Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID	:	3CXC
Title	:	The structure of an enhanced oxazolidinone inhibitor bound to the 50S ribosomal subunit of H. marismortui
Authors	:	Ippolito, J.A.; Wang, D.; Kanyo, Z.F.; Duffy, E.M.
Deposited on	:	2008-04-24
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

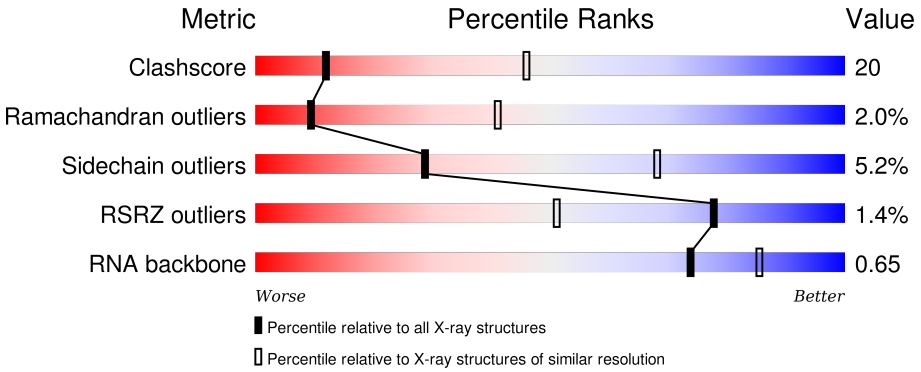
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	% 47% 40% 6% 6%
2	9	122	4% 38% 49% 11%
3	4	3	33% 33% 33%
4	A	239	% 54% 41% 5%
5	B	337	% 53% 42% 6%

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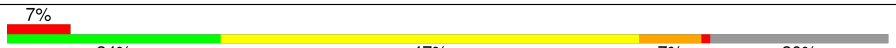
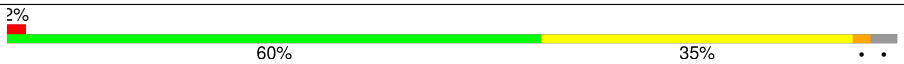
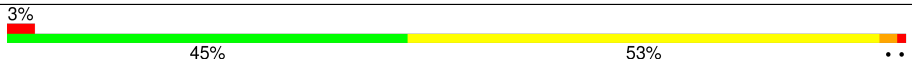
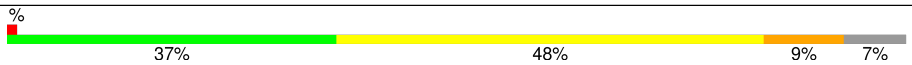
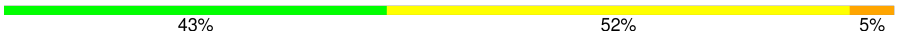
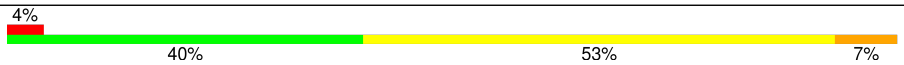
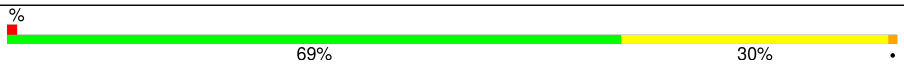
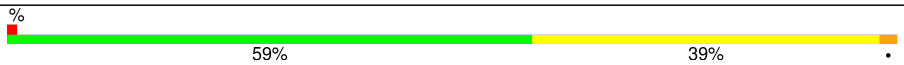
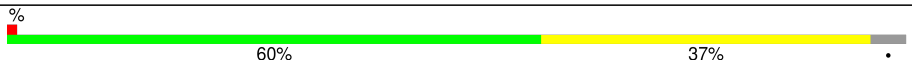
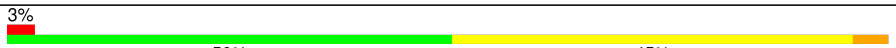
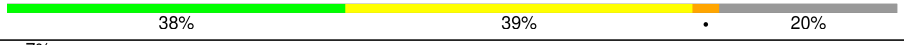
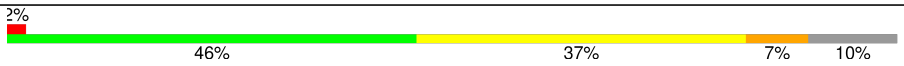
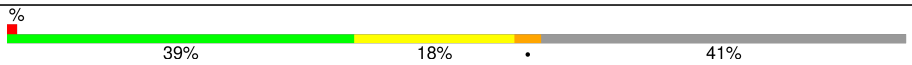
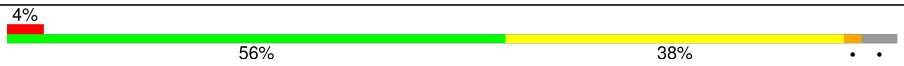
Mol	Chain	Length	Quality of chain
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	
29	Z	56	
30	1	48	

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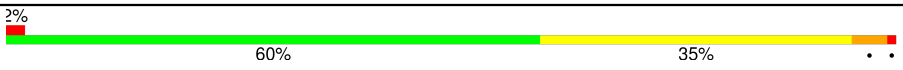
Mol	Chain	Length	Quality of chain
31	2	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8006	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8049	-	-	-	X
33	MG	0	8053	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8064	-	-	-	X
33	MG	0	8108	-	-	-	X
34	K	0	8202	-	-	-	X
35	NA	0	8303	-	-	-	X
35	NA	0	8308	-	-	-	X
35	NA	0	8310	-	-	-	X
35	NA	0	8320	-	-	-	X
35	NA	0	8321	-	-	-	X
35	NA	0	8323	-	-	-	X
35	NA	0	8324	-	-	-	X
35	NA	0	8325	-	-	-	X
35	NA	0	8326	-	-	-	X
35	NA	0	8332	-	-	-	X
35	NA	0	8333	-	-	-	X
35	NA	0	8335	-	-	-	X
35	NA	0	8350	-	-	-	X
35	NA	0	8356	-	-	-	X
35	NA	0	8361	-	-	-	X
35	NA	0	8362	-	-	-	X
35	NA	0	8364	-	-	-	X
35	NA	0	8365	-	-	-	X
35	NA	0	8366	-	-	-	X
35	NA	0	8367	-	-	-	X
35	NA	0	8368	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8372	-	-	-	X
35	NA	0	8373	-	-	-	X
35	NA	0	8376	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8377	-	-	-	X
35	NA	0	8378	-	-	-	X
35	NA	0	8379	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	K	8380	-	-	-	X
35	NA	Q	8386	-	-	-	X
36	CL	0	8505	-	-	-	X
36	CL	2	8504	-	-	-	X
36	CL	B	8519	-	-	-	X
36	CL	I	8521	-	-	-	X
36	CL	J	8512	-	-	-	X
37	CD	2	8404	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98635 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	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	3	59	28	11	18	2	0	0	0

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	CONFLICT	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

