:E:2789:HOH:O	2.02	0.59
1:0:1167:G:O2'	1:0:1168:C:H5'	2.02	0.59
1:0:1736:A:H1'	38:0:7569:HOH:O	2.03	0.59
1:0:2781:U:H2'	1:0:2782:G:C5'	2.31	0.59
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.67	0.59
38:0:9354:HOH:O	28:1:1:THR:HA	2.03	0.59
1:0:84:G:O2'	1:0:85:C:H5'	2.02	0.59
14:M:30:GLU:O	14:M:34:GLU:HG3	2.02	0.59
1:0:39:G:N2	1:0:444:C:C2	2.71	0.59
27:Z:44:GLU:HG2	27:Z:46:ARG:HD2	1.85	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
1:0:947:U:H2'	1:0:948:G:C8	2.38	0.59
1:0:121:U:OP2	29:2:10:ARG:NH2	2.35	0.59
35:0:8542:NA:NA	38:0:3317:HOH:O	1.75	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.34	0.59
1:0:364:C:H2'	1:0:365:G:O4'	2.03	0.58
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.85	0.58
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.84	0.58
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.66	0.58
11:J:107:ASN:ND2	11:J:109:TYR:H	2.01	0.58
1:0:1014:A:H2'	1:0:1015:C:H5'	1.85	0.58
1:0:1015:C:H2'	1:0:1016:U:H6	1.67	0.58
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.85	0.58
31:I:132:CYS:HB3	31:I:137:VAL:HB	1.83	0.58
1:0:1202:A:C2'	1:0:1203:G:H5'	2.33	0.58
1:0:2252:A:C5	1:0:2253:G:H1'	2.36	0.58
25:X:43:VAL:HG12	25:X:44:ASP:H	1.69	0.58
5:C:139:VAL:HG13	38:C:8648:HOH:O	2.02	0.58
19:R:14:ALA:HB3	19:R:147:LEU:HB2	1.86	0.58
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.84	0.58
5:C:180:SER:HB2	38:C:8645:HOH:O	2.02	0.58
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.32	0.58
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3035:C:H5"	38:9:4078:HOH:O	2.03	0.58
16:O:42:GLU:HB2	38:O:2176:HOH:O	2.04	0.58
13:L:136:ALA:HB3	38:L:8872:HOH:O	2.03	0.58
1:0:1168:C:H4'	38:I:5128:HOH:O	2.04	0.58
1:0:87:C:H2'	29:2:28:LYS:O	2.04	0.58
1:0:2816:A:H5"	1:0:2817:G:H5'	1.86	0.58
1:0:42:C:H3'	38:0:4179:HOH:O	2.03	0.58
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.31	0.58
4:B:25:ARG:HA	4:B:310:ARG:HH21	1.68	0.58
13:L:143:THR:HG22	13:L:144:ASP:N	2.18	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.58
1:0:282:C:H1'	1:0:368:C:H42	1.69	0.58
15:N:144:GLY:O	15:N:147:ILE:HG22	2.02	0.58
11:J:103:VAL:HG12	38:J:8868:HOH:O	2.03	0.58
1:0:661:G:C5	1:0:686:A:C2	2.92	0.58
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.84	0.58
1:0:2703:A:H2'	1:0:2704:C:H6	1.67	0.58
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.58
2:9:3057:A:H8	6:D:141:VAL:HG21	1.69	0.57
1:0:875:A:C2	3:A:194:MET:SD	2.97	0.57
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.44	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.05	0.57
1:0:1183:C:O2	1:0:1183:C:H2'	2.03	0.57
7:E:68:HIS:O	7:E:72:MET:HG3	2.04	0.57
10:H:63:GLU:HA	38:H:8582:HOH:O	2.03	0.57
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.68	0.57
38:0:7344:HOH:O	26:Y:149:GLN:HG3	2.02	0.57
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.70	0.57
11:J:131:THR:HB	11:J:134:GLU:HG3	1.85	0.57
1:0:2498:C:O2'	1:0:2499:U:H5'	2.04	0.57
1:0:877:G:C5'	1:0:878:G:OP1	2.49	0.57
4:B:258:GLY:H	4:B:260:HIS:CE1	2.21	0.57
1:0:2478:U:O2'	1:0:2479:A:H5'	2.04	0.57
1:0:1202:A:H2'	1:0:1203:G:C5'	2.34	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.57
14:M:24:GLN:NE2	14:M:27:ARG:HH11	2.02	0.57
1:0:1972:U:H2'	1:0:1973:A:C5'	2.35	0.57
1:0:2256:G:O2'	1:0:2257:G:H5'	2.04	0.57
1:0:1226:G:H5'	38:0:4537:HOH:O	2.05	0.57
2:9:3072:C:O2'	2:9:3073:G:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.05	0.57
1:0:92:G:H4'	23:V:44:GLY:HA3	1.87	0.57
30:3:70:ARG:HG2	30:3:77:ALA:HB2	1.85	0.57
1:0:31:C:H2'	38:0:7673:HOH:O	2.03	0.57
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.85	0.57
1:0:671:A:O2'	1:0:672:G:H2'	2.05	0.57
23:V:64:GLY:O	23:V:65:ASP:HB2	2.03	0.57
1:0:1028:U:H1'	38:0:3649:HOH:O	2.04	0.57
4:B:254:GLN:HG2	4:B:255:GLY:N	2.19	0.57
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.70	0.57
2:9:3095:C:O2'	2:9:3096:C:H5'	2.05	0.57
1:0:1118:A:H8	1:0:1119:G:H5"	1.69	0.57
2:9:3091:C:H1'	38:9:7454:HOH:O	2.04	0.57
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.39	0.57
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.03	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.40	0.57
1:0:1393:A:H2'	1:0:1394:C:C6	2.40	0.57
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.40	0.57
1:0:88:G:H5'	1:0:88:G:H8	1.70	0.57
1:0:1291:A:H2	38:0:5297:HOH:O	1.86	0.57
1:0:2781:U:O2'	1:0:2782:G:H5'	2.05	0.57
10:H:138:CYS:HB2	38:H:8544:HOH:O	2.03	0.57
4:B:152:PRO:HA	38:B:8866:HOH:O	2.04	0.57
1:0:1193:A:C2	1:0:1194:A:N6	2.73	0.56
1:0:2291:A:N9	1:0:2309:C:H5'	2.20	0.56
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
2:9:3052:A:H2'	2:9:3053:G:O4'	2.05	0.56
2:9:3057:A:C8	6:D:141:VAL:HG21	2.40	0.56
10:H:26:SER:HA	10:H:59:HIS:HD2	1.70	0.56
4:B:225:GLY:HA3	38:B:8863:HOH:O	2.05	0.56
1:0:564:G:H1'	38:0:6311:HOH:O	2.03	0.56
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.87	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
24:W:139:GLY:O	24:W:141:HIS:HD2	1.89	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.56
2:9:3044:A:O4'	6:D:76:ARG:NE	2.38	0.56
26:Y:187:VAL:HG23	26:Y:192:ASP:HB3	1.86	0.56
1:0:2445:U:H2'	1:0:2446:G:H8	1.69	0.56
3:A:99:ILE:O	3:A:131:HIS:HE1	1.87	0.56
21:T:64:ASN:HB3	21:T:73:HIS:HB2	1.88	0.56
1:0:2604:A:H5'	38:0:5801:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2385:G:H2'	1:0:2386:U:C6	2.40	0.56
15:N:147:ILE:HB	38:N:8842:HOH:O	2.04	0.56
1:0:941:G:O2'	1:0:942:U:H5'	2.04	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.06	0.56
4:B:254:GLN:HG3	38:B:8828:HOH:O	2.06	0.56
8:F:91:VAL:HG12	8:F:92:GLY:N	2.20	0.56
1:0:1154:A:H2'	1:0:1155:G:C8	2.40	0.56
20:S:43:GLU:HB3	38:S:8546:HOH:O	2.04	0.56
1:0:870:G:OP2	3:A:3:ARG:HD3	2.06	0.56
38:0:5467:HOH:O	9:G:12:ILE:HA	2.05	0.56
1:0:1717:A:H5"	17:P:54:LYS:HB2	1.88	0.56
1:0:776:A:OP1	28:1:28:HIS:HE1	1.87	0.56
1:0:1181:A:C2	1:0:1192:A:C8	2.94	0.56
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.31	0.56
24:W:88:THR:HG23	24:W:110:GLN:NE2	2.21	0.56
16:O:32:ARG:HD3	16:O:32:ARG:O	2.05	0.56
1:0:1329:A:H2	38:0:4691:HOH:O	1.89	0.56
1:0:821:U:H5"	38:0:3050:HOH:O	2.05	0.56
25:X:43:VAL:HG11	25:X:82:GLU:HA	1.86	0.56
1:0:111:C:O2'	28:1:20:ARG:HG2	2.06	0.56
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.88	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.06	0.56
1:0:380:A:OP2	14:M:9:ARG:HD2	2.06	0.56
1:0:573:A:O2'	1:0:574:C:H5'	2.06	0.56
1:0:1527:A:H1'	1:0:1528:A:C8	2.41	0.56
1:0:1167:G:H4'	31:I:135:LEU:HD22	1.88	0.56
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.54	0.56
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.71	0.56
1:0:2403:C:H2'	1:0:2404:G:O5'	2.06	0.56
22:U:47:ARG:HG2	38:U:4381:HOH:O	2.05	0.56
21:T:71:VAL:HG11	21:T:90:PRO:CB	2.33	0.56
5:C:114:ALA:HB1	5:C:223:LEU:HB3	1.88	0.56
1:0:2255:A:N1	1:0:2256:G:C4	2.74	0.56
1:0:1167:G:H2'	1:0:1168:C:O4'	2.06	0.56
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.58	0.56
1:0:1172:G:H1'	38:0:4978:HOH:O	2.05	0.56
1:0:21:G:H4'	19:R:2:ILE:HG22	1.88	0.56
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.88	0.56
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.87	0.56
38:0:9539:HOH:O	17:P:81:LYS:HG2	2.05	0.56
5:C:65:ARG:HG3	5:C:67:GLN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1377:C:H2'	1:0:1723:G:O6	2.06	0.55
1:0:1168:C:H5"	31:I:87:THR:HG22	1.88	0.55
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.36	0.55
2:9:3106:C:O2'	2:9:3107:C:H5'	2.07	0.55
6:D:159:PRO:O	6:D:163:VAL:HG23	2.06	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.89	0.55
1:0:333:G:O2'	1:0:334:G:H5'	2.06	0.55
4:B:62:ARG:HA	4:B:65:MET:HE3	1.87	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
25:X:74:ALA:HB2	25:X:85:VAL:HG13	1.88	0.55
38:0:6860:HOH:O	3:A:211:LYS:HD3	2.07	0.55
20:S:57:THR:HG22	20:S:59:ASP:N	2.18	0.55
4:B:79:MET:HE1	38:B:8921:HOH:O	2.06	0.55
1:0:1309:U:O2'	1:0:1310:U:H5'	2.06	0.55
6:D:149:ARG:HH12	15:N:15:GLU:HA	1.72	0.55
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.05	0.55
24:W:6:GLN:HB2	24:W:26:ILE:CD1	2.36	0.55
2:9:3001:U:H5"	2:9:3003:A:OP1	2.07	0.55
1:0:2839:C:H2'	1:0:2840:A:H5"	1.88	0.55
24:W:88:THR:HG22	24:W:89:ASP:N	2.20	0.55
1:0:1873:G:H3'	38:0:5213:HOH:O	2.06	0.55
26:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.88	0.55
1:0:1180:U:H2'	1:0:1181:A:O4'	2.07	0.55
7:E:137:ASP:O	7:E:141:VAL:HG23	2.06	0.55
1:0:926:A:O2'	13:L:41:HIS:CD2	2.60	0.55
5:C:246:ARG:NE	38:C:8623:HOH:O	2.38	0.55
8:F:27:GLY:HA3	8:F:101:ALA:O	2.07	0.55
1:0:1169:U:H2'	1:0:1170:U:O4'	2.07	0.55
22:U:52:THR:CG2	22:U:54:THR:HB	2.37	0.55
1:0:960:G:N3	1:0:960:G:C2'	2.69	0.55
1:0:1687:C:O2	28:1:9:GLY:HA2	2.06	0.55
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.88	0.55
1:0:553:G:P	26:Y:204:ARG:HH22	2.30	0.55
1:0:559:U:C5'	1:0:559:U:H6	2.18	0.55
1:0:958:G:H2'	1:0:959:C:H6	1.72	0.55
29:2:20:ARG:HG2	29:2:21:VAL:N	2.22	0.55
1:0:88:G:H2'	1:0:89:G:C8	2.41	0.55
4:B:62:ARG:HA	4:B:65:MET:CE	2.37	0.55
5:C:77:ALA:O	5:C:78:ARG:HD2	2.06	0.55
1:0:1132:A:N6	1:0:1229:C:H2'	2.22	0.55
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1119:G:H5"	2.41	0.55
1:0:947:U:H2'	1:0:948:G:H8	1.70	0.55
1:0:941:G:C5	1:0:942:U:C4	2.95	0.55
5:C:236:THR:H	5:C:239:ALA:HB3	1.72	0.55
1:0:856:G:C8	38:0:5435:HOH:O	2.54	0.55
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.55
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.10	0.54
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.69	0.54
1:0:1790:C:H2'	1:0:1791:U:C6	2.40	0.54
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
38:0:4844:HOH:O	11:J:47:THR:HB	2.07	0.54
1:0:2456:A:H5'	38:0:5705:HOH:O	2.06	0.54
24:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.54
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.87	0.54
4:B:41:PHE:HA	4:B:79:MET:HE2	1.90	0.54
1:0:120:A:H2'	1:0:120:A:N3	2.22	0.54
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.54
1:0:1588:G:C6	1:0:1589:G:N1	2.75	0.54
14:M:24:GLN:HE22	14:M:27:ARG:HH11	1.55	0.54
1:0:255:A:C5	1:0:256:C:C4	2.96	0.54
31:I:113:HIS:N	31:I:114:PRO:HD2	2.22	0.54
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.88	0.54
1:0:1137:G:H1'	38:0:3885:HOH:O	2.07	0.54
3:A:33:GLU:O	3:A:34:ASP:HB2	2.07	0.54
1:0:468:U:H3'	38:0:7553:HOH:O	2.07	0.54
2:9:3076:G:C3'	2:9:3077:A:H5"	2.30	0.54
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.22	0.54
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.37	0.54
1:0:2266:A:OP2	14:M:90:ARG:NH2	2.41	0.54
1:0:2425:A:H2'	38:0:9228:HOH:O	2.06	0.54
19:R:39:THR:HB	19:R:42:GLU:HG3	1.90	0.54
1:0:2826:G:C6	1:0:2913:A:N6	2.75	0.54
38:9:3472:HOH:O	15:N:41:LYS:HD3	2.08	0.54
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.54
5:C:233:THR:HG22	5:C:234:VAL:N	2.21	0.54
8:F:29:VAL:HG12	8:F:98:VAL:HA	1.90	0.54
1:0:226:A:H1'	1:0:393:G:C5	2.43	0.54
1:0:705:C:H2'	1:0:705:C:O2	2.08	0.54
5:C:22:PHE:HA	5:C:116:ALA:HA	1.88	0.54
21:T:53:GLY:HA3	38:T:6384:HOH:O	2.08	0.54
5:C:236:THR:CG2	5:C:239:ALA:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:H2'	1:0:1172:G:H5'	1.90	0.54
1:0:506:G:N2	1:0:509:A:H5"	2.16	0.54
1:0:1603:A:H5'	1:0:1605:G:C4'	2.38	0.54
2:9:3003:A:OP2	2:9:3025:G:N2	2.40	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
8:F:21:GLU:O	8:F:24:ARG:HG2	2.07	0.54
1:0:2346:C:O5'	1:0:2346:C:H6	1.90	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.08	0.54
1:0:2001:G:O2'	1:0:2002:C:H5'	2.07	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.88	0.54
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.43	0.54
1:0:1667:A:H2'	1:0:1668:U:H6	1.72	0.54
2:9:3076:G:H3'	2:9:3077:A:C5'	2.28	0.54
5:C:1:MET:HG2	5:C:2:GLN:N	2.21	0.54
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.90	0.54
38:0:4623:HOH:O	16:O:39:THR:HB	2.07	0.54
2:9:3055:U:H4'	2:9:3056:A:C8	2.43	0.54
38:0:4376:HOH:O	3:A:212:PRO:HB2	2.08	0.54
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.38	0.54
1:0:1568:G:O2'	1:0:1569:U:H5'	2.07	0.54
1:0:1421:C:H2'	1:0:1422:U:H6	1.73	0.54
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.23	0.54
1:0:1450:C:C4'	1:0:1451:C:OP2	2.53	0.54
1:0:1319:G:H1'	38:0:4701:HOH:O	2.07	0.54
8:F:117:GLU:C	8:F:119:ARG:H	2.10	0.54
1:0:1931:A:H2'	1:0:1932:G:H5'	1.90	0.54
5:C:236:THR:HA	38:C:8651:HOH:O	2.08	0.54
3:A:51:ARG:NH1	3:A:120:ARG:O	2.41	0.54
1:0:1762:C:H2'	1:0:1763:C:C6	2.43	0.54
1:0:2064:U:H4'	1:0:2653:A:OP1	2.08	0.54
1:0:328:U:O4'	5:C:202:THR:HG22	2.07	0.54
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.54
1:0:794:U:H3	1:0:819:A:H61	1.54	0.54
17:P:91:LYS:O	17:P:95:GLU:HG3	2.08	0.54
1:0:1173:A:H2	38:0:6282:HOH:O	1.91	0.54
1:0:645:U:OP2	13:L:4:LYS:HE2	2.08	0.54
1:0:820:G:H5'	1:0:821:U:H5'	1.90	0.53
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.43	0.53
1:0:841:A:H5"	38:0:6906:HOH:O	2.08	0.53
1:0:1396:C:H1'	17:P:1:THR:O	2.08	0.53
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:125:U:H2'	38:0:3769:HOH:O	2.07	0.53
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.08	0.53
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.53
1:0:349:U:O2'	1:0:350:C:H5'	2.09	0.53
4:B:279:THR:OG1	4:B:290:VAL:HB	2.08	0.53
4:B:74:ILE:HG22	4:B:76:THR:HG23	1.91	0.53
1:0:2488:A:H61	1:0:2534:C:H42	1.54	0.53
1:0:2361:A:H8	1:0:2361:A:H5'	1.73	0.53
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.36	0.53
23:V:4:HIS:O	23:V:8:ILE:HG13	2.08	0.53
1:0:1444:G:O2'	1:0:1445:G:H5'	2.08	0.53
20:S:57:THR:HG22	20:S:59:ASP:HB2	1.90	0.53
1:0:40:C:H4'	38:0:6998:HOH:O	2.08	0.53
1:0:660:A:H4'	1:0:661:G:O5'	2.08	0.53
22:U:9:CYS:HA	22:U:52:THR:HG23	1.90	0.53
1:0:399:C:H5'	14:M:179:GLY:O	2.09	0.53
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.53
1:0:2784:A:H1'	7:E:60:SER:OG	2.08	0.53
8:F:56:PRO:HG2	14:M:43:PRO:O	2.08	0.53
1:0:2526:C:H5'	1:0:2526:C:C6	2.43	0.53
4:B:162:MET:CE	4:B:308:LEU:HD21	2.39	0.53
1:0:2064:U:H5'	1:0:2652:U:H4'	1.91	0.53
24:W:64:THR:O	24:W:68:THR:HG22	2.08	0.53
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.90	0.53
1:0:271:C:H4'	1:0:272:A:OP1	2.08	0.53
18:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
4:B:23:THR:HG23	4:B:308:LEU:HD23	1.91	0.53
11:J:46:ILE:HA	38:J:8828:HOH:O	2.09	0.53
24:W:68:THR:HG23	24:W:69:ARG:HG2	1.91	0.53
8:F:96:ALA:HA	38:F:3111:HOH:O	2.09	0.53
5:C:40:ALA:O	5:C:43:LYS:HB2	2.08	0.53
1:0:2735:U:H2'	1:0:2736:U:C6	2.44	0.53
1:0:622:G:O2'	1:0:623:U:H5'	2.08	0.53
1:0:2382:A:H5'	38:3:8831:HOH:O	2.09	0.53
1:0:821:U:H2'	1:0:822:C:C6	2.41	0.53
1:0:420:U:H2'	1:0:421:C:C6	2.44	0.53
31:I:103:ASP:HA	31:I:106:LYS:HD2	1.91	0.53
17:P:14:LEU:HD13	17:P:51:ALA:HB2	1.91	0.53
1:0:1314:U:H2'	38:0:5885:HOH:O	2.09	0.53
1:0:2071:C:H5'	38:0:9529:HOH:O	2.09	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:129:LYS:HG2	38:W:1990:HOH:O	2.07	0.53
20:S:52:VAL:HG22	20:S:66:VAL:HG22	1.90	0.53
1:0:282:C:O2'	1:0:283:U:C5'	2.53	0.53
6:D:163:VAL:HA	38:D:6326:HOH:O	2.07	0.53
6:D:166:ILE:HB	38:D:6326:HOH:O	2.09	0.53
1:0:12:U:C2'	1:0:13:G:H5'	2.38	0.53
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.09	0.53
1:0:1342:C:O2'	1:0:1343:C:H5'	2.09	0.53
1:0:1855:G:H4'	1:0:1856:C:O5'	2.09	0.53
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.44	0.53
1:0:1456:C:H2'	1:0:1457:U:C6	2.44	0.53
1:0:1181:A:N1	1:0:1192:A:O2'	2.38	0.53
1:0:1213:C:C2'	1:0:1214:G:H5'	2.39	0.53
9:G:64:ASN:N	9:G:64:ASN:HD22	2.06	0.53
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.43	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.42	0.53
21:T:32:ARG:NH1	21:T:38:ARG:HH12	2.07	0.53
1:0:1159:G:H21	1:0:1189:A:H8	1.55	0.53
6:D:135:VAL:HG22	6:D:136:ARG:H	1.74	0.53
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.06	0.53
1:0:1309:U:C2'	1:0:1310:U:H5'	2.40	0.53
1:0:1236:A:H2'	1:0:1237:U:O4'	2.09	0.53
1:0:2269:C:C2'	1:0:2270:G:H5'	2.39	0.53
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.89	0.53
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.89	0.53
10:H:56:GLN:HE21	10:H:126:ARG:NE	2.00	0.52
1:0:1733:A:H4'	4:B:212:GLN:HA	1.90	0.52
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.52
1:0:625:U:H5"	1:0:1044:C:N4	2.24	0.52
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.39	0.52
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.90	0.52
2:9:3031:C:H2'	2:9:3032:G:O4'	2.10	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.38	0.52
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.91	0.52
1:0:2837:U:H2'	38:0:6833:HOH:O	2.08	0.52
2:9:3060:C:O2'	2:9:3061:C:H5'	2.09	0.52
14:M:169:ARG:HD2	38:M:8886:HOH:O	2.09	0.52
4:B:16:ARG:NH1	38:B:8913:HOH:O	2.42	0.52
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.38	0.52
1:0:371:U:H2'	1:0:372:A:H8	1.75	0.52
1:0:1588:G:C6	1:0:1589:G:C6	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:603:A:H4'	1:0:604:G:O5'	2.09	0.52
10:H:69:ALA:HB2	10:H:153:ALA:HB2	1.90	0.52
20:S:76:GLU:HB3	38:S:8547:HOH:O	2.09	0.52
15:N:38:LYS:HE2	15:N:107:ASN:ND2	2.24	0.52
1:0:544:G:H2'	1:0:545:G:C5'	2.40	0.52
1:0:2601:A:N1	12:K:38:SER:HB2	2.25	0.52
1:0:2894:C:O2'	1:0:2895:C:H5'	2.09	0.52
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.91	0.52
1:0:1972:U:C2'	1:0:1973:A:H5"	2.39	0.52
1:0:1755:A:H2'	1:0:1756:G:O4'	2.09	0.52
1:0:2237:G:H1'	38:0:4862:HOH:O	2.10	0.52
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.52
1:0:1384:C:H5'	25:X:30:MET:HG2	1.92	0.52
19:R:33:ARG:NH1	38:R:8838:HOH:O	2.41	0.52
30:3:3:MET:O	30:3:90:PHE:HA	2.10	0.52
1:0:304:G:H1'	1:0:347:A:N6	2.24	0.52
1:0:289:G:N2	1:0:363:A:C2	2.57	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.52
2:9:3029:C:H2'	2:9:3030:C:C5'	2.36	0.52
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.57	0.52
1:0:1421:C:H2'	1:0:1422:U:C6	2.45	0.52
6:D:82:GLU:HA	6:D:85:GLN:HE21	1.74	0.52
21:T:26:THR:HA	21:T:39:ASN:HB3	1.91	0.52
1:0:1641:A:H2'	1:0:1642:A:C5'	2.33	0.52
24:W:88:THR:HG22	24:W:90:TYR:HD1	1.74	0.52
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.90	0.52
1:0:707:C:C2	1:0:708:A:C8	2.97	0.52
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.25	0.52
13:L:148:GLU:HA	38:L:8871:HOH:O	2.10	0.52
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.91	0.52
1:0:1169:U:C5	1:0:1170:U:C4	2.97	0.52
1:0:204:A:H2'	1:0:205:U:H5'	1.91	0.52
1:0:346:U:H4'	38:0:6837:HOH:O	2.08	0.52
22:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.52
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.40	0.52
1:0:567:U:C5'	38:0:6400:HOH:O	2.57	0.52
1:0:951:A:O2'	1:0:952:G:H5'	2.10	0.52
9:G:23:ILE:O	9:G:27:ILE:HG13	2.10	0.52
1:0:2460:A:H5'	32:0:9000:13T:H231	1.90	0.52
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.16	0.52
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2766:A:O2'	1:0:2767:C:H5'	2.10	0.52
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.52
1:0:1661:A:C8	38:0:5210:HOH:O	2.55	0.52
1:0:59:A:H5'	38:0:4342:HOH:O	2.09	0.52
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.92	0.52
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.52
5:C:95:GLU:HG3	38:C:8673:HOH:O	2.09	0.52
14:M:164:THR:HG22	14:M:167:GLY:H	1.74	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.48	0.51
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.92	0.51
1:0:475:G:OP1	5:C:73:LEU:HD22	2.09	0.51
38:0:7541:HOH:O	30:3:60:LYS:HG3	2.10	0.51
2:9:3020:G:O2'	2:9:3021:G:H5'	2.10	0.51
1:0:291:C:H2'	1:0:292:G:O4'	2.10	0.51
1:0:2010:A:C2'	38:0:5968:HOH:O	2.50	0.51
1:0:2467:A:O2'	1:0:2468:A:H2'	2.10	0.51
1:0:2361:A:H5"	38:0:9001:HOH:O	2.08	0.51
38:0:4733:HOH:O	19:R:29:LYS:HD3	2.10	0.51
5:C:242:GLU:HB2	38:C:8579:HOH:O	2.09	0.51
1:0:2388:C:O2'	1:0:2389:U:H5'	2.10	0.51
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.51
8:F:91:VAL:HG12	8:F:92:GLY:H	1.76	0.51
1:0:64:G:H2'	1:0:65:C:O4'	2.10	0.51
1:0:119:A:H2'	1:0:120:A:H5"	1.93	0.51
1:0:2266:A:H2'	1:0:2267:G:C8	2.45	0.51
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.74	0.51
1:0:254:C:O2	1:0:254:C:H2'	2.09	0.51
1:0:1500:U:P	17:P:41:ARG:HH22	2.33	0.51
1:0:1545:C:H2'	1:0:1546:G:O4'	2.10	0.51
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.09	0.51
2:9:3092:G:C6	2:9:3093:A:C6	2.98	0.51
26:Y:189:ASN:HD22	26:Y:189:ASN:C	2.14	0.51
2:9:3034:A:H2'	2:9:3035:C:O4'	2.11	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.93	0.51
1:0:1398:G:O2'	1:0:1399:A:H5'	2.11	0.51
1:0:2036:C:O4'	12:K:44:LEU:HG	2.10	0.51
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.11	0.51
18:Q:75:ILE:HD13	18:Q:84:ILE:HD11	1.93	0.51
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.93	0.51
1:0:2887:G:H2'	1:0:2888:U:C6	2.45	0.51
15:N:132:ASN:O	15:N:135:VAL:HG12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:894:A:C2	5:C:87:ARG:NH2	2.78	0.51
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.51
1:0:714:U:H3'	38:0:6939:HOH:O	2.09	0.51
13:L:72:ASN:HB2	38:L:8881:HOH:O	2.09	0.51
4:B:85:ARG:NH1	38:B:8930:HOH:O	2.42	0.51
17:P:115:SER:N	17:P:118:GLN:HE21	2.00	0.51
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.10	0.51
17:P:134:VAL:O	17:P:137:LEU:HB3	2.11	0.51
11:J:54:VAL:HG11	11:J:138:THR:HG21	1.93	0.51
1:0:2379:G:N3	1:0:2418:G:H2'	2.25	0.51
1:0:2871:G:H2'	1:0:2872:U:C6	2.46	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.92	0.51
1:0:558:C:H2'	1:0:559:U:H5"	1.88	0.51
2:9:3013:A:O2'	2:9:3014:G:H5"	2.11	0.51
1:0:2578:G:C8	1:0:2578:G:H5'	2.41	0.51
2:9:3039:U:H1'	2:9:3044:A:N6	2.26	0.51
1:0:1819:G:H5'	38:0:4720:HOH:O	2.09	0.51
7:E:69:ILE:HA	7:E:72:MET:CE	2.40	0.51
1:0:1314:U:H5"	1:0:1316:G:O4'	2.11	0.51
6:D:62:ASP:HA	38:D:4233:HOH:O	2.11	0.51
15:N:169:PRO:O	15:N:172:PHE:HB3	2.11	0.51
1:0:1163:G:H5'	31:I:115:ASP:O	2.10	0.51
1:0:1543:G:N1	1:0:1641:A:OP2	2.38	0.51
1:0:1856:C:H5'	1:0:1858:A:O4'	2.10	0.51
1:0:589:U:H2'	1:0:590:A:H8	1.74	0.51
1:0:1787:C:H4'	1:0:2883:A:O4'	2.11	0.51
4:B:145:HIS:HD2	4:B:146:THR:O	1.94	0.51
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.92	0.51
1:0:324:G:C6	1:0:325:U:C5	2.99	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:1116:U:O2'	1:0:1118:A:C2	2.50	0.51
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.93	0.51
1:0:1878:G:C1'	38:0:6128:HOH:O	2.49	0.51
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.93	0.51
1:0:2893:C:O2'	1:0:2894:C:H5'	2.11	0.51
1:0:228:C:H2'	1:0:229:G:H5'	1.92	0.51
7:E:101:GLU:HB3	7:E:117:THR:HA	1.92	0.51
1:0:1119:G:H8	11:J:52:GLN:HE22	1.59	0.51
1:0:2765:C:H2'	1:0:2766:A:H8	1.76	0.51
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.08	0.51
1:0:329:A:OP2	5:C:206:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1600:G:OP2	1:0:1600:G:H8	1.94	0.51
1:0:168:C:O5'	1:0:168:C:H6	1.93	0.51
5:C:132:ASP:HB3	38:C:8560:HOH:O	2.10	0.51
1:0:1119:G:H8	11:J:52:GLN:NE2	2.08	0.50
1:0:1586:G:O2'	1:0:1587:U:H5'	2.11	0.50
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.93	0.50
1:0:2269:C:O2'	1:0:2270:G:H5'	2.11	0.50
1:0:2106:C:H5'	1:0:2284:G:H21	1.77	0.50
1:0:2135:A:O2'	1:0:2136:G:H5'	2.10	0.50
24:W:4:LEU:HB2	24:W:33:THR:HG22	1.92	0.50
6:D:103:ASN:HD22	6:D:134:LEU:H	1.57	0.50
1:0:710:G:C2'	1:0:711:G:H5'	2.41	0.50
28:1:28:HIS:CE1	28:1:31:LYS:HE2	2.46	0.50
1:0:2515:C:H2'	1:0:2516:G:O4'	2.11	0.50
1:0:1862:C:H1'	38:0:7211:HOH:O	2.10	0.50
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.93	0.50
26:Y:117:LEU:HD12	26:Y:174:VAL:CG1	2.41	0.50
1:0:17:G:H2'	1:0:18:C:C6	2.47	0.50
1:0:588:G:O6	24:W:154:ARG:NH1	2.43	0.50
1:0:1556:G:O2'	1:0:1557:G:H5'	2.11	0.50
1:0:814:G:H4'	38:0:3133:HOH:O	2.12	0.50
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.27	0.50
1:0:1413:A:H2'	1:0:1414:A:O4'	2.11	0.50
19:R:119:VAL:HG21	19:R:142:ASP:CG	2.31	0.50
1:0:1287:A:O4'	24:W:117:ARG:HD3	2.12	0.50
32:0:9000:13T:C23	32:0:9000:13T:C31	2.90	0.50
1:0:1188:A:H5'	38:0:7415:HOH:O	2.11	0.50
11:J:107:ASN:HD22	11:J:107:ASN:C	2.14	0.50
1:0:1406:A:H4'	1:0:1407:A:C5'	2.42	0.50
31:I:78:LEU:HD12	31:I:112:LYS:NZ	2.26	0.50
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.26	0.50
2:9:3023:U:O2'	2:9:3024:U:H4'	2.11	0.50
1:0:2717:C:C2'	1:0:2718:C:C5'	2.78	0.50
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.45	0.50
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.94	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.44	0.50
2:9:3104:A:O2'	2:9:3105:A:H5'	2.12	0.50
19:R:119:VAL:HG12	19:R:119:VAL:O	2.10	0.50
5:C:102:LEU:HD12	38:C:8515:HOH:O	2.11	0.50
1:0:1985:U:C2	1:0:1996:U:O4'	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:74:VAL:HG13	12:K:113:ILE:HG12	1.92	0.50
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.93	0.50
1:0:84:G:C2'	1:0:85:C:H5'	2.42	0.50
1:0:240:C:O2	1:0:240:C:H2'	2.12	0.50
1:0:2664:A:OP1	1:0:2664:A:H8	1.95	0.50
6:D:172:VAL:HG12	6:D:173:GLU:N	2.27	0.50
13:L:24:ALA:HB2	13:L:30:ARG:HD2	1.93	0.50
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.46	0.50
1:0:793:A:H5"	17:P:83:LYS:HG2	1.94	0.50
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.94	0.50
28:1:10:LYS:HG3	38:1:8731:HOH:O	2.11	0.50
21:T:69:LYS:O	21:T:71:VAL:HG23	2.12	0.50
24:W:125:HIS:CD2	24:W:127:GLY:H	2.25	0.50
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.76	0.50
1:0:370:G:O2'	1:0:371:U:H5'	2.12	0.50
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.94	0.50
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.94	0.50
19:R:59:PHE:O	19:R:63:ASN:HB3	2.12	0.50
21:T:41:ARG:NH1	21:T:42:VAL:O	2.45	0.50
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.93	0.50
1:0:363:A:O2'	1:0:364:C:H5'	2.12	0.50
1:0:2506:A:N6	1:0:2511:A:O2'	2.44	0.50
1:0:1207:A:C8	1:0:1208:C:C5	3.00	0.50
1:0:1878:G:O2'	1:0:1879:U:H6	1.93	0.50
1:0:2253:G:C2	1:0:2254:G:C8	3.00	0.50
1:0:2779:G:H21	7:E:143:GLN:NE2	2.10	0.50
1:0:1130:U:H5'	38:0:7657:HOH:O	2.11	0.50
9:G:12:ILE:N	9:G:13:PRO:HD3	2.27	0.50
3:A:89:ALA:HB3	38:A:8913:HOH:O	2.11	0.50
1:0:2336:G:H1'	38:0:6297:HOH:O	2.12	0.50
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.93	0.50
5:C:214:THR:HG23	38:C:8636:HOH:O	2.10	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.46	0.50
1:0:1163:G:N2	38:0:6056:HOH:O	2.45	0.50
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.11	0.50
1:0:1154:A:H2'	1:0:1155:G:H8	1.75	0.50
1:0:424:C:H2'	1:0:425:U:H6	1.77	0.50
25:X:25:ARG:HD3	25:X:64:ALA:O	2.12	0.50
10:H:47:ILE:HG12	10:H:165:SER:HA	1.93	0.50
1:0:93:C:H5"	23:V:1:THR:CB	2.33	0.49
21:T:71:VAL:HG12	21:T:72:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
15:N:43:VAL:HG11	15:N:81:ALA:HA	1.94	0.49
1:0:2831:C:H2'	1:0:2832:C:H5'	1.93	0.49
1:0:2296:C:H2'	1:0:2297:U:C6	2.47	0.49
1:0:635:A:H2'	1:0:636:G:H5"	1.92	0.49
13:L:80:ASP:HB2	13:L:90:ARG:O	2.12	0.49
2:9:3055:U:H4'	2:9:3056:A:H8	1.77	0.49
1:0:2896:A:N3	1:0:2896:A:H2'	2.28	0.49
1:0:710:G:O2'	1:0:711:G:H5'	2.12	0.49
4:B:26:PHE:HE1	4:B:310:ARG:HB3	1.77	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.49
1:0:1423:C:O2'	1:0:1424:A:H5'	2.12	0.49
10:H:162:ARG:HD3	38:H:8585:HOH:O	2.12	0.49
3:A:179:MET:HG2	3:A:186:TRP:CG	2.46	0.49
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.45	0.49
1:0:775:G:OP1	28:1:16:HIS:HE1	1.95	0.49
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.76	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.12	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.49
13:L:134:GLU:HG3	38:L:8855:HOH:O	2.12	0.49
1:0:1642:A:C8	1:0:1643:C:C5	3.00	0.49
1:0:2363:G:O2'	18:Q:11:ARG:HG3	2.13	0.49
1:0:2493:C:O2	1:0:2493:C:H2'	2.11	0.49
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.77	0.49
1:0:1008:C:H5"	10:H:16:ARG:HH12	1.76	0.49
1:0:2866:U:C5	22:U:50:GLU:HB2	2.47	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.12	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.49
1:0:2004:U:H2'	1:0:2004:U:O2	2.11	0.49
1:0:1972:U:H2'	1:0:1973:A:H5"	1.93	0.49
10:H:27:LYS:H	10:H:59:HIS:HD2	1.59	0.49
1:0:946:C:H2'	1:0:947:U:C6	2.47	0.49
1:0:494:C:H2'	1:0:496:G:OP2	2.13	0.49
26:Y:107:PRO:HD3	26:Y:182:PHE:CE1	2.47	0.49
11:J:19:MET:HE2	11:J:79:PHE:HA	1.94	0.49
27:Z:53:GLY:HA2	27:Z:67:GLY:O	2.12	0.49
1:0:1474:C:C5'	1:0:1474:C:C6	2.81	0.49
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.78	0.49
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:75:PRO:HD3	11:J:136:SER:OG	2.13	0.49
4:B:267:LYS:HA	38:B:8824:HOH:O	2.11	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49
1:0:318:C:H5'	1:0:339:A:C2	2.48	0.49
1:0:251:C:O2'	1:0:252:C:H5'	2.12	0.49
1:0:2122:C:H3'	38:0:5295:HOH:O	2.13	0.49
1:0:710:G:OP1	16:O:24:ALA:HB3	2.13	0.49
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.27	0.49
1:0:1488:U:H4'	1:0:1489:G:OP1	2.12	0.49
1:0:1681:G:H5"	1:0:1682:A:H5'	1.94	0.49
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.11	0.49
1:0:1278:A:H4'	1:0:1279:U:C4	2.48	0.49
1:0:645:U:O2	1:0:761:A:H2	1.96	0.49
1:0:2694:A:C6	1:0:2702:A:C8	3.01	0.49
1:0:1331:A:OP2	26:Y:142:SER:OG	2.27	0.49
38:0:5640:HOH:O	17:P:58:SER:HB3	2.11	0.49
10:H:51:VAL:HG13	10:H:159:PRO:HG3	1.95	0.49
4:B:36:PRO:HA	4:B:168:GLY:CA	2.39	0.49
1:0:558:C:H5'	38:0:5262:HOH:O	2.13	0.49
1:0:514:G:OP1	1:0:514:G:H2'	2.12	0.49
1:0:2316:G:H4'	38:0:6098:HOH:O	2.12	0.49
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.28	0.49
1:0:1422:U:H2'	1:0:1423:C:C6	2.48	0.49
1:0:1484:G:H2'	38:0:9098:HOH:O	2.13	0.49
28:1:25:LYS:O	28:1:25:LYS:HG2	2.13	0.49
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.49
1:0:2102:G:C2	1:0:2104:C:C4	3.01	0.49
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.48	0.49
4:B:294:TYR:HE2	38:B:8945:HOH:O	1.95	0.49
1:0:1834:C:H2'	1:0:1840:A:N6	2.27	0.49
1:0:949:U:O2'	18:Q:40:HIS:HE1	1.96	0.49
1:0:2300:A:H4'	1:0:2301:A:O5'	2.13	0.49
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.43	0.49
1:0:1421:C:O2'	1:0:1422:U:H5'	2.13	0.49
38:0:6679:HOH:O	21:T:38:ARG:NH1	2.45	0.49
1:0:2387:U:H2'	1:0:2388:C:C6	2.48	0.49
38:0:6699:HOH:O	26:Y:165:GLU:HB3	2.13	0.49
1:0:1311:G:C2	1:0:1312:G:C8	3.01	0.49
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.49
1:0:2453:G:H3'	38:0:5931:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:23:G:C6	1:0:24:G:N1	2.81	0.49
1:0:1098:A:H2'	1:0:1099:G:O4'	2.12	0.49
1:0:1165:G:C4'	1:0:1174:A:O2'	2.55	0.48
24:W:115:THR:HG23	38:W:5420:HOH:O	2.13	0.48
17:P:115:SER:OG	17:P:118:GLN:HG3	2.12	0.48
1:0:559:U:C3'	1:0:559:U:C6	2.96	0.48
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.39	0.48
1:0:447:A:OP2	21:T:1:SER:HB2	2.12	0.48
1:0:522:U:O2'	1:0:1366:C:H5'	2.13	0.48
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.48
1:0:816:G:C6	1:0:817:G:N1	2.80	0.48
30:3:65:THR:HB	30:3:83:TRP:H	1.78	0.48
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.95	0.48
1:0:999:C:H2'	1:0:1000:C:O4'	2.14	0.48
13:L:67:ARG:HB2	13:L:112:GLY:HA3	1.94	0.48
14:M:99:ARG:CD	14:M:167:GLY:HA2	2.42	0.48
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.34	0.48
1:0:292:G:H1'	1:0:360:A:N6	2.28	0.48
1:0:1477:C:H5'	1:0:1868:G:H5'	1.95	0.48
1:0:2703:A:H2'	1:0:2704:C:C6	2.48	0.48
25:X:23:HIS:CD2	25:X:24:LYS:HG3	2.49	0.48
1:0:474:C:O2'	5:C:73:LEU:HD21	2.13	0.48
10:H:170:ASN:N	10:H:170:ASN:HD22	2.10	0.48
5:C:107:ARG:NE	38:C:8657:HOH:O	2.35	0.48
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.48
1:0:2349:G:O2'	1:0:2350:G:H5'	2.12	0.48
12:K:130:MET:SD	22:U:25:ASP:O	2.71	0.48
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.28	0.48
14:M:164:THR:CG2	14:M:167:GLY:H	2.27	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.28	0.48
3:A:53:ALA:HB3	38:A:8897:HOH:O	2.12	0.48
1:0:2374:A:H2'	1:0:2375:G:H8	1.78	0.48
1:0:441:A:O5'	1:0:441:A:H8	1.96	0.48
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.48
31:I:113:HIS:CE1	31:I:121:LEU:HD22	2.48	0.48
38:0:9792:HOH:O	13:L:30:ARG:NH2	2.44	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:154:C:H2'	1:0:155:C:H6	1.78	0.48
14:M:49:ALA:C	14:M:54:TYR:HB3	2.34	0.48
1:0:10:U:O4	1:0:532:A:OP2	2.32	0.48
2:9:3054:A:C2	2:9:3055:U:N3	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1193:A:H2	1:0:1194:A:N6	2.12	0.48
1:0:597:A:C4	1:0:598:C:C5	3.01	0.48
16:O:47:ARG:HG3	16:O:47:ARG:NH1	2.29	0.48
4:B:17:LYS:O	4:B:260:HIS:HD2	1.95	0.48
19:R:39:THR:HB	19:R:42:GLU:CG	2.43	0.48
1:0:2055:A:H4'	19:R:132:ARG:NH2	2.28	0.48
10:H:97:GLU:HB3	10:H:121:VAL:HG11	1.96	0.48
1:0:188:C:H5"	14:M:163:LEU:HD21	1.95	0.48
1:0:366:U:H2'	1:0:367:G:O4'	2.12	0.48
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.48
1:0:1942:A:O2'	1:0:1943:C:H5'	2.14	0.48
1:0:1081:A:C6	1:0:1082:A:N1	2.82	0.48
1:0:470:U:O2'	28:1:16:HIS:CD2	2.64	0.48
1:0:2616:G:H1'	38:0:9423:HOH:O	2.14	0.48
1:0:2403:C:H3'	38:0:5214:HOH:O	2.13	0.48
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.44	0.48
2:9:3058:G:C8	2:9:3059:C:C5	3.02	0.48
7:E:11:VAL:HG12	7:E:12:ASP:N	2.29	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.95	0.48
1:0:1118:A:N6	1:0:1244:U:N3	2.57	0.48
29:2:41:HIS:HD2	29:2:44:ARG:H	1.62	0.48
24:W:3:ALA:O	24:W:54:PHE:HA	2.14	0.48
27:Z:33:MET:SD	27:Z:49:ARG:HD2	2.53	0.48
4:B:221:GLN:HE22	12:K:42:ASN:ND2	2.03	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.48
11:J:74:ARG:NH1	11:J:76:ASP:HB2	2.29	0.48
11:J:42:GLU:O	11:J:131:THR:HG23	2.14	0.48
1:0:2553:A:H2'	1:0:2553:A:N3	2.28	0.48
1:0:2324:G:N2	1:0:2377:U:H1'	2.29	0.48
1:0:963:C:O2	1:0:1005:A:N1	2.46	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:613:C:H2'	1:0:614:U:H6	1.79	0.48
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.32	0.48
1:0:1552:G:C6	1:0:1553:C:C4	3.01	0.48
1:0:1942:A:H3'	38:0:7336:HOH:O	2.12	0.48
1:0:2032:U:H2'	1:0:2033:G:C5'	2.44	0.48
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.93	0.48
3:A:200:PRO:HD3	38:A:8819:HOH:O	2.14	0.48
11:J:45:VAL:HG23	11:J:130:VAL:O	2.14	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.96	0.48
1:0:1217:G:C2	1:0:1218:U:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1921:A:O2'	1:0:1922:A:H5'	2.14	0.48
1:0:1842:A:C4	1:0:1979:G:C6	3.01	0.48
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.48
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.14	0.48
1:0:886:A:OP2	1:0:2113:G:H5'	2.14	0.48
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.42	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.43	0.48
1:0:2488:A:H2	38:0:7268:HOH:O	1.96	0.48
1:0:1044:C:H5"	38:0:9021:HOH:O	2.12	0.48
1:0:1789:G:O6	17:P:73:HIS:HE1	1.97	0.48
23:V:39:ALA:C	23:V:41:GLU:H	2.16	0.48
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.95	0.48
1:0:1747:A:C8	12:K:44:LEU:HD13	2.49	0.48
1:0:1573:A:N7	1:0:1574:C:C2	2.82	0.48
5:C:51:TYR:HA	5:C:54:LEU:HD12	1.96	0.48
1:0:1669:A:H2'	1:0:1670:G:C8	2.49	0.48
1:0:2070:G:H5"	38:0:3786:HOH:O	2.14	0.48
1:0:1587:U:H2'	1:0:1588:G:O4'	2.13	0.48
15:N:67:ALA:HA	15:N:71:TRP:CB	2.42	0.48
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.96	0.48
16:O:39:THR:O	16:O:115:ARG:NH2	2.47	0.48
6:D:51:ARG:HH11	6:D:68:PRO:HB3	1.79	0.48
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.48
2:9:3051:A:H5'	15:N:160:SER:HB3	1.96	0.48
1:0:629:A:H2'	1:0:630:A:O4'	2.14	0.48
1:0:664:U:O4	1:0:681:G:H5"	2.14	0.47
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.44	0.47
1:0:2044:G:OP1	25:X:23:HIS:HE1	1.97	0.47
1:0:324:G:O2'	1:0:325:U:H5'	2.14	0.47
1:0:2831:C:C2'	1:0:2832:C:H5'	2.44	0.47
1:0:2689:A:H2'	1:0:2690:U:H5'	1.96	0.47
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.95	0.47
25:X:66:THR:HG23	25:X:67:PRO:HD2	1.96	0.47
1:0:57:C:H5"	38:0:6753:HOH:O	2.14	0.47
1:0:2114:C:OP1	3:A:1:GLY:HA2	2.13	0.47
1:0:1188:A:C6	1:0:1189:A:C6	3.02	0.47
1:0:2765:C:H2'	1:0:2766:A:C8	2.49	0.47
1:0:1477:C:C5'	1:0:1868:G:H5"	2.43	0.47
1:0:941:G:C6	1:0:942:U:C4	3.02	0.47
28:1:25:LYS:HD2	29:2:48:ASP:HA	1.96	0.47
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.79	0.47
1:0:709:G:O2'	16:O:25:VAL:HG12	2.14	0.47
7:E:10:ASP:HA	38:E:6017:HOH:O	2.14	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.31	0.47
1:0:255:A:C8	1:0:256:C:C5	3.02	0.47
4:B:150:ALA:O	4:B:152:PRO:HD3	2.14	0.47
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.27	0.47
1:0:1398:G:H2'	1:0:1399:A:C8	2.49	0.47
1:0:2297:U:H1'	38:0:5179:HOH:O	2.13	0.47
1:0:2112:A:H2'	1:0:2113:G:C8	2.49	0.47
1:0:2330:U:H4'	1:0:2331:C:OP1	2.15	0.47
1:0:2802:C:H2'	1:0:2803:C:C6	2.50	0.47
1:0:1339:G:C6	1:0:1340:G:N1	2.82	0.47
1:0:264:G:H1'	1:0:265:U:H5	1.79	0.47
2:9:3049:G:H2'	2:9:3050:G:O4'	2.14	0.47
1:0:271:C:C2	1:0:273:G:O4'	2.67	0.47
1:0:293:A:C4	1:0:360:A:C2	3.03	0.47
2:9:3002:U:OP2	2:9:3002:U:H4'	2.15	0.47
21:T:73:HIS:CD2	21:T:88:PRO:HG3	2.49	0.47
1:0:155:C:OP2	14:M:188:ARG:HD3	2.13	0.47
1:0:106:A:O2'	1:0:107:U:H5'	2.14	0.47
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.14	0.47
38:0:9215:HOH:O	3:A:11:ARG:HD3	2.15	0.47
2:9:3114:G:O6	15:N:11:ARG:HD3	2.13	0.47
11:J:135:ILE:O	11:J:139:LEU:HG	2.15	0.47
1:0:1592:G:O2'	1:0:1593:C:O5'	2.33	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
13:L:143:THR:HG21	38:L:8836:HOH:O	2.14	0.47
30:3:3:MET:HG3	30:3:4:PRO:HD2	1.96	0.47
1:0:80:A:H3'	21:T:43:ASN:OD1	2.15	0.47
24:W:52:VAL:HG22	24:W:53:ALA:H	1.79	0.47
1:0:69:A:H8	1:0:69:A:C5'	2.25	0.47
26:Y:189:ASN:HD22	26:Y:192:ASP:H	1.63	0.47
1:0:2403:C:C2'	1:0:2404:G:O5'	2.62	0.47
1:0:1574:C:H2'	1:0:1575:C:C6	2.50	0.47
1:0:2115:U:H2'	1:0:2116:U:C6	2.49	0.47
1:0:1562:C:O2	1:0:1562:C:H2'	2.12	0.47
1:0:876:A:N3	1:0:876:A:H2'	2.29	0.47
1:0:247:A:H2'	38:0:3931:HOH:O	2.13	0.47
1:0:2026:C:O2'	1:0:2027:U:H5'	2.15	0.47
15:N:108:SER:HA	15:N:109:PRO:HD3	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1202:A:O2'	1:0:1203:G:H5'	2.14	0.47
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.97	0.47
24:W:90:TYR:CE2	24:W:99:ALA:HB2	2.50	0.47
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.45	0.47
1:0:2419:U:H5"	1:0:2420:G:H5'	1.97	0.47
1:0:2421:G:H3'	1:0:2422:U:H5"	1.97	0.47
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.47
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.15	0.47
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.47	0.47
2:9:3048:C:H4'	15:N:141:ARG:NH2	2.30	0.47
1:0:2615:U:C5	1:0:2616:G:C6	3.03	0.47
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.96	0.47
1:0:475:G:H5'	5:C:73:LEU:CD2	2.44	0.47
1:0:524:A:C5'	19:R:29:LYS:HE2	2.45	0.47
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.47
1:0:758:A:H2'	1:0:759:C:O4'	2.15	0.47
1:0:1079:A:H4'	1:0:2078:U:H5'	1.97	0.47
1:0:1069:C:C2'	1:0:1070:A:H5'	2.44	0.47
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.50	0.47
1:0:2371:G:H5'	38:0:5013:HOH:O	2.14	0.47
1:0:2274:A:O2'	1:0:2275:G:H5'	2.14	0.47
1:0:644:G:N3	1:0:644:G:H5'	2.30	0.47
1:0:729:C:C2	1:0:743:G:C2	3.03	0.47
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.97	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.15	0.47
1:0:2754:G:O2'	1:0:2755:G:H5'	2.15	0.47
14:M:65:VAL:HG21	14:M:105:ALA:HB2	1.97	0.47
16:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.47
10:H:2:PRO:HD2	10:H:5:MET:SD	2.55	0.47
1:0:951:A:H2'	1:0:952:G:H5'	1.96	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.47
28:1:28:HIS:HD2	28:1:30:LYS:H	1.61	0.47
22:U:33:SER:O	22:U:37:GLU:HG3	2.14	0.47
1:0:1746:A:O4'	1:0:1747:A:C2	2.67	0.47
26:Y:117:LEU:HD12	26:Y:174:VAL:HG11	1.97	0.47
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.79	0.47
1:0:920:C:H5'	1:0:921:G:C4	2.50	0.47
3:A:17:ARG:HD2	38:A:8836:HOH:O	2.13	0.47
1:0:2111:G:H1'	38:0:9044:HOH:O	2.14	0.47
1:0:1731:C:H1'	38:0:6446:HOH:O	2.14	0.47
1:0:1114:A:O2'	1:0:1115:U:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1593:C:OP1	17:P:117:SER:HB3	2.15	0.47
1:0:2768:A:C2'	1:0:2769:C:O4'	2.61	0.47
1:0:2502:C:H2'	1:0:2503:A:C5'	2.43	0.47
1:0:2468:A:H4'	38:0:3550:HOH:O	2.14	0.47
1:0:1268:C:O2'	1:0:1269:G:H5'	2.14	0.47
2:9:3047:A:C2	2:9:3048:C:C2	3.03	0.47
1:0:329:A:C5	1:0:347:A:C2	3.03	0.47
1:0:524:A:H5'	19:R:29:LYS:HE2	1.97	0.47
1:0:1921:A:C6	1:0:1922:A:C2	3.03	0.47
1:0:2274:A:H1'	14:M:86:GLN:NE2	2.30	0.47
1:0:1013:A:H1'	38:0:9156:HOH:O	2.15	0.47
38:0:6273:HOH:O	17:P:59:ARG:HD3	2.15	0.47
1:0:2244:A:H1'	38:M:8866:HOH:O	2.14	0.47
38:0:6996:HOH:O	18:Q:9:GLY:HA2	2.15	0.47
1:0:905:C:H3'	38:0:5188:HOH:O	2.15	0.47
24:W:149:LEU:HG	24:W:153:MET:CE	2.45	0.47
3:A:109:GLU:HG2	3:A:116:GLY:H	1.79	0.47
1:0:1878:G:H5'	38:0:4380:HOH:O	2.15	0.47
6:D:135:VAL:HG22	6:D:136:ARG:N	2.29	0.47
1:0:1015:C:O5'	1:0:1015:C:H6	1.98	0.47
1:0:1857:A:N6	1:0:2247:C:H1'	2.30	0.47
8:F:34:ASN:HA	14:M:4:ALA:HB2	1.97	0.47
1:0:312:U:C2	1:0:320:G:N2	2.83	0.47
7:E:37:ASP:OD1	11:J:125:SER:HB3	2.15	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
3:A:215:ILE:HG13	3:A:216:SER:N	2.30	0.47
1:0:377:C:H5	38:0:3309:HOH:O	1.98	0.47
21:T:71:VAL:HG13	21:T:91:LEU:O	2.15	0.46