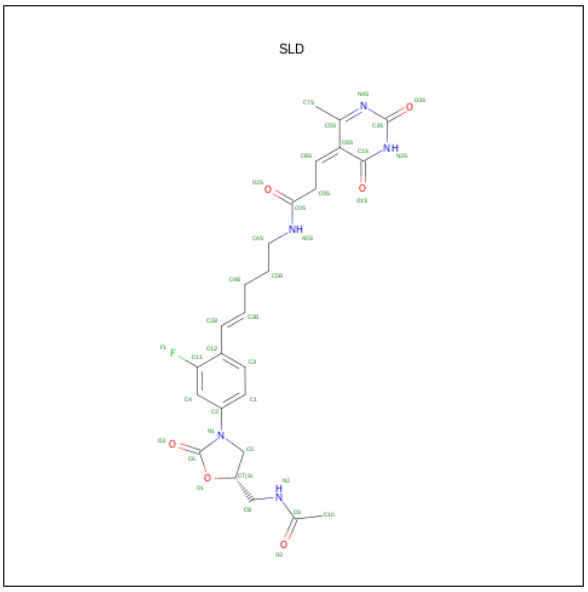
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is (3Z)-N-[(4E)-5-(4-{(5S)-5-[(ACETYLAMINO)METHYL]-2-OXO-1,3-OXAZOLIDIN-3-YL}-2-FLUOROPHENYL)PENT-4-EN-1-YL]-3-(4-METHYL-2,6-DIOXO-1,6-DIHYDROPYRIMIDIN-5(2H)-YLIDENE)PROPANAMIDE (three-letter code: SLD) (formula: $C_{25}H_{28}FN_5O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	F	N	O	0	0
			37	25	1	5	6		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	J	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	2	1	Total Mg 1 1	0	0
33	9	2	Total Mg 2 2	0	0
33	S	1	Total Mg 1 1	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	73	Total Na 73 73	0	0
35	P	1	Total Na 1 1	0	0
35	Q	2	Total Na 2 2	0	0
35	K	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	I	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0
35	L	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	8	Total Cl 8 8	0	0
36	P	1	Total Cl 1 1	0	0
36	J	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0
36	L	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	Z	1	Total Cd 1 1	0	0
37	Y	1	Total Cd 1 1	0	0
37	T	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	N	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5806	Total O 5806 5806	0	0
38	9	147	Total O 147 147	0	0
38	4	1	Total O 1 1	0	0
38	A	136	Total O 136 136	0	0
38	B	160	Total O 160 160	0	0
38	C	180	Total O 180 180	0	0
38	D	49	Total O 49 49	0	0
38	E	47	Total O 47 47	0	0
38	F	26	Total O 26 26	0	0
38	G	21	Total O 21 21	0	0
38	H	82	Total O 82 82	0	0
38	I	61	Total O 61 61	0	0
38	J	63	Total O 63 63	0	0
38	K	85	Total O 85 85	0	0
38	L	130	Total O 130 130	0	0
38	M	69	Total O 69 69	0	0
38	N	45	Total O 45 45	0	0
38	O	70	Total O 70 70	0	0
38	P	56	Total O 56 56	0	0
38	Q	92	Total O 92 92	0	0
38	R	40	Total O 40 40	0	0
38	S	37	Total O 37 37	0	0

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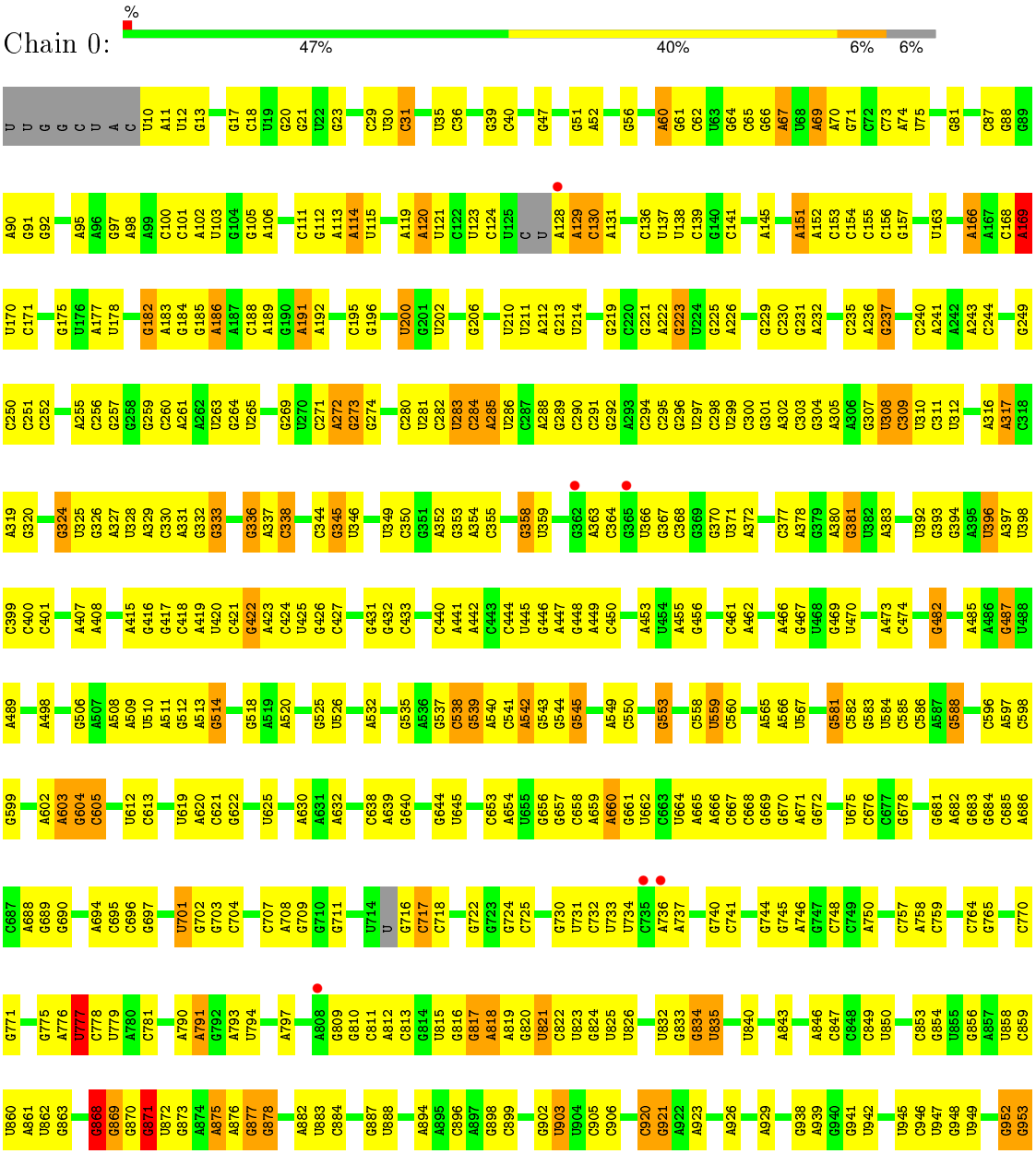
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	T	27	Total O 27 27	0	0
38	U	13	Total O 13 13	0	0
38	V	74	Total O 74 74	0	0
38	W	29	Total O 29 29	0	0
38	X	105	Total O 105 105	0	0
38	Y	41	Total O 41 41	0	0
38	Z	57	Total O 57 57	0	0
38	1	45	Total O 45 45	0	0
38	2	76	Total O 76 76	0	0

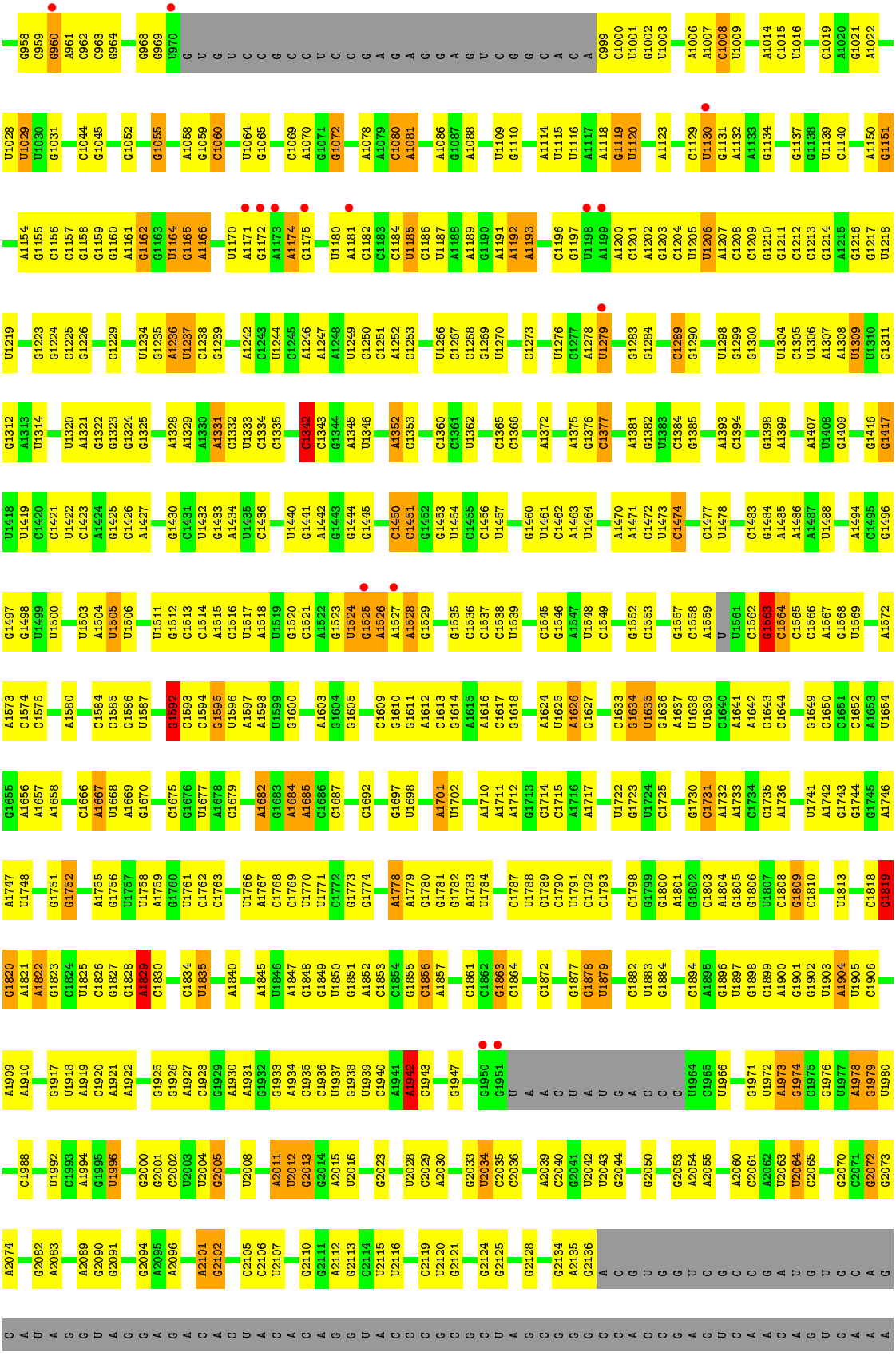
3 Residue-property plots (i)