1:0:559:U:H3'	1:0:559:U:C6	2.51	0.46
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.46
1:0:2255:A:C6	1:0:2256:G:C5	3.03	0.46
18:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.15	0.46
1:0:513:A:N3	38:0:3663:HOH:O	2.36	0.46
1:0:2047:C:H2'	1:0:2048:C:H6	1.80	0.46
26:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.48	0.46
1:0:851:C:H5	38:0:6802:HOH:O	1.96	0.46
24:W:38:THR:HG22	24:W:39:ASP:N	2.30	0.46
1:0:2063:U:O4	1:0:2083:A:H2	1.98	0.46
1:0:1773:G:N2	1:0:1774:G:C8	2.83	0.46
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.46
2:9:3097:U:H2'	2:9:3098:C:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:812:A:H1'	38:0:3966:HOH:O	2.14	0.46
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.97	0.46
32:0:9000:13T:C23	32:0:9000:13T:H311	2.46	0.46
1:0:1183:C:C2	1:0:1184:C:C5	3.03	0.46
2:9:3028:U:H2'	2:9:3029:C:C6	2.50	0.46
1:0:2255:A:C2	1:0:2256:G:C4	3.03	0.46
1:0:31:C:H4'	38:0:7414:HOH:O	2.16	0.46
1:0:111:C:O2'	1:0:112:G:H5'	2.16	0.46
1:0:1447:U:H3'	1:0:1506:U:O2	2.15	0.46
1:0:1838:U:O2'	1:0:2644:C:H5'	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.16	0.46
1:0:1207:A:N6	38:0:5644:HOH:O	2.48	0.46
1:0:1878:G:O2'	1:0:1879:U:C5	2.65	0.46
1:0:2764:C:H1'	38:0:7458:HOH:O	2.16	0.46
1:0:1523:G:C6	1:0:1524:U:O4	2.67	0.46
1:0:694:A:C2'	1:0:695:C:H5'	2.43	0.46
1:0:1198:U:C6	1:0:1200:A:OP2	2.68	0.46
1:0:1211:G:H2'	1:0:1212:C:C6	2.47	0.46
1:0:2269:C:H2'	1:0:2270:G:C5'	2.46	0.46
3:A:126:ALA:HB1	3:A:138:VAL:CG1	2.45	0.46
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.46
8:F:111:ILE:O	8:F:115:VAL:HG23	2.15	0.46
1:0:1913:C:H2'	1:0:1914:C:H6	1.80	0.46
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.48	0.46
1:0:2459:G:C2'	32:0:9000:13T:C23	2.94	0.46
1:0:559:U:H2'	1:0:560:C:O4'	2.14	0.46
1:0:704:C:H2'	1:0:705:C:H6	1.81	0.46
1:0:1931:A:C2'	1:0:1932:G:H5'	2.45	0.46
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.31	0.46
1:0:1913:C:H2'	1:0:1914:C:C6	2.50	0.46
1:0:843:A:C2	1:0:846:A:C8	3.04	0.46
16:O:105:ASN:HD21	16:O:109:SER:H	1.62	0.46
31:I:100:LEU:HD22	31:I:105:VAL:CG2	2.46	0.46
1:0:2459:G:H2'	32:0:9000:13T:H232	1.98	0.46
1:0:1204:C:H2'	1:0:1205:U:O4'	2.16	0.46
1:0:317:A:OP1	21:T:52:ARG:O	2.33	0.46
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.46
15:N:65:ASP:HB3	38:N:8821:HOH:O	2.14	0.46
1:0:2821:C:H2'	1:0:2822:C:H6	1.80	0.46
3:A:3:ARG:H	3:A:3:ARG:HG2	1.55	0.46
3:A:179:MET:HG2	3:A:186:TRP:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:183:THR:HG22	14:M:194:ALA:HB1	1.96	0.46
1:0:39:G:C2	1:0:444:C:C2	3.04	0.46
1:0:1173:A:H3'	38:0:4360:HOH:O	2.16	0.46
1:0:2114:C:O2'	1:0:2115:U:H5'	2.16	0.46
1:0:2332:A:H3'	1:0:2333:G:H8	1.80	0.46
1:0:1619:G:C5	1:0:1620:C:C4	3.03	0.46
22:U:13:ILE:HG12	22:U:32:CYS:HB3	1.97	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.98	0.46
1:0:281:U:C2'	1:0:282:C:H5'	2.46	0.46
19:R:39:THR:HG23	19:R:107:GLU:O	2.16	0.46
1:0:1850:U:H2'	1:0:1851:G:C8	2.50	0.46
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.98	0.46
1:0:857:A:H4'	3:A:176:HIS:CD2	2.51	0.46
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.96	0.46
6:D:10:PHE:CG	6:D:11:HIS:N	2.84	0.46
3:A:36:ASP:O	3:A:38:ILE:N	2.49	0.46
1:0:1684:A:O2'	1:0:1685:A:H5"	2.15	0.46
13:L:56:LYS:NZ	38:L:8873:HOH:O	2.49	0.46
22:U:52:THR:HG22	22:U:54:THR:N	2.31	0.46
1:0:475:G:H5'	5:C:73:LEU:HD23	1.96	0.46
31:I:78:LEU:HD12	31:I:112:LYS:HZ2	1.79	0.46
1:0:2121:G:O2'	1:0:2122:C:H5'	2.16	0.46
1:0:2729:C:O2'	1:0:2730:G:H5'	2.15	0.46
26:Y:216:ARG:HD2	38:Y:8868:HOH:O	2.14	0.46
26:Y:184:GLU:OE2	26:Y:204:ARG:HD2	2.15	0.46
1:0:1218:U:H2'	1:0:1219:U:C6	2.51	0.46
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.46
1:0:2263:G:H1'	38:0:6618:HOH:O	2.16	0.46
1:0:1182:C:O2'	1:0:1183:C:H5	1.99	0.46
1:0:1166:A:H1'	1:0:1192:A:C2	2.50	0.46
20:S:57:THR:CG2	20:S:59:ASP:HB2	2.45	0.46
14:M:134:ILE:CG2	14:M:141:ILE:HD13	2.43	0.46
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.45	0.46
7:E:69:ILE:HA	7:E:72:MET:HE3	1.98	0.46
1:0:2672:C:H1'	38:B:8930:HOH:O	2.15	0.46
1:0:17:G:H2'	1:0:18:C:H6	1.81	0.46
10:H:170:ASN:N	10:H:170:ASN:ND2	2.64	0.46
6:D:51:ARG:NH1	6:D:68:PRO:HB3	2.31	0.46
8:F:107:ASP:O	8:F:111:ILE:HG13	2.15	0.46
1:0:101:C:H2'	1:0:102:A:C8	2.51	0.46
1:0:113:A:H2'	1:0:115:U:O4	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:7403:HOH:O	31:I:90:GLY:HA2	2.16	0.46
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.98	0.46
1:0:2549:C:H4'	38:0:7504:HOH:O	2.16	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
11:J:26:VAL:HG13	11:J:36:VAL:HG11	1.98	0.46
1:0:2050:G:H5"	19:R:80:TYR:O	2.16	0.46
1:0:189:A:OP1	14:M:171:ARG:NH2	2.49	0.45
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.97	0.45
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.98	0.45
1:0:2253:G:O2'	1:0:2254:G:H5'	2.16	0.45
1:0:583:G:H2'	1:0:584:U:C6	2.51	0.45
11:J:45:VAL:HG22	11:J:46:ILE:N	2.30	0.45
2:9:3107:C:H2'	2:9:3108:C:C6	2.51	0.45
1:0:2000:G:O2'	1:0:2001:G:H5'	2.16	0.45
10:H:1:LYS:HA	10:H:2:PRO:HD3	1.73	0.45
1:0:2730:G:O2'	1:0:2731:G:H5'	2.15	0.45
1:0:1583:U:H1'	38:0:9979:HOH:O	2.15	0.45
20:S:77:VAL:O	20:S:80:ARG:HG2	2.17	0.45
1:0:1741:U:C4	1:0:2033:G:C8	3.04	0.45
1:0:2570:G:H8	38:0:4917:HOH:O	2.00	0.45
16:O:32:ARG:HB2	38:O:4656:HOH:O	2.17	0.45
1:0:2092:G:H5"	1:0:2613:G:OP1	2.15	0.45
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.45
1:0:2820:A:H2'	1:0:2821:C:O4'	2.17	0.45
1:0:939:A:H5'	38:0:5419:HOH:O	2.16	0.45
23:V:7:GLU:O	23:V:11:MET:HG3	2.15	0.45
1:0:1127:C:C5	1:0:1128:U:C4	3.04	0.45
10:H:95:LEU:HD11	10:H:124:ALA:HB2	1.99	0.45
26:Y:220:GLU:HG3	38:Y:8849:HOH:O	2.16	0.45
1:0:1321:A:H2'	1:0:1322:G:C8	2.51	0.45
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.51	0.45
27:Z:56:GLN:HA	27:Z:62:TYR:O	2.16	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.82	0.45
1:0:365:G:C6	1:0:366:U:C4	3.04	0.45
1:0:706:G:O2'	1:0:707:C:H6	1.99	0.45
1:0:814:G:N2	1:0:815:U:H1'	2.31	0.45
23:V:39:ALA:N	23:V:40:PRO:CD	2.80	0.45
29:2:20:ARG:HB3	38:2:5444:HOH:O	2.17	0.45
1:0:512:G:O3'	1:0:513:A:C8	2.69	0.45
2:9:3107:C:C5	38:9:3167:HOH:O	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1855:G:H8	3:A:144:GLU:OE2	1.99	0.45
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.98	0.45
17:P:83:LYS:O	17:P:86:ALA:HB3	2.16	0.45
1:0:2831:C:H2'	1:0:2832:C:C5'	2.46	0.45
1:0:920:C:H5"	1:0:921:G:O5'	2.17	0.45
1:0:419:A:H1'	1:0:1921:A:C2	2.51	0.45
23:V:45:ARG:HH11	23:V:45:ARG:HG3	1.82	0.45
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.52	0.45
1:0:2314:G:C2'	1:0:2315:C:H5'	2.46	0.45
1:0:2582:G:H5"	4:B:3:PRO:HB3	1.98	0.45
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.16	0.45
1:0:1588:G:C5	1:0:1589:G:C6	3.05	0.45
1:0:1477:C:H5'	1:0:1868:G:H5"	1.97	0.45
1:0:2237:G:O2'	1:0:2238:A:C8	2.69	0.45
1:0:2428:G:N7	30:3:60:LYS:NZ	2.61	0.45
1:0:229:G:O2'	1:0:230:C:H5'	2.16	0.45
1:0:2105:C:H2'	1:0:2106:C:C6	2.52	0.45
26:Y:130:ARG:HB2	26:Y:142:SER:O	2.16	0.45
1:0:2649:A:C8	1:0:2649:A:H5'	2.52	0.45
1:0:200:U:H2'	38:0:3446:HOH:O	2.15	0.45
3:A:82:VAL:HG13	3:A:93:THR:HB	1.98	0.45
1:0:51:G:O2'	1:0:52:A:H5'	2.16	0.45
4:B:162:MET:CE	4:B:310:ARG:HD3	2.47	0.45
1:0:407:A:H5'	38:0:6034:HOH:O	2.15	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.81	0.45
2:9:3008:G:O6	15:N:11:ARG:NH1	2.39	0.45
3:A:109:GLU:HG2	3:A:116:GLY:N	2.31	0.45
1:0:2864:U:C5	1:0:2865:G:C6	3.04	0.45
38:0:9988:HOH:O	13:L:22:ARG:HG2	2.15	0.45
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.45
2:9:3026:C:O2'	2:9:3027:C:H5'	2.17	0.45
1:0:2016:U:H2'	1:0:2017:U:C6	2.51	0.45
25:X:76:ARG:NH1	25:X:76:ARG:HG3	2.28	0.45
25:X:76:ARG:HH11	25:X:76:ARG:CG	2.28	0.45
26:Y:117:LEU:HA	26:Y:174:VAL:HG11	1.98	0.45
1:0:1730:G:H4'	1:0:1731:C:H6	1.82	0.45
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.51	0.45
1:0:453:A:H4'	1:0:455:A:N7	2.32	0.45
1:0:1164:U:OP1	31:I:74:PRO:HA	2.17	0.45
1:0:560:C:H2'	1:0:561:G:H8	1.82	0.45
1:0:2110:G:C2	1:0:2478:U:C2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:111:C:C2'	1:0:112:G:H5'	2.47	0.45
1:0:1544:U:O2'	1:0:1545:C:H5'	2.17	0.45
1:0:1771:U:O2'	1:0:1773:G:N7	2.48	0.45
1:0:2326:U:H4'	1:0:2412:G:C4'	2.46	0.45
1:0:2891:A:C2	1:0:2892:G:C4	3.05	0.45
1:0:2772:G:O2'	1:0:2773:G:H5'	2.16	0.45
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
1:0:289:G:N1	1:0:363:A:C2	2.81	0.45
15:N:110:THR:HB	15:N:113:SER:OG	2.17	0.45
1:0:1940:C:H4'	38:0:7336:HOH:O	2.17	0.45
1:0:2073:G:OP2	1:0:2490:A:H5'	2.16	0.45
1:0:1973:A:H5'	1:0:1973:A:C8	2.45	0.45
1:0:696:C:O2'	1:0:731:U:OP1	2.33	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45
7:E:15:GLN:HG2	7:E:19:ASP:O	2.17	0.45
13:L:143:THR:HG22	13:L:144:ASP:H	1.81	0.45
30:3:69:TYR:O	30:3:77:ALA:HA	2.16	0.45
1:0:1682:A:O2'	1:0:1683:G:H5"	2.17	0.45
24:W:5:VAL:HG11	24:W:153:MET:CE	2.47	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.16	0.45
1:0:244:C:OP2	8:F:38:LYS:HE3	2.17	0.45
1:0:1123:A:N1	1:0:1238:C:H5'	2.32	0.45
1:0:1150:A:C2	9:G:20:VAL:HG21	2.52	0.45
1:0:1252:A:H2'	1:0:1253:C:O4'	2.17	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.32	0.45
1:0:542:A:C5'	1:0:542:A:C8	2.95	0.45
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.45
1:0:292:G:H1'	1:0:360:A:H61	1.81	0.45
5:C:2:GLN:HB3	38:C:8582:HOH:O	2.15	0.45
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.45
1:0:2075:G:C6	1:0:2076:U:C4	3.05	0.45
1:0:2906:A:H5'	1:0:2907:C:O4'	2.17	0.45
1:0:1076:G:C2	1:0:1084:C:C2	3.05	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
5:C:236:THR:HG22	5:C:239:ALA:CB	2.47	0.45
24:W:139:GLY:O	24:W:141:HIS:CD2	2.70	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.98	0.45
1:0:670:G:H2'	1:0:671:A:C8	2.52	0.45
1:0:926:A:O2'	13:L:41:HIS:HD2	2.00	0.45
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1238:C:H5"	1:0:1239:G:OP2	2.17	0.45
1:0:488:U:O2'	21:T:82:THR:HG21	2.17	0.45
17:P:9:LEU:O	17:P:13:VAL:HG23	2.17	0.45
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.44
1:0:538:C:N4	1:0:2061:C:H1'	2.32	0.44
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:660:A:N6	1:0:746:A:O4'	2.50	0.44
22:U:52:THR:HG22	22:U:54:THR:HB	1.98	0.44
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.44
1:0:2346:C:O2'	6:D:52:THR:HG21	2.17	0.44
18:Q:75:ILE:CD1	18:Q:84:ILE:HD11	2.47	0.44
1:0:1279:U:H2'	1:0:1279:U:O2	2.17	0.44
1:0:2354:A:C2	1:0:2367:A:C8	3.04	0.44
26:Y:235:GLU:CD	26:Y:235:GLU:H	2.21	0.44
1:0:2594:C:O2'	1:0:2595:U:H5'	2.17	0.44
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.17	0.44
11:J:53:ILE:O	11:J:57:TYR:HD1	2.00	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.17	0.44
15:N:179:LEU:HD23	15:N:184:ILE:CD1	2.47	0.44
25:X:78:GLU:HG2	25:X:79:GLU:H	1.82	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.18	0.44
11:J:45:VAL:CG2	11:J:129:PHE:HD1	2.30	0.44
2:9:3058:G:H1'	38:9:3839:HOH:O	2.16	0.44
1:0:1494:A:O2'	1:0:1505:U:O2	2.34	0.44
3:A:107:ASN:OD1	3:A:116:GLY:HA3	2.17	0.44
2:9:3097:U:H2'	2:9:3098:C:C6	2.51	0.44
1:0:957:A:O5'	1:0:957:A:H8	2.00	0.44
1:0:2719:A:C2	4:B:70:PRO:HG3	2.52	0.44
26:Y:151:SER:HB3	26:Y:154:ARG:HB3	2.00	0.44
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.98	0.44
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.52	0.44
1:0:536:A:H3'	38:0:5051:HOH:O	2.16	0.44
4:B:60:SER:HA	4:B:61:PRO:HD3	1.85	0.44
1:0:2716:G:O2'	1:0:2717:C:H5'	2.18	0.44
1:0:1244:U:H4'	1:0:1246:A:O4'	2.17	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.44
1:0:1972:U:C2'	1:0:1973:A:C5'	2.96	0.44
1:0:1269:G:H2'	1:0:1270:U:C6	2.53	0.44
1:0:2133:U:H4'	1:0:2134:G:C5'	2.47	0.44
1:0:111:C:H2'	1:0:112:G:C5'	2.46	0.44
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.52	0.44
1:0:1334:C:O2'	1:0:1335:C:H5'	2.18	0.44
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.44
1:0:2900:G:C2'	1:0:2901:C:H5'	2.47	0.44
15:N:154:LEU:C	15:N:156:GLU:H	2.20	0.44
14:M:15:PRO:HA	14:M:20:LEU:HD23	2.00	0.44
1:0:263:U:C2	8:F:59:ILE:CD1	3.01	0.44
1:0:697:G:H4'	1:0:730:G:O3'	2.17	0.44
4:B:307:ARG:HA	38:B:8850:HOH:O	2.17	0.44
1:0:2256:G:H2'	1:0:2257:G:O5'	2.17	0.44
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.85	0.44
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.15	0.44
1:0:2610:U:H4'	38:0:9479:HOH:O	2.18	0.44
5:C:34:ALA:HB3	5:C:220:THR:HG21	2.00	0.44
1:0:1667:A:H8	1:0:1667:A:C5'	2.18	0.44
1:0:710:G:N2	1:0:719:C:C2	2.86	0.44
4:B:144:THR:HB	38:B:8921:HOH:O	2.18	0.44
1:0:1309:U:C4	1:0:1310:U:C5	3.06	0.44
1:0:1748:U:C5	1:0:1749:U:C4	3.06	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.18	0.44
1:0:2846:C:H4'	4:B:156:LYS:HB3	1.98	0.44
1:0:1117:A:C2	1:0:1244:U:C2	3.06	0.44
32:0:9000:13T:H323	32:0:9000:13T:O2	2.18	0.44
1:0:1602:C:OP2	27:Z:46:ARG:NH2	2.51	0.44
1:0:1523:G:H2'	1:0:1524:U:C6	2.53	0.44
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.97	0.44
12:K:14:LYS:CB	12:K:45:PRO:HG2	2.46	0.44
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.44
1:0:538:C:H5"	1:0:539:G:C8	2.53	0.44
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.18	0.44
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.51	0.44
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.44
23:V:45:ARG:NH1	23:V:45:ARG:HG3	2.32	0.44
1:0:2504:A:H4'	10:H:71:ARG:HH11	1.83	0.44
4:B:199:TYR:CE2	4:B:268:ARG:HB2	2.53	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.98	0.44
7:E:132:THR:HB	38:E:2227:HOH:O	2.17	0.44
1:0:929:A:O5'	1:0:929:A:H8	2.01	0.44
1:0:2432:C:H1'	32:0:9000:13T:O9	2.17	0.44
24:W:90:TYR:N	24:W:90:TYR:CD1	2.85	0.44
5:C:129:HIS:CE1	5:C:232:LEU:H	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1419:U:H2'	1:0:1685:A:C2	2.53	0.44
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.17	0.44
24:W:13:MET:CE	24:W:17:ILE:HG22	2.48	0.44
4:B:321:PRO:HA	38:B:8952:HOH:O	2.16	0.44
1:0:500:G:H21	19:R:98:ASN:ND2	2.13	0.44
38:0:7396:HOH:O	21:T:2:LYS:HE2	2.17	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.52	0.44
1:0:622:G:P	26:Y:148:GLY:HA3	2.58	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
1:0:920:C:H4'	1:0:921:G:N2	2.32	0.44
1:0:2802:C:H2'	1:0:2803:C:H6	1.81	0.44
1:0:1069:C:O2'	1:0:1070:A:H5'	2.18	0.44
1:0:1730:G:H4'	1:0:1731:C:C6	2.53	0.44
1:0:1773:G:C8	27:Z:16:ALA:HA	2.53	0.44
1:0:2899:A:O2'	1:0:2900:G:H5'	2.18	0.44
1:0:1280:A:H3'	1:0:1280:A:OP1	2.18	0.44
1:0:413:G:H2'	1:0:414:C:C6	2.52	0.44
15:N:171:HIS:CE1	38:N:8862:HOH:O	2.71	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.44
1:0:2577:A:H5'	38:0:7734:HOH:O	2.17	0.44
1:0:637:C:H2'	1:0:638:C:C6	2.52	0.44
2:9:3039:U:H3	2:9:3042:C:H5"	1.83	0.44
1:0:307:G:C2	1:0:309:C:C4	3.05	0.44
1:0:821:U:H4'	27:Z:17:ARG:NH1	2.33	0.44
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.99	0.44
1:0:2385:G:H2'	1:0:2386:U:H6	1.79	0.44
1:0:1236:A:C8	11:J:63:ILE:HD11	2.53	0.44
1:0:303:C:O2'	1:0:304:G:H5'	2.18	0.44
1:0:2691:A:OP1	1:0:2691:A:H8	2.01	0.44
1:0:276:C:O5'	1:0:276:C:H6	2.01	0.44
4:B:185:GLY:HA2	38:B:8929:HOH:O	2.17	0.44
1:0:238:C:H4'	1:0:287:C:OP1	2.18	0.44
1:0:1191:A:H2'	1:0:1193:A:H5'	2.00	0.43
1:0:1205:U:C2'	1:0:1206:U:C5'	2.87	0.43
1:0:1159:G:H1	1:0:1208:C:H42	1.64	0.43
1:0:1761:U:H5'	17:P:81:LYS:O	2.18	0.43
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
27:Z:36:ASP:HB3	27:Z:45:ASP:HB3	1.99	0.43
1:0:1183:C:H42	1:0:1184:C:N4	2.12	0.43
1:0:338:C:H4'	5:C:174:ILE:HD12	1.98	0.43
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:303:C:H2'	1:0:304:G:O4'	2.18	0.43
5:C:51:TYR:CE2	28:1:53:LYS:HB3	2.53	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.43
1:0:2821:C:H4'	4:B:116:PRO:HG3	2.00	0.43
1:0:2850:C:H6	1:0:2850:C:H5'	1.83	0.43
1:0:1215:A:O3'	1:0:1216:G:C4'	2.66	0.43
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.43
1:0:2101:A:H2'	5:C:63:SER:OG	2.18	0.43
1:0:37:A:H2'	1:0:38:G:C8	2.52	0.43
1:0:1829:A:H5"	38:0:3081:HOH:O	2.17	0.43
32:0:9000:13T:C26	32:0:9000:13T:H2	2.42	0.43
1:0:1377:C:C5'	1:0:1377:C:H6	2.28	0.43
38:0:7442:HOH:O	4:B:211:THR:HG21	2.19	0.43
1:0:2089:A:O2'	1:0:2090:G:H5'	2.18	0.43
1:0:1624:A:H5'	1:0:1626:A:O4'	2.17	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.19	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.00	0.43
1:0:1118:A:N6	1:0:1244:U:C2	2.86	0.43
5:C:115:LEU:HA	5:C:115:LEU:HD12	1.87	0.43
1:0:1343:C:H2'	1:0:1344:G:O5'	2.19	0.43
1:0:2252:A:C6	1:0:2253:G:H1'	2.54	0.43
12:K:34:VAL:HG21	12:K:46:LYS:O	2.19	0.43
8:F:101:ALA:HA	38:F:5413:HOH:O	2.18	0.43
1:0:2002:C:H2'	1:0:2003:U:H5'	2.00	0.43
1:0:304:G:H1'	1:0:347:A:H61	1.83	0.43
7:E:22:VAL:O	7:E:76:VAL:HG11	2.18	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.01	0.43
6:D:170:TYR:O	6:D:171:ASP:HB3	2.18	0.43
1:0:772:G:H2'	1:0:773:A:O4'	2.17	0.43
1:0:99:A:C8	1:0:100:C:C5	3.06	0.43
1:0:1409:G:C2	1:0:1410:G:C8	3.06	0.43
20:S:33:SER:O	20:S:37:VAL:HG23	2.18	0.43
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.34	0.43
12:K:132:VAL:HG21	22:U:22:VAL:HG11	2.00	0.43
1:0:1903:U:O2'	1:0:1904:A:N7	2.49	0.43
27:Z:30:GLU:HG2	27:Z:33:MET:HE2	1.99	0.43
6:D:49:PRO:HA	6:D:73:VAL:HG22	2.01	0.43
7:E:80:TRP:O	7:E:134:SER:HA	2.17	0.43
1:0:137:U:H2'	1:0:139:C:C5	2.53	0.43
15:N:7:LYS:HE3	18:Q:21:ARG:O	2.19	0.43
19:R:132:ARG:HG2	19:R:133:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:187:A:H3'	1:0:188:C:H6	1.83	0.43
1:0:2786:G:H2'	38:0:7180:HOH:O	2.17	0.43
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.43
5:C:193:LEU:HD13	5:C:222:ASP:HB2	2.00	0.43
1:0:242:A:N6	1:0:269:G:H1'	2.34	0.43
5:C:185:LYS:HD3	5:C:186:TYR:CE1	2.53	0.43
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.43
1:0:1183:C:O2	1:0:1183:C:C2'	2.67	0.43
1:0:1186:C:H5"	31:I:119:TYR:CE1	2.53	0.43
1:0:2812:A:H2	1:0:2814:A:N6	1.91	0.43
24:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
1:0:69:A:C8	1:0:69:A:C5'	2.95	0.43
1:0:2779:G:N2	1:0:2796:U:C2	2.87	0.43
1:0:1130:U:H4'	38:0:6133:HOH:O	2.18	0.43
1:0:2840:A:OP1	4:B:211:THR:HG23	2.19	0.43
1:0:645:U:H2'	1:0:646:G:C8	2.54	0.43
8:F:56:PRO:CG	14:M:44:THR:HA	2.48	0.43
4:B:4:SER:O	4:B:5:ARG:HB2	2.19	0.43
9:G:20:VAL:O	9:G:24:VAL:HG23	2.19	0.43
4:B:88:GLU:HG3	4:B:88:GLU:O	2.18	0.43
1:0:1439:C:H6	1:0:1439:C:O5'	2.01	0.43
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.43
1:0:2460:A:C4	32:0:9000:13T:H20	2.53	0.43
1:0:365:G:C5	1:0:366:U:C5	3.07	0.43
1:0:947:U:O2'	1:0:948:G:H5'	2.18	0.43
11:J:47:THR:HG22	11:J:48:GLY:N	2.34	0.43
1:0:1778:A:H2'	1:0:1779:A:H5'	2.00	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
1:0:1215:A:O3'	1:0:1216:G:H4'	2.19	0.43
1:0:1904:A:H2'	1:0:1905:U:O4'	2.19	0.43
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.34	0.43
24:W:106:THR:OG1	24:W:109:GLU:HB2	2.19	0.43
1:0:1386:G:O2'	1:0:1387:G:H5'	2.19	0.43
1:0:1257:C:O2'	1:0:1258:G:H5'	2.18	0.43
14:M:46:LEU:HG	38:M:8913:HOH:O	2.18	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
1:0:1883:U:H5'	1:0:2012:U:OP2	2.19	0.43
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.43
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:2856:A:OP1	25:X:15:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:127:ILE:CG2	36:J:8801:CL:CL	3.00	0.43
2:9:3069:U:OP1	15:N:4:PRO:HG3	2.18	0.43
1:0:2036:C:C4'	12:K:44:LEU:HG	2.48	0.43
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.54	0.43
1:0:1850:U:O4'	1:0:1941:A:C2	2.71	0.43
1:0:445:U:O2'	1:0:446:G:H5'	2.18	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
1:0:1565:C:O2'	1:0:1566:C:H5'	2.19	0.43
31:I:125:ALA:O	31:I:129:VAL:HG23	2.19	0.43
38:0:6721:HOH:O	18:Q:2:SER:HA	2.19	0.43
38:0:9208:HOH:O	4:B:248:ARG:NH2	2.51	0.43
1:0:1434:A:H2'	1:0:1436:C:C5	2.53	0.43
4:B:33:ASP:HB3	4:B:34:GLY:H	1.60	0.43
1:0:1415:G:H5'	28:1:12:ASN:O	2.18	0.43
32:0:9000:13T:H3	30:3:56:PRO:CB	2.48	0.43
1:0:1191:A:H2	1:0:1206:U:H3	1.67	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:0:2254:G:C2	1:0:2255:A:C8	3.06	0.43
7:E:20:ILE:HD11	7:E:40:VAL:HG11	2.01	0.43
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.49	0.43
12:K:125:ALA:C	12:K:127:ALA:H	2.22	0.43
1:0:228:C:C2'	1:0:229:G:H5'	2.49	0.43
1:0:2372:A:H2'	1:0:2373:U:H6	1.82	0.43
24:W:5:VAL:HG11	24:W:153:MET:HE3	1.99	0.43
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.43
1:0:134:U:C2	1:0:145:A:C2	3.07	0.43
6:D:138:GLY:N	38:D:7597:HOH:O	2.51	0.43
1:0:1825:U:O2'	1:0:1826:C:H5'	2.19	0.43
1:0:1667:A:C2	1:0:1668:U:C2	3.07	0.43
1:0:1114:A:H2'	1:0:1115:U:C6	2.54	0.43
1:0:1163:G:H1	1:0:1184:C:N4	2.17	0.43
29:2:40:ARG:HG3	29:2:45:ASN:CB	2.48	0.43
24:W:4:LEU:O	24:W:32:CYS:HA	2.18	0.43
22:U:17:THR:HG22	22:U:18:GLY:N	2.34	0.43
1:0:1080:C:O5'	1:0:1080:C:H6	2.02	0.43
1:0:2255:A:O2'	1:0:2256:G:H5'	2.18	0.43
1:0:2255:A:H2'	1:0:2256:G:O4'	2.18	0.43
1:0:815:U:O2'	1:0:1598:A:H4'	2.18	0.43
11:J:45:VAL:HG21	11:J:129:PHE:HD1	1.82	0.43
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.52	0.43
26:Y:107:PRO:HD3	26:Y:182:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.43
1:0:73:C:O2'	1:0:74:A:H5'	2.18	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.34	0.43
1:0:2348:C:H1'	6:D:131:THR:HG21	2.01	0.43
14:M:80:GLY:O	14:M:81:ARG:HD3	2.18	0.43
4:B:177:HIS:O	4:B:181:ILE:HG13	2.19	0.43
1:0:1805:G:H2'	1:0:1806:G:H8	1.83	0.43
1:0:1242:A:OP2	11:J:60:ARG:NH2	2.47	0.42
32:0:9000:13T:H233	32:0:9000:13T:H311	2.01	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.42
6:D:103:ASN:HD22	6:D:133:ASN:HA	1.84	0.42
1:0:2291:A:H8	38:0:6467:HOH:O	2.01	0.42
1:0:559:U:C5	1:0:560:C:C5	3.07	0.42
1:0:2712:G:H5'	38:0:5223:HOH:O	2.18	0.42
5:C:194:PHE:HA	5:C:234:VAL:HG13	2.01	0.42
38:0:6400:HOH:O	24:W:122:ARG:NH2	2.45	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
1:0:1930:A:H2'	1:0:1931:A:C8	2.54	0.42
28:1:53:LYS:HD3	28:1:53:LYS:HA	1.85	0.42
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.34	0.42
1:0:2504:A:H4'	10:H:71:ARG:NH1	2.34	0.42
1:0:571:C:O5'	1:0:571:C:H6	2.01	0.42
1:0:2519:C:O2'	1:0:2520:G:H5'	2.19	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:169:A:H1'	30:3:48:ASN:ND2	2.34	0.42
2:9:3041:C:C2	6:D:50:VAL:HG21	2.54	0.42
6:D:44:ILE:HG23	6:D:45:THR:HG23	2.00	0.42
1:0:952:G:OP1	18:Q:42:LYS:HE2	2.20	0.42
21:T:28:SER:O	21:T:32:ARG:HG3	2.18	0.42
10:H:47:ILE:HG21	38:H:8579:HOH:O	2.20	0.42
1:0:1552:G:H2'	1:0:1553:C:C6	2.54	0.42
16:O:105:ASN:HD21	16:O:109:SER:N	2.18	0.42
16:O:21:SER:OG	16:O:106:PRO:HB2	2.18	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
1:0:1138:G:H4'	38:0:5719:HOH:O	2.19	0.42
26:Y:178:HIS:CG	26:Y:179:PRO:HD2	2.54	0.42
19:R:4:TYR:CE1	19:R:15:LYS:HD3	2.53	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.42
1:0:284:C:C4'	1:0:285:A:O5'	2.64	0.42
25:X:30:MET:HE1	25:X:55:ASN:HA	2.00	0.42
1:0:1544:U:H2'	1:0:1545:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:151:A:H2'	1:0:152:A:O4'	2.18	0.42
4:B:165:ARG:HG2	4:B:166:VAL:N	2.35	0.42
1:0:644:G:O2'	36:0:8814:CL:CL	2.67	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
20:S:37:VAL:O	20:S:41:VAL:HG23	2.19	0.42
1:0:2785:C:H4'	1:0:2786:G:OP2	2.19	0.42
4:B:204:GLY:HA3	38:B:8948:HOH:O	2.18	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.35	0.42
1:0:2608:C:H3'	38:0:7790:HOH:O	2.18	0.42
38:0:4740:HOH:O	15:N:21:HIS:HD2	2.01	0.42
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.19	0.42
14:M:167:GLY:O	14:M:171:ARG:HG3	2.19	0.42
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.42
2:9:3001:U:H4'	2:9:3003:A:OP1	2.19	0.42
1:0:2296:C:H2'	1:0:2297:U:H6	1.82	0.42
22:U:6:CYS:HB2	22:U:32:CYS:HB3	2.00	0.42
1:0:1486:A:C5	29:2:2:LYS:HG3	2.55	0.42
16:O:44:ASN:HA	16:O:65:LEU:O	2.19	0.42
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.55	0.42
1:0:2909:G:O2'	1:0:2910:A:H5'	2.20	0.42
1:0:2502:C:O2'	1:0:2503:A:H5'	2.18	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
2:9:3031:C:H1'	38:9:1137:HOH:O	2.18	0.42
1:0:263:U:C4	8:F:54:VAL:HG13	2.54	0.42
1:0:395:A:H4'	38:0:9964:HOH:O	2.20	0.42
12:K:28:GLU:HB3	12:K:59:LYS:HB2	2.01	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.19	0.42
17:P:103:THR:O	17:P:107:GLU:HG3	2.20	0.42
28:1:26:SER:HB3	28:1:35:SER:OG	2.20	0.42
13:L:73:VAL:HG11	13:L:118:LEU:HD21	2.01	0.42
1:0:2395:A:C6	1:0:2396:C:C4	3.07	0.42
1:0:2035:C:O5'	1:0:2035:C:H6	2.02	0.42
1:0:1175:G:H1'	1:0:1193:A:H2'	2.01	0.42
1:0:1046:G:N3	1:0:1082:A:H2	2.17	0.42
2:9:3034:A:H8	2:9:3034:A:O5'	2.02	0.42
1:0:2265:U:H2'	1:0:2266:A:C8	2.55	0.42
1:0:475:G:C5'	5:C:73:LEU:HD23	2.50	0.42
1:0:482:G:O4'	1:0:511:A:C2	2.72	0.42
1:0:2105:C:O2'	1:0:2284:G:N2	2.52	0.42
26:Y:151:SER:HB3	26:Y:154:ARG:CB	2.49	0.42
11:J:39:VAL:HG13	11:J:106:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:2607:U:H4'	38:0:9438:HOH:O	2.18	0.42
14:M:28:GLN:O	14:M:32:ARG:HG3	2.18	0.42
15:N:170:GLU:O	15:N:174:GLU:HG3	2.20	0.42
3:A:9:ARG:NH1	38:A:8822:HOH:O	2.53	0.42
25:X:80:GLU:HB3	38:X:5564:HOH:O	2.17	0.42
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.42
32:0:9000:13T:H323	32:0:9000:13T:C1	2.49	0.42
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.42
30:3:22:VAL:HG11	30:3:67:LEU:HD13	2.01	0.42
1:0:316:A:H5'	21:T:54:ASP:OD2	2.20	0.42
1:0:535:G:C6	1:0:2064:U:C5	3.08	0.42
38:0:3186:HOH:O	14:M:9:ARG:HG3	2.19	0.42
11:J:59:LYS:O	11:J:63:ILE:HG13	2.19	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.18	0.42
1:0:1323:G:N2	1:0:1335:C:C2	2.88	0.42
1:0:876:A:N3	1:0:876:A:C2'	2.83	0.42
2:9:3110:G:C5	2:9:3111:U:C5	3.07	0.42
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.42
1:0:1161:A:O5'	1:0:1161:A:H8	2.02	0.42
2:9:3013:A:H3'	2:9:3014:G:H5'	2.02	0.42
13:L:120:LEU:HD12	13:L:133:VAL:HG21	2.02	0.42
1:0:2256:G:C2'	1:0:2257:G:C5'	2.93	0.42
1:0:447:A:OP1	21:T:2:LYS:HG2	2.20	0.42
38:0:3652:HOH:O	16:O:3:THR:HG21	2.19	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.42
5:C:218:VAL:HG12	38:C:8623:HOH:O	2.19	0.42
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.02	0.42
1:0:2078:U:O2'	1:0:2079:G:H5'	2.20	0.42
12:K:4:LEU:HD23	12:K:4:LEU:HA	1.83	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.42
38:0:4574:HOH:O	5:C:50:GLU:HG2	2.20	0.42
1:0:1579:C:H4'	1:0:1580:A:OP1	2.19	0.42
1:0:595:U:H2'	1:0:596:C:H6	1.85	0.42
1:0:282:C:O2'	1:0:283:U:C4'	2.68	0.42
1:0:856:G:H2'	38:0:5435:HOH:O	2.18	0.42
2:9:3059:C:H2'	2:9:3060:C:C6	2.55	0.42
1:0:589:U:H2'	1:0:590:A:C8	2.54	0.42
1:0:318:C:H5'	1:0:339:A:N3	2.35	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.20	0.42
22:U:6:CYS:C	22:U:8:TYR:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:25:MET:HE1	6:D:37:ALA:O	2.20	0.42
1:0:1923:G:H2'	1:0:1924:A:H8	1.84	0.42
6:D:64:ARG:HD3	6:D:67:ASP:HB3	2.02	0.42
26:Y:170:SER:OG	26:Y:175:ARG:HG3	2.19	0.42
1:0:2758:G:H2'	1:0:2759:C:C6	2.55	0.42
1:0:825:U:H5"	1:0:826:U:OP1	2.20	0.42
1:0:561:G:C2	1:0:562:A:C5	3.08	0.42
6:D:23:VAL:HG21	6:D:45:THR:HG21	2.02	0.42
1:0:2521:A:P	10:H:3:ALA:HB3	2.60	0.42
1:0:2240:U:O2'	1:0:2241:C:H5'	2.19	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.42
4:B:79:MET:HE3	4:B:79:MET:HB2	1.99	0.42
1:0:2824:C:O3'	1:0:2825:C:H6	2.01	0.42
19:R:132:ARG:NH2	38:R:8879:HOH:O	2.52	0.42
2:9:3114:G:H2'	2:9:3115:C:C6	2.55	0.42
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.01	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
4:B:305:ASP:O	4:B:306:LYS:CB	2.68	0.42
1:0:2612:A:H4'	38:0:3685:HOH:O	2.19	0.42
1:0:1055:G:OP2	10:H:96:ARG:NH1	2.53	0.42
1:0:2032:U:O2'	1:0:2033:G:H5"	2.20	0.41
19:R:18:LEU:HD12	19:R:143:VAL:HG11	2.02	0.41
6:D:48:MET:HA	6:D:49:PRO:HD3	1.87	0.41
1:0:1762:C:H4'	38:0:4662:HOH:O	2.19	0.41
1:0:517:U:C2'	1:0:518:G:H5'	2.50	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
3:A:131:HIS:O	3:A:132:ASP:HB2	2.20	0.41
4:B:260:HIS:HE1	38:B:8883:HOH:O	2.03	0.41
1:0:941:G:C2'	1:0:942:U:H5'	2.50	0.41
2:9:3105:A:C2'	2:9:3106:C:H5'	2.49	0.41
1:0:2589:U:H2'	1:0:2590:U:C6	2.55	0.41
2:9:3059:C:O5'	2:9:3059:C:H6	2.03	0.41
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.55	0.41
6:D:25:MET:SD	6:D:40:ILE:HD11	2.60	0.41
3:A:76:VAL:HG23	27:Z:63:LYS:HB3	2.00	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:1019:C:O2	18:Q:94:GLN:NE2	2.53	0.41
1:0:381:G:OP2	14:M:45:ARG:NH2	2.50	0.41
14:M:164:THR:HG22	14:M:167:GLY:N	2.35	0.41
22:U:17:THR:CG2	22:U:18:GLY:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:49:PRO:HG3	38:D:5828:HOH:O	2.21	0.41
1:0:2254:G:O2'	1:0:2255:A:H5'	2.20	0.41
8:F:48:VAL:HG23	8:F:74:PHE:HB3	2.01	0.41
1:0:553:G:H2'	1:0:554:G:H5'	2.02	0.41
28:1:25:LYS:HD2	29:2:49:GLU:H	1.84	0.41
1:0:2112:A:H2'	1:0:2113:G:H8	1.85	0.41
1:0:2689:A:C2'	1:0:2690:U:H5'	2.50	0.41
1:0:699:C:C6	1:0:744:G:C4	3.08	0.41
1:0:2754:G:C2'	1:0:2755:G:H5'	2.50	0.41
31:I:100:LEU:HD22	31:I:105:VAL:HG23	2.02	0.41
1:0:1904:A:C8	1:0:1905:U:C5	3.08	0.41
1:0:2402:A:H1'	38:0:3163:HOH:O	2.20	0.41
1:0:497:A:H2'	1:0:498:A:C5'	2.50	0.41
8:F:14:ASP:O	8:F:18:GLU:HG3	2.20	0.41
31:I:91:GLU:HA	31:I:92:PRO:HD2	1.84	0.41
24:W:4:LEU:CD1	24:W:24:LEU:HD13	2.50	0.41
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
27:Z:30:GLU:HB2	38:Z:8715:HOH:O	2.20	0.41
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.35	0.41
2:9:3042:C:O2	6:D:76:ARG:NH1	2.52	0.41
1:0:694:A:H4'	1:0:2441:U:OP1	2.21	0.41
1:0:2434:A:O3'	30:3:28:GLY:HA3	2.20	0.41
26:Y:112:GLU:CD	26:Y:115:ARG:NH1	2.74	0.41
1:0:1225:C:H2'	1:0:1226:G:O4'	2.21	0.41
2:9:3105:A:H2'	2:9:3106:C:H5'	2.03	0.41
1:0:902:G:N7	13:L:18:HIS:CD2	2.85	0.41
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.41
11:J:19:MET:CE	11:J:132:LEU:HD11	2.51	0.41
28:1:25:LYS:HE2	38:2:7213:HOH:O	2.20	0.41
1:0:1576:G:H2'	1:0:1577:U:H6	1.85	0.41
2:9:3033:U:H2'	38:9:3797:HOH:O	2.19	0.41
10:H:171:ALA:HA	38:H:8570:HOH:O	2.20	0.41
1:0:459:A:H5"	38:0:9047:HOH:O	2.20	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.41
7:E:84:MET:HG2	7:E:168:ILE:HA	2.02	0.41
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.41
25:X:7:GLU:HA	25:X:74:ALA:O	2.20	0.41
1:0:1943:C:C4'	3:A:212:PRO:HA	2.50	0.41
11:J:74:ARG:HH11	11:J:74:ARG:CB	2.30	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.54	0.41
1:0:2825:C:H4'	1:0:2826:G:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1422:U:H4'	38:0:7732:HOH:O	2.19	0.41
1:0:2634:G:OP2	3:A:204:GLY:N	2.53	0.41
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.86	0.41
11:J:19:MET:HE1	11:J:132:LEU:HD11	2.02	0.41
1:0:81:G:N3	1:0:98:A:C2	2.89	0.41
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.41
15:N:42:HIS:CG	15:N:62:HIS:HE1	2.38	0.41
2:9:3092:G:C6	2:9:3093:A:N6	2.88	0.41
25:X:74:ALA:CB	25:X:85:VAL:HG22	2.51	0.41
1:0:308:U:C4	1:0:342:C:C1'	3.03	0.41
2:9:3001:U:H5'	2:9:3121:C:O2	2.20	0.41
2:9:3001:U:O3'	2:9:3003:A:C5'	2.69	0.41
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.48	0.41
14:M:182:LYS:HB2	14:M:194:ALA:HB2	2.01	0.41
1:0:1024:G:C6	1:0:1025:C:C4	3.08	0.41
27:Z:67:GLY:N	27:Z:70:LYS:O	2.54	0.41
24:W:149:LEU:HG	24:W:153:MET:HE2	2.03	0.41
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.86	0.41
1:0:1923:G:H2'	1:0:1924:A:C8	2.56	0.41
1:0:1052:G:N3	1:0:1052:G:H2'	2.35	0.41
1:0:61:G:C6	1:0:62:C:C4	3.09	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.56	0.41
1:0:849:C:O2'	1:0:850:U:H5'	2.21	0.41
1:0:1400:C:O2'	1:0:1401:G:H5'	2.21	0.41
1:0:1206:U:C5'	1:0:1206:U:H6	2.23	0.41
1:0:255:A:C5	1:0:256:C:C5	3.09	0.41
31:I:129:VAL:O	31:I:129:VAL:HG12	2.21	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.51	0.41
1:0:2775:A:C6	1:0:2776:A:C6	3.08	0.41
24:W:19:ASP:O	24:W:23:MET:HG3	2.20	0.41
1:0:863:G:C6	1:0:864:U:C4	3.08	0.41
18:Q:16:ASN:OD1	18:Q:45:PRO:HB2	2.20	0.41
1:0:1181:A:C2'	1:0:1182:C:H5'	2.51	0.41
1:0:1224:G:H2'	1:0:1225:C:C6	2.55	0.41
1:0:2549:C:O2'	1:0:2550:U:H5'	2.20	0.41
1:0:298:C:O5'	1:0:298:C:H6	2.04	0.41
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.85	0.41
7:E:5:LEU:HD21	7:E:66:GLN:HG3	2.01	0.41
14:M:123:ASP:OD1	14:M:126:GLN:HG2	2.19	0.41
24:W:119:HIS:HD2	24:W:120:PRO:O	2.03	0.41
1:0:25:A:O2'	1:0:640:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2716:G:H5"	4:B:206:THR:CG2	2.44	0.41
2:9:3003:A:H61	2:9:3022:G:H1'	1.83	0.41
1:0:539:G:H2'	1:0:540:A:C8	2.56	0.41
1:0:2036:C:C1'	12:K:44:LEU:HG	2.51	0.41
14:M:158:ARG:HB2	14:M:163:LEU:HB2	2.03	0.41
1:0:247:A:H1'	38:0:3892:HOH:O	2.21	0.41
26:Y:144:ARG:NH2	38:Y:8912:HOH:O	2.54	0.41
20:S:45:TYR:O	20:S:80:ARG:NH2	2.53	0.41
12:K:132:VAL:HG21	22:U:22:VAL:CG1	2.50	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.41
1:0:2365:G:H4'	18:Q:45:PRO:O	2.20	0.41
1:0:912:A:C4	1:0:1294:A:C2	3.09	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.20	0.41
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.41
1:0:1622:G:H2'	1:0:1623:C:H5'	2.02	0.41
19:R:72:VAL:CG1	19:R:75:TRP:HB3	2.50	0.41
13:L:92:ASP:HA	13:L:121:ILE:HB	2.02	0.41
1:0:2303:A:H2	38:Q:5641:HOH:O	2.03	0.41
1:0:1666:C:H2'	1:0:1667:A:H8	1.86	0.41
1:0:1115:U:O2'	1:0:1116:U:H5'	2.20	0.41
1:0:1116:U:C2	1:0:1246:A:N6	2.89	0.41
1:0:1166:A:P	1:0:1174:A:H4'	2.61	0.41
1:0:368:C:H2'	1:0:369:G:H5'	2.02	0.41
1:0:1157:C:O2'	1:0:1158:G:H5'	2.20	0.41
1:0:2768:A:H5"	38:0:4432:HOH:O	2.21	0.41
1:0:2569:A:H2'	1:0:2570:G:O5'	2.20	0.41
1:0:2727:A:N1	1:0:2756:U:C2	2.89	0.41
1:0:169:A:H4'	38:M:8837:HOH:O	2.20	0.41
2:9:3040:C:OP1	2:9:3041:C:H5	2.04	0.41
3:A:186:TRP:CG	3:A:187:PRO:HA	2.56	0.41
4:B:23:THR:HG23	4:B:308:LEU:CD2	2.51	0.41
1:0:2415:A:O2'	15:N:29:SER:HB3	2.21	0.41
2:9:3001:U:C4'	2:9:3003:A:OP1	2.69	0.41
1:0:567:U:O2'	1:0:568:G:H5'	2.20	0.41
2:9:3065:A:O2'	2:9:3066:G:P	2.79	0.41
19:R:113:HIS:O	19:R:145:LEU:HD12	2.20	0.41
31:I:131:THR:O	31:I:135:LEU:HG	2.21	0.41
11:J:42:GLU:HG2	11:J:43:ARG:HG3	2.03	0.41
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.51	0.41
2:9:3104:A:C2'	2:9:3105:A:H5'	2.50	0.41
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:66:G:C2	1:0:109:U:C4	3.08	0.41
21:T:32:ARG:NH1	21:T:38:ARG:NH1	2.69	0.41
1:0:327:A:H4'	1:0:329:A:C8	2.55	0.41
1:0:1619:G:C6	1:0:1620:C:N3	2.89	0.41
1:0:287:C:H6	1:0:287:C:O5'	2.04	0.41
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.41
1:0:2607:U:C4	4:B:242:TRP:CZ2	3.08	0.41
1:0:1786:C:OP1	17:P:74:GLN:HG2	2.21	0.41
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.56	0.41
5:C:228:ALA:HA	5:C:229:PRO:HD3	1.90	0.41
4:B:265:LEU:HD21	4:B:316:ARG:HD3	2.01	0.41
6:D:151:ILE:HA	6:D:152:PRO:HD3	1.92	0.41
21:T:3:GLN:HA	21:T:4:PRO:HD3	1.76	0.41
4:B:52:VAL:O	4:B:53:LEU:HD12	2.21	0.41
1:0:483:C:C4	1:0:484:A:C6	3.09	0.41
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.41
24:W:81:ASP:OD1	24:W:92:ASP:HB2	2.20	0.41
1:0:1630:A:O2'	1:0:1631:A:H5'	2.21	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.21	0.41
1:0:911:G:H5'	1:0:932:U:OP1	2.21	0.41
32:0:9000:13T:H261	32:0:9000:13T:H10	1.80	0.41
1:0:1182:C:H6	1:0:1182:C:O5'	2.02	0.41
17:P:115:SER:O	17:P:117:SER:N	2.46	0.41
1:0:2004:U:H5"	1:0:2005:G:C8	2.56	0.41
1:0:2363:G:H2'	1:0:2364:A:O4'	2.21	0.41
1:0:1299:G:N2	38:0:4691:HOH:O	2.53	0.41
1:0:1662:C:H2'	1:0:1663:G:O4'	2.21	0.41
1:0:380:A:O4'	1:0:382:U:H1'	2.21	0.41
1:0:1594:C:OP1	17:P:109:ARG:NH1	2.54	0.41
26:Y:144:ARG:NE	38:Y:8912:HOH:O	2.54	0.41
1:0:397:A:H1'	1:0:417:G:H1'	2.02	0.41
1:0:2791:U:H1'	1:0:2792:A:H5"	2.03	0.41
1:0:2791:U:H4'	1:0:2792:A:OP1	2.21	0.41
1:0:2897:C:O2'	1:0:2898:G:H5'	2.21	0.41
1:0:716:G:C6	1:0:717:C:N4	2.89	0.41
13:L:119:THR:HA	13:L:139:SER:O	2.21	0.41
3:A:68:ILE:HD11	38:A:8863:HOH:O	2.20	0.41
1:0:545:G:H2'	1:0:546:C:O4'	2.21	0.40
1:0:2072:G:H3'	1:0:2073:G:C5'	2.52	0.40
1:0:1925:G:O2'	1:0:1926:G:H5'	2.21	0.40
4:B:336:GLN:NE2	38:B:8822:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:189:ASN:ND2	26:Y:192:ASP:N	2.69	0.40
7:E:69:ILE:HA	7:E:72:MET:HE2	2.03	0.40
4:B:198:GLU:HA	38:B:8952:HOH:O	2.20	0.40
3:A:33:GLU:CD	3:A:33:GLU:H	2.24	0.40
1:0:2887:G:H2'	1:0:2888:U:O4'	2.21	0.40
1:0:228:C:H2'	1:0:229:G:C5'	2.51	0.40
7:E:22:VAL:O	7:E:28:SER:HA	2.22	0.40
1:0:2549:C:H2'	1:0:2550:U:O4'	2.22	0.40
1:0:445:U:C1'	38:0:7326:HOH:O	2.68	0.40
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.40
4:B:305:ASP:O	4:B:306:LYS:HB2	2.21	0.40
1:0:1449:G:N3	1:0:1449:G:H2'	2.36	0.40
19:R:89:LEU:HA	19:R:89:LEU:HD23	1.84	0.40
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.21	0.40
1:0:1745:G:H5'	38:0:4341:HOH:O	2.20	0.40
9:G:67:LEU:O	9:G:71:LEU:HG	2.21	0.40
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.40
1:0:1642:A:N7	1:0:1643:C:C4	2.89	0.40
1:0:567:U:O5'	1:0:567:U:H6	2.04	0.40
26:Y:134:HIS:H	26:Y:134:HIS:CD2	2.38	0.40
1:0:2064:U:H2'	1:0:2065:C:H6	1.86	0.40
1:0:535:G:O6	1:0:2064:U:C6	2.75	0.40
1:0:1310:U:P	5:C:168:ARG:HH11	2.44	0.40
1:0:2361:A:H2'	1:0:2362:A:O4'	2.21	0.40
1:0:1457:U:H5	38:0:7859:HOH:O	2.04	0.40
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.54	0.40
1:0:2453:G:O3'	13:L:50:GLY:HA2	2.21	0.40
1:0:1494:A:H1'	1:0:1495:C:C6	2.56	0.40
1:0:1574:C:H6	1:0:1574:C:O5'	2.04	0.40
1:0:699:C:H6	1:0:744:G:O4'	2.03	0.40
1:0:2344:G:H2'	1:0:2344:G:N3	2.36	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:1268:C:O2'	26:Y:169:ARG:HB2	2.21	0.40
1:0:574:C:H2'	1:0:575:G:O4'	2.21	0.40
24:W:13:MET:CE	24:W:18:GLN:HA	2.49	0.40
3:A:105:VAL:HG12	3:A:106:CYS:N	2.36	0.40
6:D:25:MET:HE3	6:D:37:ALA:HB1	2.04	0.40
1:0:1902:G:H2'	1:0:1903:U:O4'	2.21	0.40
1:0:74:A:H2'	1:0:75:U:C6	2.55	0.40
1:0:844:A:C6	1:0:882:A:C6	3.09	0.40
17:P:121:ASP:HB2	38:P:5891:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:65:VAL:HG12	24:W:116:LEU:HD13	2.04	0.40
1:0:2902:A:H4'	1:0:2903:C:OP1	2.21	0.40
26:Y:177:LYS:HD3	26:Y:181:GLY:O	2.22	0.40
1:0:2642:G:H2'	1:0:2643:G:O4'	2.22	0.40
14:M:72:ALA:HB2	14:M:93:ARG:HG2	2.03	0.40
1:0:1180:U:O2'	31:I:92:PRO:HD2	2.21	0.40
1:0:1189:A:C3'	38:0:7666:HOH:O	2.62	0.40
1:0:559:U:C4'	1:0:559:U:C6	3.04	0.40
1:0:1741:U:H3'	38:0:9763:HOH:O	2.20	0.40
1:0:485:A:HO2'	1:0:487:G:H8	1.68	0.40
38:9:466:HOH:O	18:Q:25:PRO:HB3	2.21	0.40
1:0:1308:A:O4'	5:C:226:GLY:HA3	2.21	0.40
1:0:517:U:H2'	1:0:518:G:H5'	2.03	0.40
1:0:1309:U:H2'	1:0:1310:U:O4'	2.21	0.40
1:0:705:C:C2'	1:0:705:C:O2	2.70	0.40
1:0:474:C:O3'	5:C:73:LEU:HD21	2.22	0.40
25:X:30:MET:CE	25:X:58:ALA:HB3	2.52	0.40
1:0:2754:G:HO2'	1:0:2755:G:H5'	1.85	0.40
1:0:1705:C:P	17:P:59:ARG:HH12	2.45	0.40
6:D:25:MET:CE	6:D:37:ALA:HB1	2.51	0.40
2:9:3110:G:C2'	2:9:3111:U:H5'	2.51	0.40
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.22	0.40
1:0:1006:A:N1	1:0:2311:A:H1'	2.37	0.40
16:O:45:LEU:CD1	16:O:88:LYS:HD2	2.51	0.40
12:K:62:PRO:HG3	12:K:65:ARG:NH2	2.37	0.40
1:0:243:A:H2	1:0:274:G:N3	2.19	0.40
16:O:14:LEU:HB3	16:O:26:TRP:O	2.21	0.40
1:0:260:C:C4	1:0:261:A:C5	3.10	0.40
1:0:1087:G:H4'	1:0:1088:A:OP1	2.22	0.40
1:0:2673:U:C4	1:0:2674:G:C6	3.10	0.40
5:C:175:LYS:HD2	5:C:187:ARG:HB3	2.04	0.40
1:0:1617:C:C4	1:0:1643:C:H4'	2.57	0.40
27:Z:49:ARG:NH2	27:Z:52:THR:HA	2.37	0.40
8:F:58:GLU:HA	8:F:61:MET:CE	2.47	0.40
1:0:1329:A:H5"	38:0:3790:HOH:O	2.20	0.40
1:0:820:G:H5'	1:0:821:U:C5'	2.51	0.40
23:V:39:ALA:O	23:V:41:GLU:N	2.51	0.40
1:0:1544:U:H2'	1:0:1545:C:H6	1.87	0.40
29:2:49:GLU:HB2	38:2:131:HOH:O	2.21	0.40
1:0:1334:C:H2'	1:0:1335:C:H6	1.86	0.40
1:0:160:A:C4	1:0:177:A:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:28:GLN:HA	14:M:31:TRP:HB2	2.03	0.40
17:P:40:VAL:O	17:P:44:VAL:HG23	2.22	0.40
19:R:17:MET:HE3	19:R:19:ARG:HH21	1.86	0.40
7:E:6:GLU:HA	7:E:46:THR:HG22	2.03	0.40
25:X:8:ARG:NH1	38:X:2479:HOH:O	2.49	0.40
1:0:245:C:H2'	1:0:246:G:H5'	2.04	0.40
1:0:2739:A:C6	1:0:2740:G:C5	3.09	0.40
1:0:1453:G:H2'	1:0:1454:U:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	235/240 (98%)	212 (90%)	21 (9%)	2 (1%)	21 57
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	16 48
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	24 60
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	8 31
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	30 67
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	7 26
9	G	25/348 (7%)	25 (100%)	0	0	100 100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	10 35
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	14 44
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100 100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100 100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100 100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	8 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	26	63
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	17	51
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	57
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	15	46
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	15	46
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	6	24
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	21	57