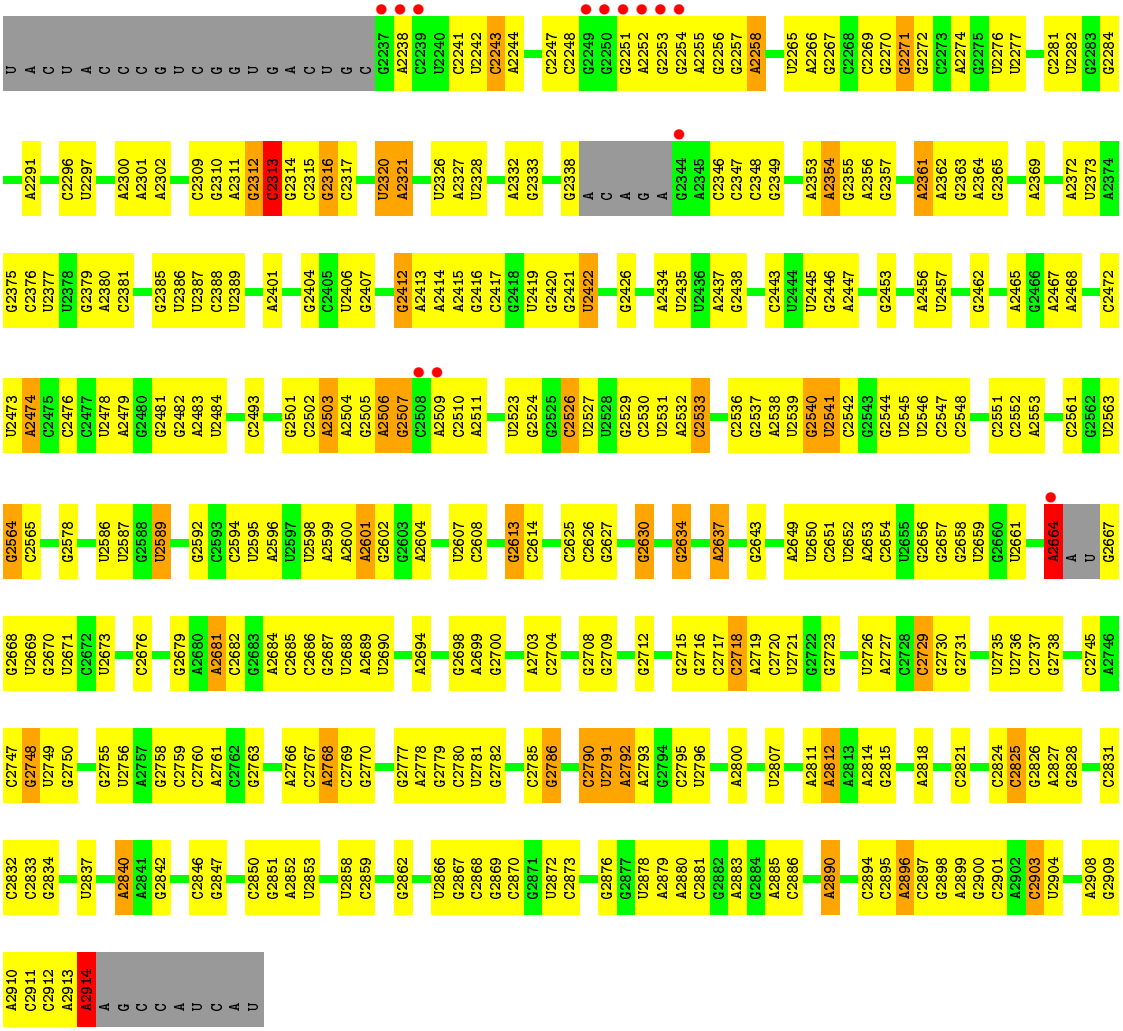
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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:

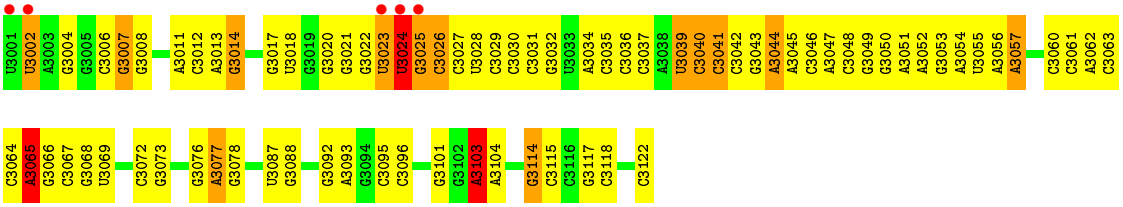






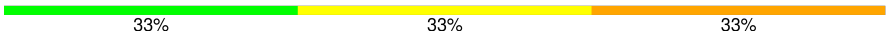
• Molecule 2: 5S RIBOSOMAL RNA

Chain 9:



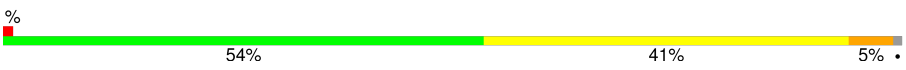
• Molecule 3: 5'-R(*CP*CP*A)-3'

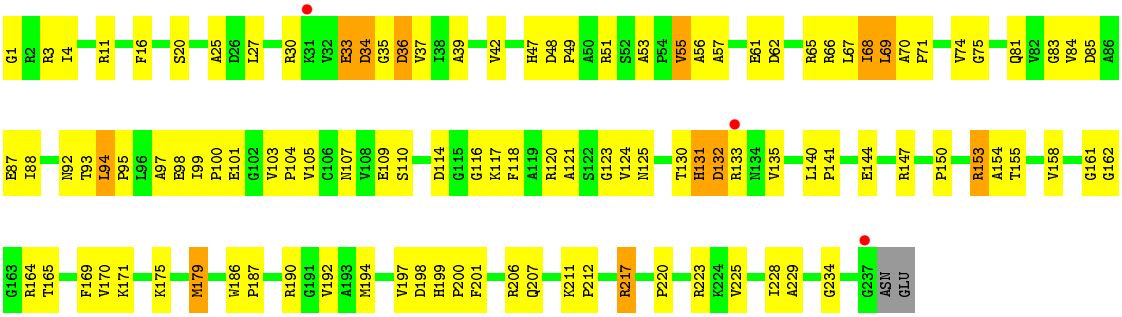
Chain 4:



• Molecule 4: RIBOSOMAL PROTEIN L2

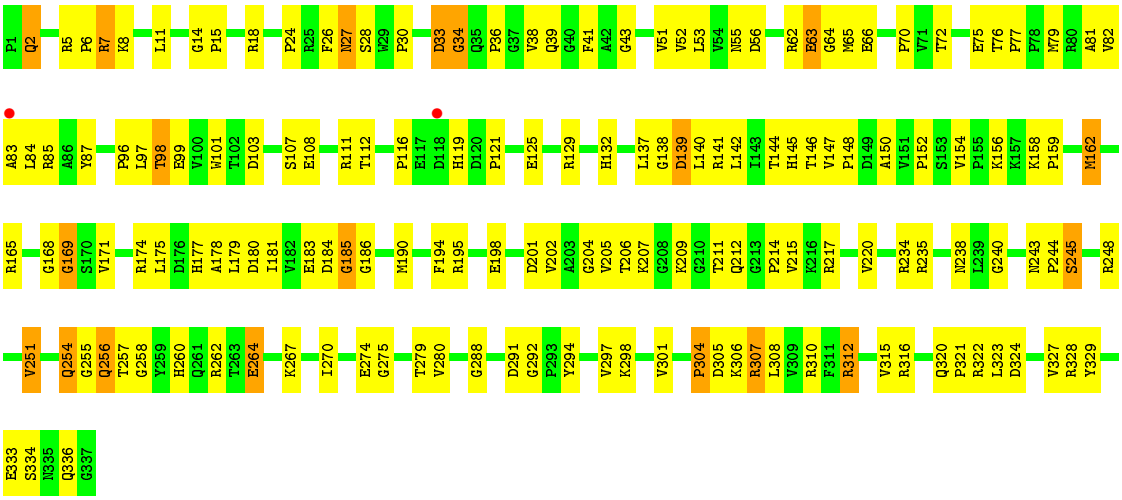
Chain A:





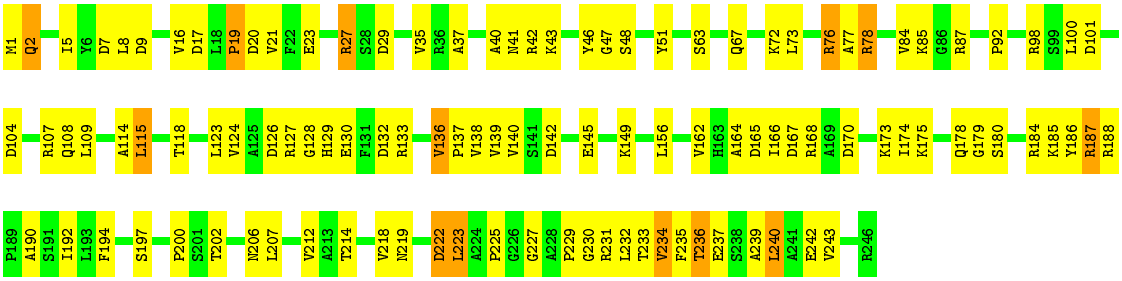
• Molecule 5: RIBOSOMAL PROTEIN L3

Chain B:



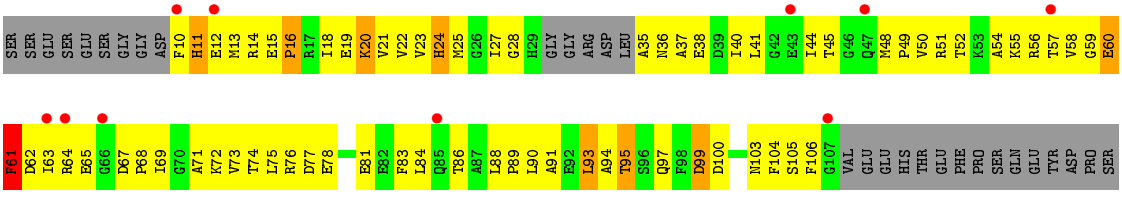
• Molecule 6: RIBOSOMAL PROTEIN L4

Chain C:



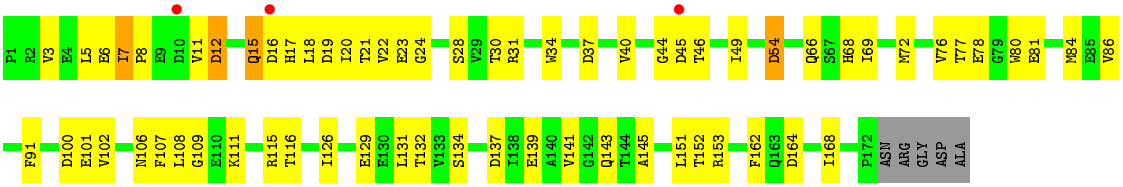
• Molecule 7: RIBOSOMAL PROTEIN L5

Chain D:



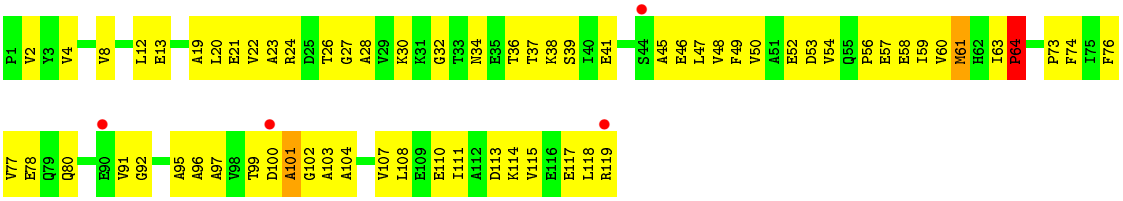
• Molecule 8: RIBOSOMAL PROTEIN L6

Chain E:



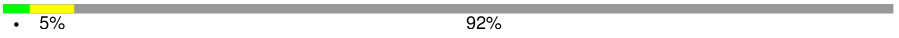
• Molecule 9: RIBOSOMAL PROTEIN L7AE

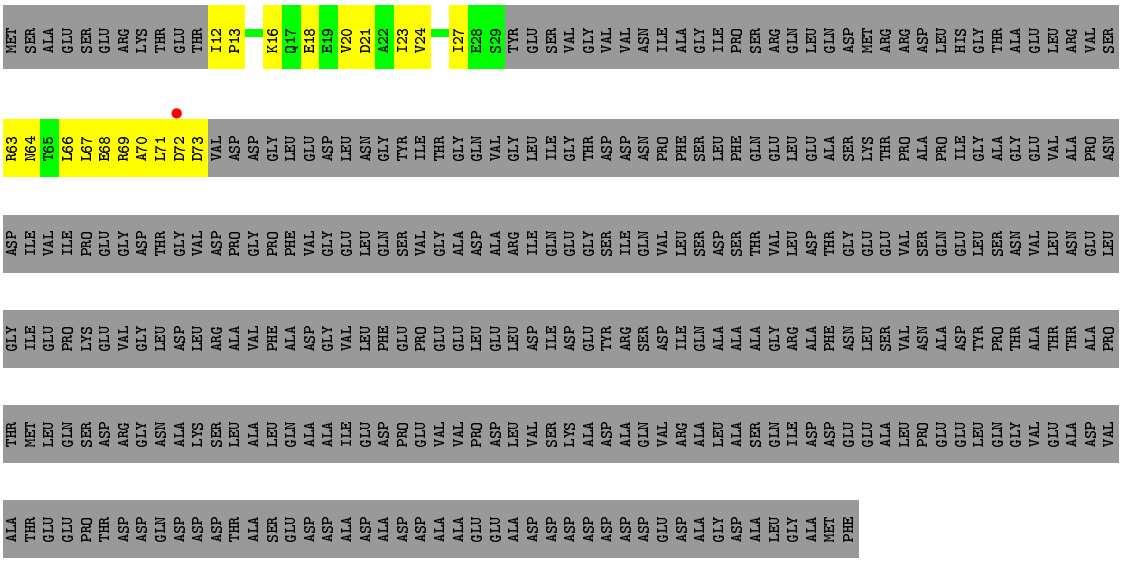
Chain F:



• Molecule 10: RIBOSOMAL PROTEIN L10

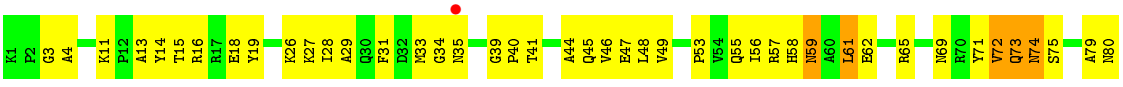
Chain G:

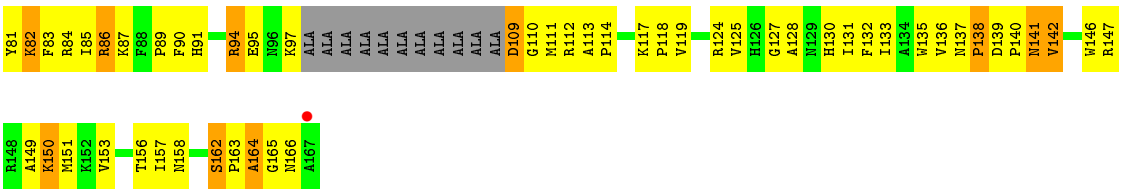




• Molecule 11: RIBOSOMAL PROTEIN L10E

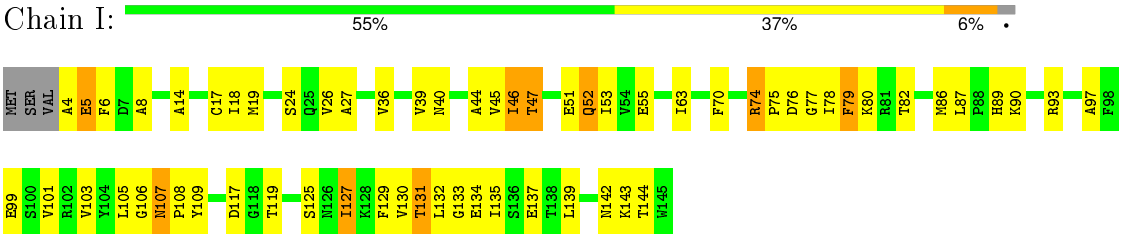
Chain H:





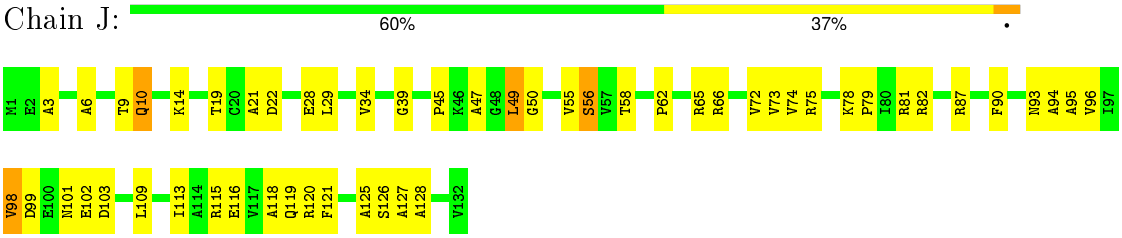
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I:



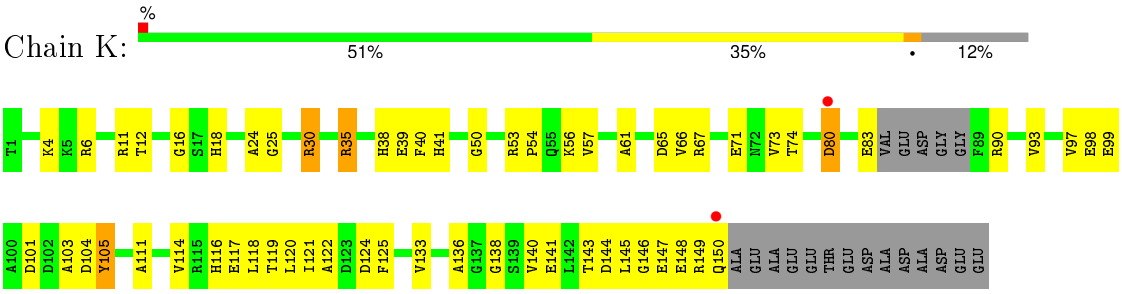
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J:



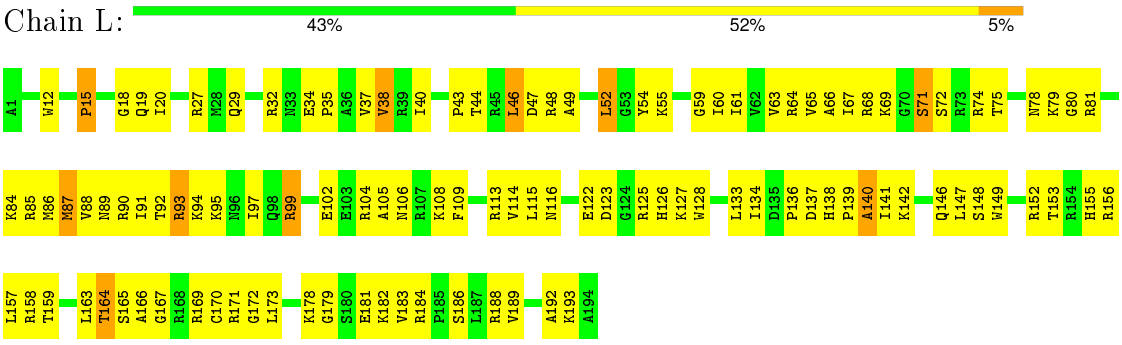
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K:



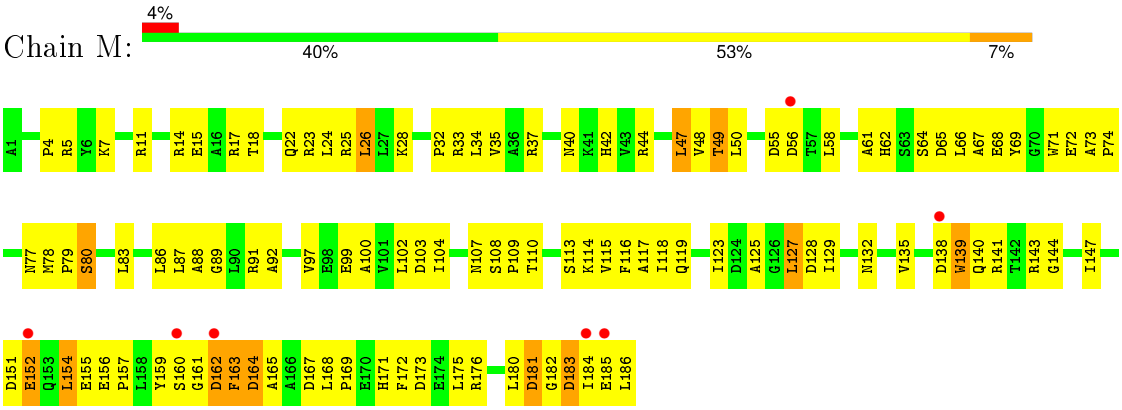
• Molecule 15: RIBOSOMAL PROTEIN L15E

Chain L:



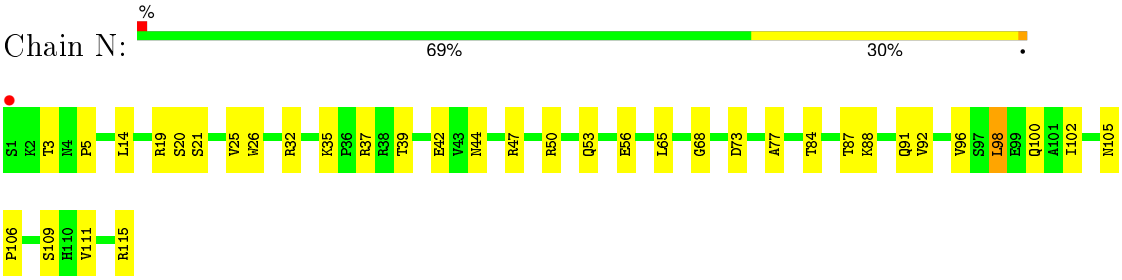
• Molecule 16: RIBOSOMAL PROTEIN L18

Chain M:



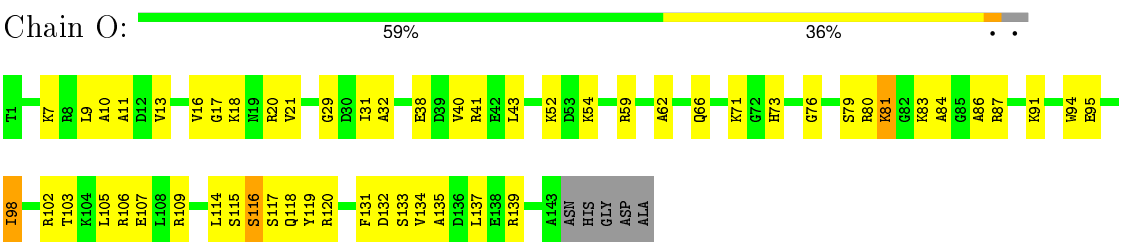
• Molecule 17: RIBOSOMAL PROTEIN L18E

Chain N:



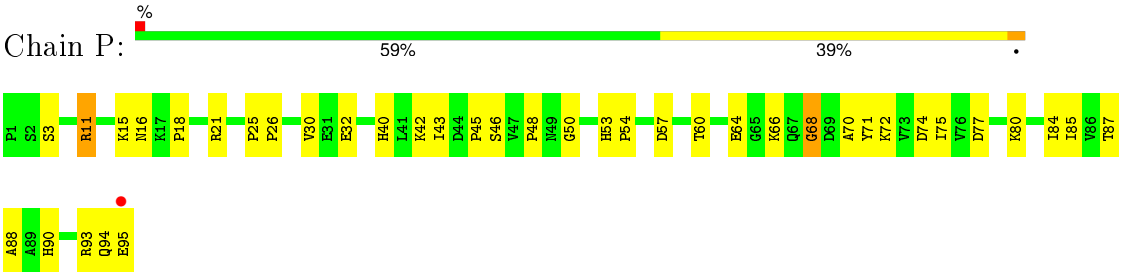
• Molecule 18: RIBOSOMAL PROTEIN L19E

Chain O:



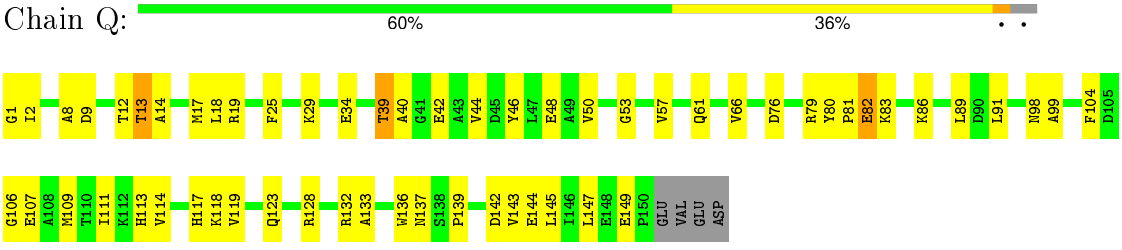
• Molecule 19: RIBOSOMAL PROTEIN L21E

Chain P:



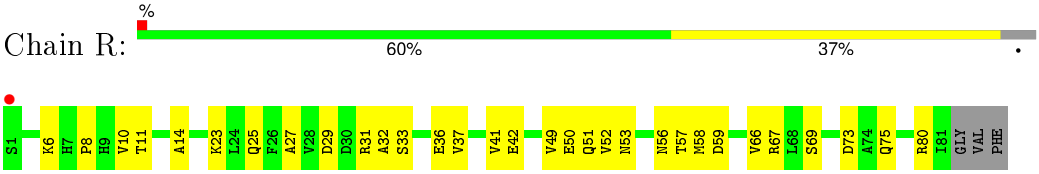
• Molecule 20: RIBOSOMAL PROTEIN L22

Chain Q:



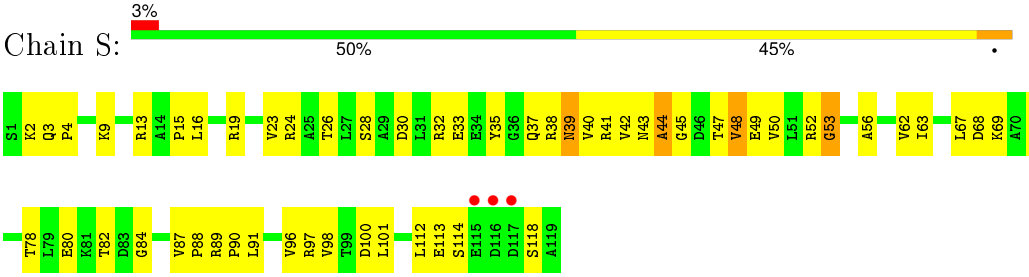
• Molecule 21: RIBOSOMAL PROTEIN L23

Chain R:



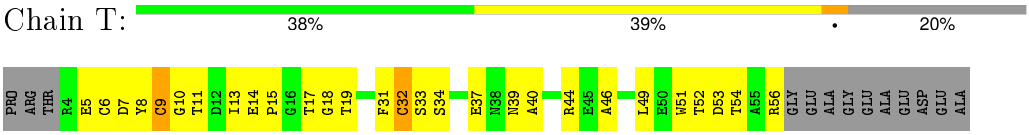
• Molecule 22: RIBOSOMAL PROTEIN L24

Chain S:



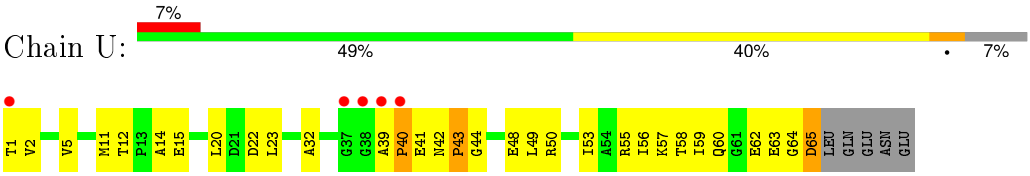
• Molecule 23: RIBOSOMAL PROTEIN L24E

Chain T:



• Molecule 24: RIBOSOMAL PROTEIN L29

Chain U:

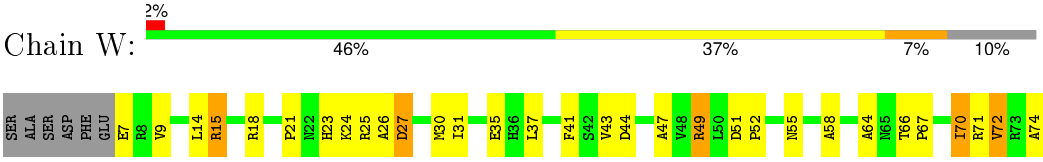


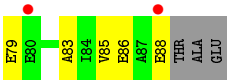
• Molecule 25: RIBOSOMAL PROTEIN L30

Chain V:

• Molecule 26: RIBOSOMAL PROTEIN L31E

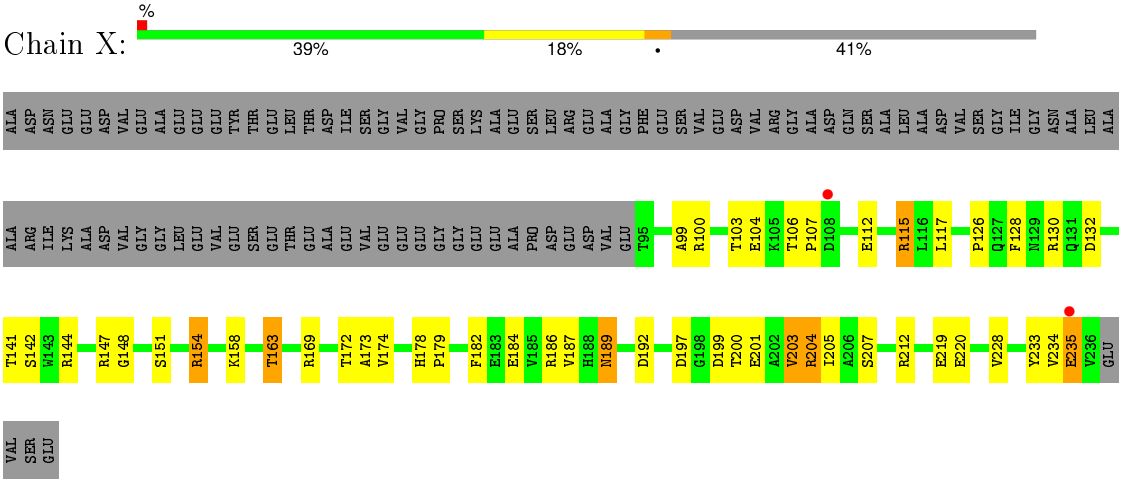
Chain W:





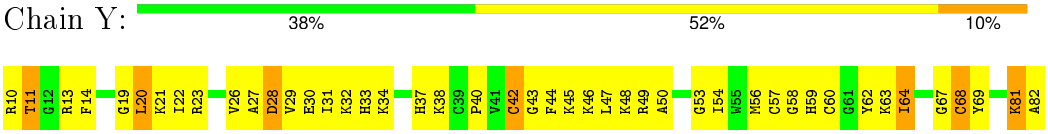
• Molecule 27: RIBOSOMAL PROTEIN L32E

Chain X:



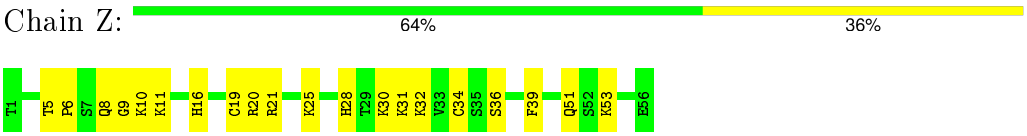
• Molecule 28: RIBOSOMAL PROTEIN L37AE

Chain Y:



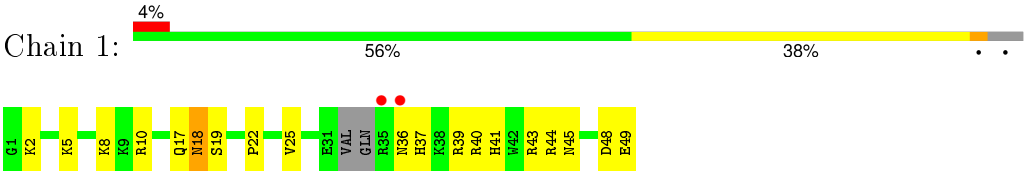
• Molecule 29: RIBOSOMAL PROTEIN L37E

Chain Z:



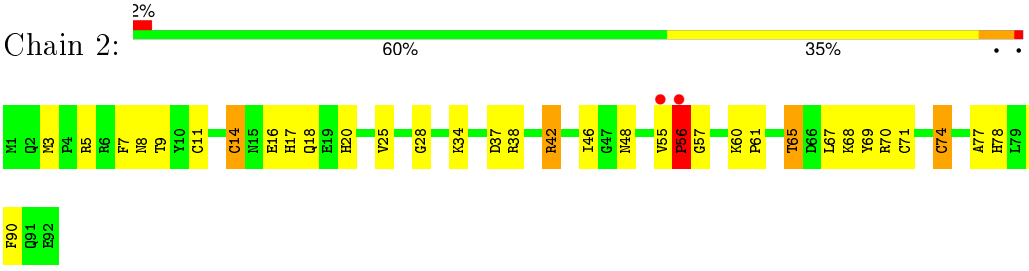
• Molecule 30: RIBOSOMAL PROTEIN L39E

Chain 1:



• Molecule 31: RIBOSOMAL PROTEIN L44E

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.66Å 300.71Å 575.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.00) 90.8 (20.00-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.98Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.186 , 0.229 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.5	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 360129 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	98635	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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, CL, NA, K, CD, SLD

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	0.52	4/66076 (0.0%)	0.71	23/103052 (0.0%)
2	9	0.46	0/2905	0.76	3/4528 (0.1%)
3	4	0.89	0/65	1.01	0/99
4	A	0.39	0/1787	0.70	0/2409
5	B	0.40	0/2690	0.68	0/3652
6	C	0.45	0/1884	0.71	0/2551
7	D	0.37	0/1111	0.62	0/1498
8	E	0.38	0/1382	0.61	0/1880
9	F	0.38	0/897	0.60	0/1219
10	G	0.38	0/241	0.58	0/324
11	H	0.44	0/1247	0.79	3/1686 (0.2%)
12	I	0.43	0/1136	0.65	0/1530
13	J	0.41	0/1004	0.72	0/1351
14	K	0.41	0/1130	0.71	0/1509
15	L	0.49	0/1634	0.75	1/2180 (0.0%)
16	M	0.39	0/1474	0.68	0/1999
17	N	0.41	0/874	0.67	0/1181
18	O	0.41	0/1143	0.60	0/1521
19	P	0.44	0/749	0.74	1/1005 (0.1%)
20	Q	0.44	0/1172	0.69	0/1578
21	R	0.38	0/648	0.62	0/875
22	S	0.40	0/958	0.69	0/1289
23	T	0.61	2/417 (0.5%)	0.68	0/562
24	U	0.36	0/502	0.60	0/675
25	V	0.43	0/1219	0.67	0/1655
26	W	0.41	0/664	0.65	0/895
27	X	0.43	0/1146	0.68	0/1536
28	Y	0.54	1/576 (0.2%)	0.80	0/763
29	Z	0.54	0/438	0.78	2/578 (0.3%)
30	1	0.43	0/399	0.58	0/527
31	2	0.73	2/771 (0.3%)	0.72	0/1024
All	All	0.49	9/98339 (0.0%)	0.70	33/147131 (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	0	70
2	9	0	2
25	V	0	1
All	All	0	73

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	14	CYS	CB-SG	-12.55	1.60	1.82
1	0	2102	G	C6-O6	-6.72	1.18	1.24
28	Y	60	CYS	CB-SG	-6.10	1.71	1.82
1	0	2474	A	N1-C2	5.85	1.39	1.34
23	T	9	CYS	CB-SG	-5.75	1.72	1.81
31	2	74	CYS	CB-SG	-5.65	1.72	1.81
1	0	456	G	C6-O6	-5.58	1.19	1.24
23	T	32	CYS	CB-SG	-5.19	1.73	1.81
1	0	2474	A	C5-C6	5.03	1.45	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9	3024	U	C2'-C3'-O3'	8.48	128.16	109.50
1	0	1979	G	C2'-C3'-O3'	6.90	124.75	113.70
11	H	74	ASN	N-CA-C	-6.85	92.50	111.00
2	9	3103	A	C5'-C4'-O4'	6.75	117.20	109.10
1	0	1563	G	C2'-C3'-O3'	6.72	124.45	113.70
1	0	871	G	C5'-C4'-O4'	-6.35	101.48	109.10
1	0	1942	A	C5'-C4'-O4'	-6.12	101.76	109.10
29	Z	34	CYS	CA-CB-SG	-6.09	103.05	114.00
1	0	1559	A	C2'-C3'-O3'	6.08	123.42	113.70
19	P	68	GLY	N-CA-C	-6.05	97.98	113.10
1	0	1120	U	C5'-C4'-C3'	-5.95	106.48	116.00
15	L	52	LEU	CB-CG-CD1	-5.86	101.05	111.00
1	0	2338	G	C2'-C3'-O3'	5.85	123.06	113.70
1	0	1942	A	C5'-C4'-C3'	5.81	125.30	116.00
11	H	141	ASN	N-CA-C	-5.75	95.47	111.00
29	Z	19	CYS	CA-CB-SG	-5.71	103.72	114.00
1	0	2313	C	C5'-C4'-O4'	5.69	115.93	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1819	G	C5'-C4'-C3'	5.58	124.92	116.00
1	0	2664	A	N9-C1'-C2'	5.56	121.22	114.00
1	0	2914	A	C2'-C3'-O3'	5.53	122.55	113.70
1	0	1342	C	N1-C1'-C2'	-5.53	105.92	112.00
1	0	2316	G	C5'-C4'-C3'	-5.44	107.29	116.00
1	0	2313	C	O4'-C1'-N1	5.41	112.52	108.20
2	9	3039	U	N1-C1'-C2'	5.40	121.02	114.00
11	H	110	GLY	N-CA-C	-5.39	99.61	113.10
1	0	206	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	0	535	G	N9-C1'-C2'	5.34	120.94	114.00
1	0	1592	G	N9-C1'-C2'	5.25	120.82	114.00
1	0	169	A	C5'-C4'-O4'	-5.21	102.85	109.10
1	0	868	G	O4'-C1'-N9	5.19	112.36	108.20
1	0	1863	G	N9-C1'-C2'	-5.16	106.33	112.00
1	0	777	U	O4'-C1'-N1	5.10	112.28	108.20
1	0	2313	C	C5'-C4'-C3'	5.07	124.11	116.00

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1226	G	Sidechain
1	0	1236	A	Sidechain
1	0	1309	U	Sidechain
1	0	1342	C	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1595	G	Sidechain
1	0	1635	U	Sidechain
1	0	1744	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1822	A	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1933	G	Sidechain
1	0	1978	A	Sidechain
1	0	202	U	Sidechain
1	0	2023	G	Sidechain
1	0	223	G	Sidechain
1	0	2312	G	Sidechain
1	0	2313	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	261	A	Sidechain
1	0	2630	G	Sidechain
1	0	2637	A	Sidechain
1	0	2643	G	Sidechain
1	0	2673	U	Sidechain
1	0	2727	A	Sidechain
1	0	2729	C	Sidechain
1	0	2790	C	Sidechain
1	0	2793	A	Sidechain
1	0	2840	A	Sidechain
1	0	2853	U	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	422	G	Sidechain
1	0	469	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	532	A	Sidechain
1	0	619	U	Sidechain
1	0	664	U	Sidechain
1	0	722	G	Sidechain
1	0	781	C	Sidechain
1	0	791	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	868	G	Sidechain
1	0	903	U	Sidechain
1	0	939	A	Sidechain
1	0	952	G	Sidechain
2	9	3065	A	Sidechain
2	9	3087	U	Sidechain
25	V	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	59017	0	29800	1222	0
2	9	2600	0	1326	88	0
3	4	59	0	35	2	0
4	A	1754	0	1763	127	0
5	B	2625	0	2533	170	0
6	C	1859	0	1816	112	0
7	D	1094	0	1085	125	0
8	E	1357	0	1266	65	0
9	F	886	0	854	67	0
10	G	240	0	231	22	0
11	H	1216	0	1215	155	0
12	I	1120	0	1098	69	0
13	J	994	0	1027	57	0
14	K	1118	0	1076	64	0
15	L	1606	0	1676	142	0
16	M	1445	0	1401	139	0
17	N	865	0	873	35	0
18	O	1133	0	1127	57	0
19	P	735	0	729	29	0
20	Q	1149	0	1122	61	0
21	R	641	0	605	24	0
22	S	950	0	923	53	0
23	T	410	0	364	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	U	499	0	511	32	0
25	V	1196	0	1137	97	0
26	W	654	0	653	46	0
27	X	1130	0	1133	51	0
28	Y	564	0	598	54	0
29	Z	431	0	426	24	0
30	1	394	0	406	32	0
31	2	755	0	729	51	0
32	0	37	0	28	4	0
33	0	107	0	0	0	0
33	2	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	8	0	0	1	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	P	1	0	0	0	0
36	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	X	1	0	0	0	0
37	2	1	0	0	2	0
37	N	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5806	0	0	72	0
38	1	45	0	0	1	0
38	2	76	0	0	4	0
38	4	1	0	0	0	0
38	9	147	0	0	5	0
38	A	136	0	0	11	0
38	B	160	0	0	17	0
38	C	180	0	0	10	0
38	D	49	0	0	8	0
38	E	47	0	0	1	0
38	F	26	0	0	6	0
38	G	21	0	0	2	0
38	H	82	0	0	9	0
38	I	61	0	0	3	0
38	J	63	0	0	4	0
38	K	85	0	0	9	0
38	L	130	0	0	5	0
38	M	69	0	0	8	0
38	N	45	0	0	5	0
38	O	70	0	0	0	0
38	P	56	0	0	1	0
38	Q	92	0	0	4	0
38	R	40	0	0	1	0
38	S	37	0	0	3	0
38	T	27	0	0	2	0
38	U	13	0	0	1	0
38	V	74	0	0	6	0
38	W	29	0	0	3	0
38	X	105	0	0	4	0
38	Y	41	0	0	5	0
38	Z	57	0	0	1	0
All	All	98635	0	59566	2990	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 20.

All (2990) 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)
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.24	1.14
13:J:10:GLN:NE2	13:J:10:GLN:H	1.47	1.13
1:0:871:G:H8	1:0:871:G:H5'	1.13	1.10
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.66	1.08
15:L:87:MET:HB3	31:2:46:ILE:HD13	1.31	1.07
6:C:236:THR:HG22	6:C:239:ALA:H	1.17	1.07
15:L:164:THR:HG22	15:L:167:GLY:H	1.20	1.06
1:0:1160:G:H5'	1:0:1161:A:H5'	1.33	1.06
1:0:871:G:C8	1:0:871:G:H5'	1.90	1.06
13:J:10:GLN:N	13:J:10:GLN:HE21	1.54	1.05
22:S:71:VAL:HG11	22:S:90:PRO:HB3	1.37	1.05
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.74	1.03
1:0:156:C:H5"	15:L:171:ARG:HD3	1.36	1.03
2:9:3023:U:H3'	2:9:3024:U:H5"	1.39	1.03
11:H:86:ARG:HH11	11:H:133:ILE:HG13	0.87	1.02
2:9:3056:A:H2'	2:9:3057:A:H5"	1.40	1.02
1:0:1119:G:H2'	12:I:52:GLN:HE22	1.25	1.02
15:L:106:ASN:ND2	36:L:8518:CL:CL	2.30	1.02
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.43	1.01
11:H:45:GLN:HB3	11:H:163:PRO:HD2	1.42	0.99
1:0:1751:G:H2'	1:0:1752:G:H5"	1.44	0.99
2:9:3076:G:H3'	2:9:3077:A:H5"	1.44	0.99
5:B:238:ASN:HD22	5:B:240:GLY:H	1.08	0.98
13:J:62:PRO:HG3	13:J:65:ARG:HH21	1.29	0.96
11:H:162:SER:HB2	11:H:163:PRO:HD3	1.46	0.95
7:D:105:SER:HB2	7:D:131:THR:HG23	1.49	0.95
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.46	0.95
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.49	0.95
11:H:86:ARG:HH11	11:H:133:ILE:CG1	1.80	0.94
1:0:1164:U:H4'	1:0:1165:G:OP1	1.68	0.94
31:2:71:CYS:HG	37:2:8404:CD:CD	0.84	0.94
1:0:289:G:H22	1:0:363:A:H2	1.14	0.93
16:M:47:LEU:HD11	16:M:127:LEU:HD21	1.49	0.93
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.50	0.93
11:H:29:ALA:HB3	11:H:65:ARG:HH12	1.31	0.92
1:0:545:G:H8	1:0:545:G:H5'	1.34	0.92
1:0:870:G:H2'	1:0:871:G:H5"	1.51	0.92
1:0:1242:A:H5'	12:I:82:THR:HG23	1.51	0.92
2:9:3006:C:H5"	16:M:37:ARG:NH1	1.85	0.92
11:H:26:LYS:HD2	11:H:28:ILE:HD12	1.50	0.91
28:Y:46:LYS:HD3	28:Y:59:HIS:HB2	1.52	0.91
26:W:37:LEU:HD13	26:W:85:VAL:HG21	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1134:G:H4'	11:H:151:MET:HE1	1.53	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.14	0.90
31:2:71:CYS:SG	37:2:8404:CD:CD	1.79	0.90
18:O:115:SER:H	18:O:118:GLN:HE21	0.96	0.89
1:0:182:G:H4'	15:L:157:LEU:HD13	1.51	0.89
11:H:55:GLN:HE21	11:H:124:ARG:HE	1.14	0.89
28:Y:38:LYS:HG2	28:Y:45:LYS:HG2	1.54	0.89
2:9:3024:U:O2'	2:9:3025:G:H4'	1.73	0.88
7:D:25:MET:HE2	7:D:41:LEU:HG	1.54	0.88
1:0:1120:U:H6	1:0:1120:U:H5"	1.39	0.88
15:L:102:GLU:OE1	15:L:164:THR:HG21	1.72	0.88
27:X:187:VAL:HG23	27:X:192:ASP:HB2	1.56	0.88
26:W:15:ARG:HH11	26:W:15:ARG:HB3	1.37	0.87
7:D:154:LYS:HD2	7:D:154:LYS:H	1.38	0.87
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.57	0.87
11:H:139:ASP:N	11:H:140:PRO:HD3	1.90	0.87
7:D:27:ILE:HG22	7:D:28:GLY:H	1.37	0.87
1:0:1116:U:O2'	1:0:1118:A:H2	1.56	0.86
16:M:49:THR:HG22	16:M:56:ASP:HB2	1.56	0.86
20:Q:99:ALA:HB1	20:Q:109:MET:HE1	1.55	0.86
25:V:72:PRO:HG2	25:V:77:ALA:HB3	1.57	0.86
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.86
11:H:162:SER:HB2	11:H:163:PRO:CD	2.06	0.85
25:V:4:LEU:HD22	25:V:52:VAL:HG21	1.59	0.85
25:V:88:THR:HG23	25:V:110:GLN:NE2	1.91	0.85
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.58	0.85
11:H:26:LYS:HG2	11:H:28:ILE:H	1.42	0.84
1:0:2717:C:C2'	1:0:2718:C:H5"	2.07	0.84
30:1:41:HIS:H	30:1:45:ASN:HD22	1.24	0.84
18:O:103:THR:HA	18:O:106:ARG:NH1	1.91	0.84
1:0:506:G:H22	1:0:509:A:H5'	1.42	0.84
25:V:6:GLN:HB2	25:V:26:ILE:HD12	1.58	0.84
15:L:35:PRO:CG	15:L:38:VAL:HG23	2.06	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.85	0.83
1:0:56:G:H5"	24:U:50:ARG:HH12	1.43	0.83
28:