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP
15	N	184	ILE
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
6	D	27	ILE
6	D	137	PRO
6	D	173	GLU
8	F	44	SER
24	W	49	ASN
3	A	37	VAL

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Mol	Chain	Res	Type
15	N	139	TRP
27	Z	42	CYS
5	C	79	ARG
10	H	16	ARG
10	H	168	ALA
17	P	117	SER
25	X	70	ILE
4	B	2	GLN
5	C	8	LEU
8	F	64	PRO
21	T	44	ALA
24	W	77	ALA
4	B	306	LYS
7	E	44	GLY
11	J	89	HIS
18	Q	18	PRO
27	Z	43	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	170 (95%)	9 (5%)	30	65
4	B	282/283 (100%)	268 (95%)	14 (5%)	30	65
5	C	193/193 (100%)	178 (92%)	15 (8%)	16	41
6	D	117/148 (79%)	115 (98%)	2 (2%)	68	91
7	E	152/156 (97%)	149 (98%)	3 (2%)	63	88
8	F	93/94 (99%)	89 (96%)	4 (4%)	35	71
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	126 (96%)	6 (4%)	34	70
11	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
12	K	106/106 (100%)	104 (98%)	2 (2%)	65	89
13	L	113/127 (89%)	107 (95%)	6 (5%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	M	158/158 (100%)	149 (94%)	9 (6%)	25 59
15	N	149/150 (99%)	146 (98%)	3 (2%)	63 88
16	O	93/94 (99%)	92 (99%)	1 (1%)	80 95
17	P	113/117 (97%)	109 (96%)	4 (4%)	43 78
18	Q	79/80 (99%)	78 (99%)	1 (1%)	76 94
19	R	117/122 (96%)	113 (97%)	4 (3%)	44 79
20	S	71/74 (96%)	70 (99%)	1 (1%)	74 93
21	T	105/106 (99%)	99 (94%)	6 (6%)	25 59
22	U	44/52 (85%)	43 (98%)	1 (2%)	58 87
23	V	51/57 (90%)	49 (96%)	2 (4%)	39 75
24	W	130/130 (100%)	124 (95%)	6 (5%)	33 69
25	X	66/74 (89%)	61 (92%)	5 (8%)	16 43
26	Y	120/196 (61%)	114 (95%)	6 (5%)	30 65
27	Z	60/60 (100%)	60 (100%)	0	100 100
28	1	46/47 (98%)	45 (98%)	1 (2%)	60 88
29	2	42/46 (91%)	40 (95%)	2 (5%)	31 67
30	3	79/79 (100%)	78 (99%)	1 (1%)	76 94
31	I	58/129 (45%)	56 (97%)	2 (3%)	44 79
All	All	3093/3602 (86%)	2969 (96%)	124 (4%)	38 74

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	36	ASP
3	A	69	LEU
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP

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Mol	Chain	Res	Type
4	B	56	ASP
4	B	97	LEU
4	B	98	THR
4	B	149	ASP
4	B	162	MET
4	B	175	LEU
4	B	195	ARG
4	B	254	GLN
4	B	257	THR
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	91	PRO
5	C	94	THR
5	C	115	LEU
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	236	THR
5	C	240	LEU
6	D	61	PHE
6	D	149	ARG
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	24	ARG
8	F	46	GLU
8	F	103	GLU
10	H	59	HIS
10	H	62	LEU
10	H	84	LYS
10	H	96	ARG
10	H	119	LYS
10	H	154	TYR
11	J	46	ILE
11	J	52	GLN

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Mol	Chain	Res	Type
11	J	74	ARG
11	J	79	PHE
11	J	93	ARG
11	J	107	ASN
11	J	120	SER
11	J	132	LEU
12	K	10	GLN
12	K	132	VAL
13	L	30	ARG
13	L	35	ARG
13	L	51	PHE
13	L	99	GLU
13	L	101	ASP
13	L	140	VAL
14	M	10	ASP
14	M	46	LEU
14	M	68	ARG
14	M	75	ARG
14	M	81	ARG
14	M	93	ARG
14	M	99	ARG
14	M	116	ASN
14	M	164	THR
15	N	26	LEU
15	N	49	THR
15	N	138	ASP
16	O	43	VAL
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	95	GLU
19	R	13	THR
19	R	82	GLU
19	R	132	ARG
19	R	143	VAL
20	S	72	ASP
21	T	39	ASN
21	T	48	VAL
21	T	73	HIS
21	T	89	ARG
21	T	96	VAL

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Mol	Chain	Res	Type
21	T	117	ASP
22	U	47	ARG
23	V	12	THR
23	V	65	ASP
24	W	26	ILE
24	W	35	VAL
24	W	73	LEU
24	W	109	GLU
24	W	142	ASP
24	W	146	ILE
25	X	15	ARG
25	X	27	ASP
25	X	52	PRO
25	X	72	VAL
25	X	82	GLU
26	Y	154	ARG
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
26	Y	204	ARG
26	Y	220	GLU
28	1	47	ASP
29	2	18	ASN
29	2	31	ARG
30	3	3	MET
31	I	87	THR
31	I	100	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	176	HIS
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	129	HIS

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Mol	Chain	Res	Type
6	D	85	GLN
6	D	103	ASN
6	D	133	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	170	ASN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	42	ASN
13	L	18	HIS
13	L	41	HIS
13	L	42	ASN
13	L	116	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	21	HIS
15	N	107	ASN
17	P	50	GLN
17	P	73	HIS
17	P	118	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	123	GLN
20	S	9	HIS
20	S	53	ASN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	28	HIS
24	W	110	GLN
24	W	119	HIS

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Mol	Chain	Res	Type
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	134	HIS
26	Y	149	GLN
26	Y	188	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	30	GLN
30	3	48	ASN
31	I	93	GLN
31	I	107	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	241 (8%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	259 (9%)	34 (1%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C

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Mol	Chain	Res	Type
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
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	285	A
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A

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Mol	Chain	Res	Type
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	885	G
1	0	898	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	1003	U
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G

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Mol	Chain	Res	Type
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G

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Mol	Chain	Res	Type
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	1742	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
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

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Mol	Chain	Res	Type
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2468	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
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	2638	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C

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Mol	Chain	Res	Type
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U

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Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1165	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1506	U
1	0	1563	G
1	0	1667	A
1	0	1685	A
1	0	1942	A
1	0	2313	C
1	0	2361	A
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
2	9	3065	A

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

5 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	OMU	0	2587	1	12,22,23	0.96	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	1.00	1 (5%)	21,38,41	2.54	3 (14%)
1	UR3	0	2619	1	12,22,23	0.77	0	16,32,35	0.78	0
1	PSU	0	2621	1	13,21,22	1.65	2 (15%)	18,30,33	6.12	3 (16%)
1	1MA	0	628	1	14,25,26	0.94	1 (7%)	15,37,40	1.20	1 (6%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.05	1.47	1.52
1	0	2587	OMU	C4-N3	2.31	1.37	1.33
1	0	2621	PSU	C4-N3	2.38	1.37	1.33
1	0	628	1MA	C6-N6	2.49	1.33	1.29
1	0	2588	OMG	C6-N1	3.08	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-21.44	114.65	128.33
1	0	2588	OMG	C5-C6-N1	-8.74	111.64	123.59
1	0	628	1MA	C2-N3-C4	-3.75	110.59	116.40
1	0	2587	OMU	C5-C4-N3	-3.32	114.61	123.12
1	0	2588	OMG	N3-C2-N1	-2.34	123.89	127.44
1	0	2621	PSU	C6-N1-C2	2.66	119.75	115.47
1	0	2588	OMG	C6-N1-C2	6.70	125.24	115.94
1	0	2587	OMU	C4-N3-C2	13.08	127.09	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C4-N3-C2	13.91	127.28	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	13T	0	9000	-	40,43,43	2.02	11 (27%)	43,63,63	1.90	5 (11%)

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
32	13T	0	9000	-	-	0/73/81/81	0/0/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	13T	O1-C1	2.06	1.37	1.33
32	0	9000	13T	C26-C8	2.21	1.54	1.50
32	0	9000	13T	C27-C10	2.33	1.57	1.53
32	0	9000	13T	C10-C11	2.35	1.54	1.52
32	0	9000	13T	C29-C16	2.42	1.55	1.52
32	0	9000	13T	O7-C11	2.92	1.26	1.21
32	0	9000	13T	O5-C5	3.02	1.26	1.21
32	0	9000	13T	C9-C8	3.15	1.40	1.33
32	0	9000	13T	O2-C1	3.33	1.29	1.21
32	0	9000	13T	C10-C9	3.65	1.57	1.51
32	0	9000	13T	C18-C19	7.17	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	9000	13T	O11-C18-C19	-4.16	56.62	59.46
32	0	9000	13T	O11-C19-C18	-2.35	58.01	59.87
32	0	9000	13T	C27-C10-C9	2.61	113.14	110.72
32	0	9000	13T	O4-C3-C4	3.86	115.61	106.02
32	0	9000	13T	C18-O11-C19	8.40	65.36	60.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	13T	24	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	2749/2922 (94%)	-0.44	9 (0%) 94 94	23, 50, 93, 150	0
2	9	122/122 (100%)	-0.64	2 (1%) 74 72	43, 69, 91, 151	0
3	A	237/240 (98%)	-0.20	7 (2%) 54 47	32, 55, 86, 105	0
4	B	337/338 (99%)	-0.27	1 (0%) 94 94	33, 60, 82, 90	0
5	C	246/246 (100%)	-0.43	0 100 100	30, 50, 73, 82	0
6	D	140/177 (79%)	1.29	42 (30%) 1 0	63, 103, 124, 130	0
7	E	172/178 (96%)	-0.12	3 (1%) 73 70	55, 73, 90, 96	0
8	F	119/120 (99%)	0.40	6 (5%) 32 26	57, 74, 96, 106	0
9	G	29/348 (8%)	0.81	4 (13%) 4 2	81, 94, 103, 103	0
10	H	160/171 (93%)	0.45	15 (9%) 11 6	52, 67, 93, 100	0
11	J	142/145 (97%)	-0.36	2 (1%) 78 76	45, 56, 74, 94	0
12	K	132/132 (100%)	-0.43	1 (0%) 87 86	41, 54, 75, 81	0
13	L	145/165 (87%)	0.29	12 (8%) 14 9	32, 71, 107, 118	0
14	M	194/194 (100%)	-0.51	0 100 100	36, 47, 60, 64	0
15	N	186/187 (99%)	0.11	10 (5%) 29 23	50, 67, 110, 119	0
16	O	115/116 (99%)	-0.33	0 100 100	44, 59, 71, 76	0
17	P	143/149 (95%)	-0.29	1 (0%) 89 88	46, 60, 70, 75	0
18	Q	95/96 (98%)	-0.43	0 100 100	43, 52, 64, 72	0
19	R	150/155 (96%)	-0.42	0 100 100	38, 50, 68, 73	0
20	S	81/85 (95%)	-0.04	1 (1%) 81 78	52, 65, 81, 85	0
21	T	119/120 (99%)	-0.06	3 (2%) 61 55	47, 62, 83, 96	0
22	U	53/66 (80%)	-0.19	0 100 100	51, 61, 75, 81	0
23	V	65/71 (91%)	1.30	14 (21%) 1 0	59, 79, 109, 114	0
24	W	154/154 (100%)	-0.38	0 100 100	42, 56, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	82/92 (89%)	0.18	7 (8%) 13 8	52, 64, 87, 97	0
26	Y	142/241 (58%)	-0.56	2 (1%) 78 76	30, 51, 70, 86	0
27	Z	73/73 (100%)	0.31	7 (9%) 10 6	58, 69, 80, 94	0
28	1	56/57 (98%)	-0.42	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	0.17	3 (6%) 22 16	41, 69, 90, 99	0
30	3	92/92 (100%)	-0.34	0 100 100	42, 60, 71, 82	0
31	I	70/161 (43%)	3.26	50 (71%) 0 0	109, 119, 135, 135	0
All	All	6646/7463 (89%)	-0.21	202 (3%) 54 47	23, 57, 100, 151	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	I	75	THR	9.3
31	I	79	ILE	8.8
23	V	1	THR	8.5
31	I	109	ALA	8.2
6	D	63	ILE	8.0
31	I	113	HIS	7.8
31	I	71	GLY	7.8
31	I	118	SER	7.7
23	V	40	PRO	6.9
31	I	96	PHE	6.8
13	L	100	ALA	6.8
23	V	39	ALA	6.7
23	V	43	PRO	6.6
15	N	166	ALA	6.5
13	L	97	VAL	6.5
31	I	93	GLN	6.1
25	X	88	GLU	5.9
31	I	102	VAL	5.9
6	D	57	THR	5.7
31	I	137	VAL	5.7
31	I	76	ALA	5.5
31	I	105	VAL	5.3
10	H	73	LEU	5.3
6	D	64	ARG	5.1
31	I	133	THR	5.1
25	X	80	GLU	5.0
31	I	103	ASP	4.8
23	V	38	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
31	I	107	GLN	4.7
6	D	85	GLN	4.6
31	I	77	GLU	4.6
31	I	85	PHE	4.5
6	D	18	ILE	4.4
27	Z	22	SER	4.4
20	S	81	ILE	4.3
6	D	90	LEU	4.3
27	Z	11	SER	4.3
4	B	1	PRO	4.3
23	V	41	GLU	4.2
27	Z	26	VAL	4.2
31	I	111	GLN	4.2
3	A	37	VAL	4.1
1	0	1172	G	4.1
13	L	102	ASP	4.0
31	I	83	ALA	3.9
31	I	84	GLY	3.9
31	I	115	ASP	3.8
8	F	17	LEU	3.8
31	I	116	LEU	3.8
29	2	39	ARG	3.7
10	H	138	CYS	3.7
6	D	69	ILE	3.6
31	I	104	GLN	3.6
23	V	37	GLY	3.6
27	Z	21	VAL	3.6
6	D	88	LEU	3.5
31	I	74	PRO	3.4
10	H	32	LYS	3.4
6	D	87	ALA	3.4
8	F	49	PHE	3.4
31	I	108	ILE	3.4
31	I	132	CYS	3.3
9	G	27	ILE	3.3
31	I	121	LEU	3.3
27	Z	19	GLY	3.2
13	L	76	LEU	3.2
6	D	23	VAL	3.2
31	I	91	GLU	3.2
10	H	65	SER	3.2
15	N	183	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	237	GLY	3.1
6	D	157	LEU	3.1
10	H	37	GLN	3.1
31	I	117	LEU	3.1
15	N	165	ALA	3.1
23	V	52	ALA	3.1
31	I	81	ASP	3.1
29	2	35	ARG	3.1
6	D	66	GLY	3.1
3	A	31	LYS	3.0
6	D	81	GLU	3.0
31	I	126	LYS	3.0
7	E	45	ASP	2.9
15	N	185	GLU	2.9
6	D	17	ARG	2.9
25	X	71	ARG	2.9
29	2	49	GLU	2.9
26	Y	108	ASP	2.9
31	I	110	GLU	2.9
23	V	34	GLN	2.9
21	T	116	ASP	2.9
8	F	106	ALA	2.9
9	G	25	GLU	2.9
6	D	95	THR	2.9
1	0	960	G	2.8
31	I	122	THR	2.8
6	D	53	LYS	2.8
13	L	101	ASP	2.8
10	H	79	GLU	2.8
25	X	65	ASN	2.8
9	G	23	ILE	2.8
31	I	97	VAL	2.8
31	I	99	ASP	2.8
6	D	45	THR	2.8
31	I	138	THR	2.7
6	D	134	LEU	2.7
6	D	135	VAL	2.7
6	D	166	ILE	2.7
31	I	72	VAL	2.7
31	I	89	SER	2.7
1	0	1199	A	2.7
31	I	82	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
13	L	80	ASP	2.7
23	V	59	ILE	2.6
31	I	86	GLU	2.6
6	D	62	ASP	2.6
6	D	11	HIS	2.6
10	H	86	THR	2.6
13	L	60	GLU	2.6
6	D	128	LEU	2.6
1	0	1177	A	2.6
6	D	40	ILE	2.6
13	L	105	TYR	2.6
10	H	146	VAL	2.6
6	D	101	THR	2.6
6	D	44	ILE	2.5
6	D	58	VAL	2.5
6	D	75	LEU	2.5
10	H	36	LYS	2.5
1	0	1171	A	2.5
8	F	29	VAL	2.5
6	D	93	LEU	2.5
8	F	16	ALA	2.5
7	E	100	ASP	2.5
10	H	171	ALA	2.4
26	Y	235	GLU	2.4
15	N	95	ALA	2.4
6	D	26	GLY	2.4
31	I	78	LEU	2.4
1	0	497	A	2.4
13	L	106	VAL	2.4
25	X	74	ALA	2.4
6	D	74	THR	2.4
31	I	129	VAL	2.4
6	D	129	ASP	2.4
25	X	10	VAL	2.4
6	D	165	PHE	2.3
31	I	136	GLY	2.3
21	T	119	ALA	2.3
6	D	170	TYR	2.3
6	D	104	PHE	2.3
3	A	35	GLY	2.3
23	V	8	ILE	2.3
6	D	158	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
21	T	118	SER	2.3
10	H	63	GLU	2.3
10	H	29	ALA	2.3
27	Z	34	ASN	2.3
1	0	1198	U	2.2
15	N	68	GLU	2.2
6	D	98	PHE	2.2
31	I	80	LYS	2.2
6	D	86	THR	2.2
31	I	92	PRO	2.2
31	I	135	LEU	2.2
15	N	178	THR	2.2
23	V	58	THR	2.2
10	H	81	GLY	2.2
17	P	49	ILE	2.2
1	0	282	C	2.2
12	K	119	GLN	2.2
6	D	27	ILE	2.2
3	A	82	VAL	2.2
23	V	3	LEU	2.2
31	I	100	LEU	2.2
10	H	74	ILE	2.2
13	L	149	ARG	2.2
2	9	3001	U	2.1
15	N	138	ASP	2.1
2	9	3024	U	2.1
15	N	137	ALA	2.1
1	0	2637	A	2.1
9	G	26	MET	2.1
3	A	36	ASP	2.1
31	I	112	LYS	2.1
11	J	70	PHE	2.1
11	J	5	GLU	2.1
13	L	96	VAL	2.1
25	X	72	VAL	2.1
23	V	36	ALA	2.1
10	H	34	GLY	2.1
31	I	95	ASP	2.1
27	Z	20	ARG	2.1
6	D	171	ASP	2.1
15	N	155	GLU	2.1
6	D	72	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	99	ILE	2.0
13	L	81	VAL	2.0
6	D	65	GLU	2.0
7	E	87	PHE	2.0
8	F	75	ILE	2.0
31	I	88	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PSU	0	2621	20/21	0.97	0.12	-	30,32,39,40	0
1	OMG	0	2588	24/25	0.97	0.13	-	37,38,39,40	0
1	UR3	0	2619	21/22	0.96	0.15	-	36,38,39,40	0
1	OMU	0	2587	21/22	0.95	0.12	-	38,39,40,41	0
1	1MA	0	628	23/24	0.96	0.17	-	33,35,36,37	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8577	1/1	0.63	0.73	58.21	81,81,81,81	0
34	K	0	8401	1/1	0.87	0.73	46.07	84,84,84,84	0
35	NA	0	8574	1/1	0.92	0.62	40.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8550	1/1	0.66	0.61	29.90	65,65,65,65	0
35	NA	0	8525	1/1	0.98	0.39	20.43	59,59,59,59	0
35	NA	0	8531	1/1	0.54	0.38	19.66	57,57,57,57	0
35	NA	0	8559	1/1	0.47	0.38	19.17	53,53,53,53	0
35	NA	0	8562	1/1	0.82	0.48	16.17	70,70,70,70	0
35	NA	0	8556	1/1	0.87	0.46	15.97	61,61,61,61	0
35	NA	0	8571	1/1	0.61	0.30	15.84	59,59,59,59	0
33	MG	0	8114	1/1	0.91	0.34	14.37	54,54,54,54	0
35	NA	0	8565	1/1	0.82	0.59	13.87	47,47,47,47	0
35	NA	0	8526	1/1	0.94	0.30	12.44	70,70,70,70	0
35	NA	0	8521	1/1	0.83	0.41	12.28	77,77,77,77	0
35	NA	0	8555	1/1	0.88	1.00	12.03	85,85,85,85	0
35	NA	0	8572	1/1	0.88	0.39	11.50	73,73,73,73	0
35	NA	0	8564	1/1	0.78	0.37	10.28	49,49,49,49	0
35	NA	0	8503	1/1	0.99	0.30	10.12	1,1,1,1	0
35	NA	0	8568	1/1	0.84	0.20	9.83	87,87,87,87	0
35	NA	0	8540	1/1	0.93	0.26	9.76	50,50,50,50	0
35	NA	0	8532	1/1	0.90	0.23	9.20	44,44,44,44	0
35	NA	0	8561	1/1	0.87	0.33	9.02	50,50,50,50	0
35	NA	0	8539	1/1	0.93	0.30	8.52	40,40,40,40	0
33	MG	0	8102	1/1	0.72	0.28	8.08	50,50,50,50	0
35	NA	0	8573	1/1	0.97	0.20	7.40	56,56,56,56	0
35	NA	0	8535	1/1	0.74	0.34	7.34	54,54,54,54	0
33	MG	0	8062	1/1	0.90	0.22	7.18	13,13,13,13	0
35	NA	0	8566	1/1	0.83	0.17	5.90	48,48,48,48	0
35	NA	0	8520	1/1	0.96	0.23	5.50	36,36,36,36	0
35	NA	0	8527	1/1	0.79	0.24	5.24	61,61,61,61	0
35	NA	0	8515	1/1	0.87	0.22	4.77	49,49,49,49	0
35	NA	0	8579	1/1	0.86	0.23	4.76	65,65,65,65	0
35	NA	0	8523	1/1	0.99	0.23	4.29	38,38,38,38	0
35	NA	0	8582	1/1	0.73	0.21	4.22	85,85,85,85	0
35	NA	R	8586	1/1	0.95	0.35	3.70	23,23,23,23	0
33	MG	0	8013	1/1	0.88	0.20	3.66	38,38,38,38	0
35	NA	0	8543	1/1	0.98	0.20	3.63	35,35,35,35	0
35	NA	L	8580	1/1	0.98	0.24	3.60	1,1,1,1	0
32	13T	0	9000	42/42	0.86	0.25	3.41	58,67,73,74	0
35	NA	0	8569	1/1	0.69	0.25	2.85	64,64,64,64	0
35	NA	0	8505	1/1	0.91	0.23	2.73	37,37,37,37	0
35	NA	9	8583	1/1	0.74	0.15	1.91	73,73,73,73	0
36	CL	0	8805	1/1	0.99	0.13	1.56	71,71,71,71	0
33	MG	B	8055	1/1	0.95	0.15	1.56	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8012	1/1	0.99	0.14	1.30	39,39,39,39	0
33	MG	0	8018	1/1	0.90	0.15	1.13	39,39,39,39	0
33	MG	0	8060	1/1	0.98	0.17	0.92	45,45,45,45	0
35	NA	0	8510	1/1	0.73	0.14	0.83	45,45,45,45	0
33	MG	0	8084	1/1	0.82	0.14	0.78	58,58,58,58	0
33	MG	0	8054	1/1	0.97	0.16	0.70	30,30,30,30	0
35	NA	J	8546	1/1	0.76	0.25	0.70	39,39,39,39	0
35	NA	0	8533	1/1	0.92	0.12	0.60	39,39,39,39	0
33	MG	0	8004	1/1	0.96	0.18	0.55	37,37,37,37	0
35	NA	A	8545	1/1	0.94	0.16	0.29	61,61,61,61	0
36	CL	J	8821	1/1	0.87	0.21	0.14	77,77,77,77	0
33	MG	Y	8109	1/1	0.88	0.16	-0.01	44,44,44,44	0
33	MG	0	8007	1/1	0.97	0.17	-0.14	26,26,26,26	0
33	MG	0	8096	1/1	0.48	0.11	-0.39	48,48,48,48	0
33	MG	0	8107	1/1	0.98	0.12	-0.40	38,38,38,38	0
33	MG	0	8038	1/1	0.95	0.12	-0.51	31,31,31,31	0
35	NA	0	8576	1/1	0.98	0.16	-0.61	33,33,33,33	0
36	CL	0	8816	1/1	0.80	0.13	-0.63	69,69,69,69	0
37	CD	U	8701	1/1	0.99	0.10	-0.83	67,67,67,67	0
33	MG	0	8015	1/1	0.85	0.17	-0.83	35,35,35,35	0
35	NA	0	8524	1/1	0.80	0.11	-1.00	48,48,48,48	0
33	MG	0	8017	1/1	0.97	0.16	-1.09	31,31,31,31	0
33	MG	A	8065	1/1	0.96	0.14	-1.14	45,45,45,45	0
33	MG	0	8086	1/1	0.96	0.07	-1.14	42,42,42,42	0
35	NA	0	8509	1/1	0.72	0.11	-1.16	48,48,48,48	0
35	NA	Q	8548	1/1	0.94	0.11	-1.17	46,46,46,46	0
33	MG	0	8080	1/1	0.63	0.15	-1.18	39,39,39,39	0
34	K	0	8402	1/1	0.95	0.13	-1.20	61,61,61,61	0
35	NA	0	8517	1/1	0.77	0.12	-1.30	37,37,37,37	0
36	CL	0	8812	1/1	0.86	0.09	-1.33	49,49,49,49	0
33	MG	0	8077	1/1	0.96	0.16	-1.37	36,36,36,36	0
33	MG	0	8001	1/1	0.93	0.12	-1.39	44,44,44,44	0
37	CD	Z	8703	1/1	0.96	0.09	-1.42	71,71,71,71	0
33	MG	0	8020	1/1	0.90	0.12	-1.47	39,39,39,39	0
36	CL	3	8804	1/1	0.96	0.09	-1.51	56,56,56,56	0
37	CD	3	8704	1/1	0.98	0.08	-1.54	65,65,65,65	0
37	CD	O	8705	1/1	0.88	0.10	-1.63	186,186,186,186	0
33	MG	3	8078	1/1	0.94	0.10	-1.68	16,16,16,16	0
37	CD	1	8702	1/1	0.99	0.08	-1.76	65,65,65,65	0
33	MG	0	8053	1/1	0.96	0.13	-1.87	43,43,43,43	0
33	MG	0	8010	1/1	0.91	0.16	-1.95	11,11,11,11	0
33	MG	0	8074	1/1	0.95	0.04	-1.97	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	CL	M	8818	1/1	0.96	0.09	-2.00	44,44,44,44	0
36	CL	O	8808	1/1	0.88	0.09	-2.06	67,67,67,67	0
33	MG	0	8064	1/1	0.99	0.10	-2.10	41,41,41,41	0
33	MG	0	8035	1/1	0.84	0.11	-2.11	46,46,46,46	0
33	MG	T	8073	1/1	0.96	0.10	-2.15	57,57,57,57	0
33	MG	0	8091	1/1	0.91	0.10	-2.34	65,65,65,65	0
33	MG	0	8056	1/1	0.97	0.10	-2.47	56,56,56,56	0
33	MG	0	8032	1/1	0.97	0.07	-2.47	35,35,35,35	0
35	NA	0	8538	1/1	0.46	0.09	-2.60	55,55,55,55	0
36	CL	B	8819	1/1	0.91	0.10	-2.77	53,53,53,53	0
33	MG	0	8006	1/1	0.95	0.09	-2.80	36,36,36,36	0
33	MG	0	8028	1/1	0.90	0.06	-2.97	33,33,33,33	0
33	MG	0	8067	1/1	0.93	0.09	-3.03	37,37,37,37	0
35	NA	0	8578	1/1	0.97	0.10	-3.04	57,57,57,57	0
33	MG	0	8003	1/1	0.98	0.10	-3.06	36,36,36,36	0
33	MG	0	8014	1/1	1.00	0.10	-3.12	41,41,41,41	0
33	MG	0	8101	1/1	0.96	0.08	-3.28	45,45,45,45	0
33	MG	0	8008	1/1	0.89	0.08	-3.34	29,29,29,29	0
35	NA	0	8514	1/1	0.96	0.10	-3.35	38,38,38,38	0
33	MG	0	8058	1/1	0.86	0.11	-3.69	42,42,42,42	0
33	MG	0	8039	1/1	0.99	0.07	-3.79	64,64,64,64	0
35	NA	0	8553	1/1	0.98	0.11	-4.08	44,44,44,44	0
35	NA	M	8547	1/1	0.90	0.07	-4.37	41,41,41,41	0
33	MG	0	8021	1/1	0.94	0.09	-4.46	37,37,37,37	0
33	MG	0	8112	1/1	0.84	0.06	-5.25	39,39,39,39	0
33	MG	0	8088	1/1	0.92	0.10	-5.30	33,33,33,33	0
33	MG	0	8057	1/1	0.85	0.05	-5.46	41,41,41,41	0
33	MG	K	8069	1/1	0.82	0.06	-5.62	51,51,51,51	0
33	MG	0	8048	1/1	0.95	0.09	-5.78	49,49,49,49	0
33	MG	0	8002	1/1	0.97	0.03	-6.34	40,40,40,40	0
33	MG	0	8044	1/1	0.93	0.08	-7.01	55,55,55,55	0
35	NA	0	8544	1/1	0.86	0.07	-7.38	29,29,29,29	0
33	MG	0	8033	1/1	0.94	0.04	-8.56	38,38,38,38	0
33	MG	0	8108	1/1	0.95	0.03	-8.68	77,77,77,77	0
33	MG	0	8019	1/1	0.94	0.04	-10.99	34,34,34,34	0
35	NA	0	8541	1/1	0.94	0.10	-	46,46,46,46	0
35	NA	S	8512	1/1	0.87	0.43	-	57,57,57,57	0
33	MG	0	8041	1/1	0.96	0.22	-	68,68,68,68	0
33	MG	0	8090	1/1	0.90	0.23	-	73,73,73,73	0
35	NA	0	8516	1/1	0.78	0.43	-	49,49,49,49	0
35	NA	H	8522	1/1	0.79	0.35	-	77,77,77,77	0
33	MG	0	8024	1/1	0.84	0.99	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8100	1/1	0.71	0.10	-	42,42,42,42	0
33	MG	0	8117	1/1	0.69	0.09	-	34,34,34,34	0
36	CL	0	8815	1/1	0.64	0.14	-	89,89,89,89	0
35	NA	0	8585	1/1	0.61	0.38	-	65,65,65,65	0
33	MG	0	8046	1/1	0.72	0.07	-	56,56,56,56	0
33	MG	0	8113	1/1	0.23	0.16	-	44,44,44,44	0
35	NA	0	8560	1/1	0.74	0.24	-	60,60,60,60	0
35	NA	0	8507	1/1	0.54	0.24	-	69,69,69,69	0
35	NA	0	8529	1/1	0.83	0.10	-	68,68,68,68	0
33	MG	9	8095	1/1	0.77	0.15	-	77,77,77,77	0
33	MG	0	8116	1/1	0.86	0.10	-	56,56,56,56	0
33	MG	0	8106	1/1	0.99	0.07	-	71,71,71,71	0
33	MG	0	8045	1/1	0.76	0.12	-	67,67,67,67	0
33	MG	0	8076	1/1	0.87	0.06	-	49,49,49,49	0
35	NA	0	8534	1/1	0.94	0.07	-	40,40,40,40	0
33	MG	0	8023	1/1	0.92	0.24	-	61,61,61,61	0
33	MG	0	8093	1/1	0.92	0.10	-	61,61,61,61	0
33	MG	0	8068	1/1	0.98	0.09	-	56,56,56,56	0
35	NA	0	8542	1/1	0.91	0.29	-	15,15,15,15	0
33	MG	0	8071	1/1	0.82	0.07	-	50,50,50,50	0
33	MG	0	8011	1/1	0.89	0.18	-	39,39,39,39	0
33	MG	0	8043	1/1	0.95	0.13	-	47,47,47,47	0
36	CL	0	8813	1/1	0.95	0.06	-	54,54,54,54	0
35	NA	0	8519	1/1	0.99	0.16	-	17,17,17,17	0
33	MG	0	8083	1/1	0.93	0.07	-	41,41,41,41	0
33	MG	0	8059	1/1	0.97	0.05	-	39,39,39,39	0
33	MG	0	8087	1/1	0.96	0.09	-	63,63,63,63	0
33	MG	0	8027	1/1	0.99	0.03	-	40,40,40,40	0
33	MG	0	8098	1/1	0.95	0.11	-	42,42,42,42	0
33	MG	0	8111	1/1	0.68	0.08	-	46,46,46,46	0
33	MG	0	8115	1/1	0.90	0.07	-	45,45,45,45	0
35	NA	0	8528	1/1	0.68	0.51	-	54,54,54,54	0
36	CL	0	8822	1/1	0.86	0.48	-	90,90,90,90	0
35	NA	0	8552	1/1	0.92	0.13	-	68,68,68,68	0
36	CL	J	8801	1/1	0.95	0.06	-	58,58,58,58	0
33	MG	0	8104	1/1	0.54	0.37	-	78,78,78,78	0
35	NA	0	8549	1/1	0.93	0.26	-	53,53,53,53	0
33	MG	0	8029	1/1	0.89	0.12	-	42,42,42,42	0
33	MG	0	8082	1/1	0.97	0.34	-	84,84,84,84	0
33	MG	0	8009	1/1	0.97	0.15	-	36,36,36,36	0
33	MG	0	8042	1/1	0.95	0.05	-	33,33,33,33	0
36	CL	N	8807	1/1	0.88	0.14	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8050	1/1	0.93	0.19	-	74,74,74,74	0
33	MG	0	8061	1/1	0.84	0.15	-	44,44,44,44	0
33	MG	3	8118	1/1	0.98	0.21	-	50,50,50,50	0
33	MG	0	8092	1/1	0.95	0.12	-	72,72,72,72	0
33	MG	0	8103	1/1	0.92	0.19	-	78,78,78,78	0
36	CL	L	8810	1/1	0.84	0.10	-	59,59,59,59	0
35	NA	0	8536	1/1	0.95	0.07	-	54,54,54,54	0
33	MG	0	8049	1/1	0.93	0.17	-	36,36,36,36	0
33	MG	0	8094	1/1	0.79	0.15	-	59,59,59,59	0
33	MG	A	8066	1/1	0.96	0.05	-	73,73,73,73	0
35	NA	0	8563	1/1	0.90	0.42	-	68,68,68,68	0
36	CL	Y	8817	1/1	0.95	0.15	-	70,70,70,70	0
35	NA	R	8537	1/1	0.94	0.14	-	45,45,45,45	0
33	MG	0	8016	1/1	0.97	0.07	-	18,18,18,18	0
36	CL	0	8814	1/1	0.96	0.11	-	57,57,57,57	0
35	NA	0	8584	1/1	0.77	0.69	-	90,90,90,90	0
35	NA	0	8567	1/1	0.91	0.46	-	61,61,61,61	0
33	MG	0	8040	1/1	0.92	0.34	-	53,53,53,53	0
35	NA	0	8518	1/1	0.89	0.35	-	58,58,58,58	0
33	MG	0	8110	1/1	0.99	0.10	-	53,53,53,53	0
35	NA	0	8554	1/1	0.90	0.15	-	42,42,42,42	0
35	NA	0	8506	1/1	0.77	0.74	-	49,49,49,49	0
33	MG	0	8079	1/1	0.93	0.15	-	27,27,27,27	0
35	NA	9	8551	1/1	0.39	0.39	-	92,92,92,92	0
33	MG	0	8047	1/1	0.83	0.12	-	57,57,57,57	0
36	CL	A	8809	1/1	0.95	0.19	-	82,82,82,82	0
35	NA	0	8530	1/1	0.95	0.09	-	45,45,45,45	0
33	MG	0	8022	1/1	0.90	0.08	-	37,37,37,37	0
36	CL	0	8803	1/1	0.92	0.16	-	56,56,56,56	0
33	MG	0	8075	1/1	0.77	0.06	-	56,56,56,56	0
33	MG	0	8031	1/1	0.91	0.10	-	30,30,30,30	0
33	MG	0	8081	1/1	0.90	0.13	-	43,43,43,43	0
35	NA	0	8558	1/1	0.89	0.55	-	75,75,75,75	0
36	CL	0	8811	1/1	0.99	0.11	-	58,58,58,58	0
35	NA	0	8557	1/1	0.87	0.13	-	45,45,45,45	0
33	MG	0	8063	1/1	0.82	0.09	-	63,63,63,63	0
35	NA	C	8504	1/1	0.85	0.08	-	35,35,35,35	0
33	MG	0	8025	1/1	0.93	0.10	-	43,43,43,43	0
33	MG	0	8070	1/1	0.93	0.15	-	43,43,43,43	0
33	MG	0	8034	1/1	0.96	0.10	-	25,25,25,25	0
36	CL	R	8806	1/1	0.99	0.03	-	49,49,49,49	0
35	NA	0	8501	1/1	0.99	0.06	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8099	1/1	0.95	0.33	-	70,70,70,70	0
35	NA	0	8502	1/1	0.67	0.20	-	57,57,57,57	0
33	MG	0	8005	1/1	0.96	0.10	-	32,32,32,32	0
35	NA	0	8570	1/1	0.94	0.39	-	65,65,65,65	0
33	MG	0	8072	1/1	0.85	0.09	-	57,57,57,57	0
35	NA	0	8511	1/1	0.98	0.12	-	56,56,56,56	0
33	MG	0	8030	1/1	0.99	0.07	-	35,35,35,35	0
35	NA	0	8513	1/1	0.55	0.07	-	72,72,72,72	0
36	CL	J	8802	1/1	0.91	0.15	-	76,76,76,76	0
33	MG	0	8036	1/1	0.92	0.06	-	41,41,41,41	0
33	MG	0	8085	1/1	0.95	0.12	-	48,48,48,48	0
35	NA	0	8581	1/1	0.81	0.08	-	42,42,42,42	0
35	NA	0	8508	1/1	0.96	0.26	-	58,58,58,58	0
33	MG	0	8089	1/1	0.92	0.13	-	62,62,62,62	0
33	MG	0	8097	1/1	0.85	0.07	-	45,45,45,45	0
33	MG	0	8051	1/1	0.95	0.12	-	56,56,56,56	0
33	MG	0	8052	1/1	0.81	0.13	-	68,68,68,68	0
35	NA	0	8575	1/1	0.75	0.32	-	72,72,72,72	0
36	CL	Y	8820	1/1	0.98	0.05	-	44,44,44,44	0
33	MG	0	8026	1/1	0.98	0.09	-	33,33,33,33	0
33	MG	0	8037	1/1	0.93	0.07	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.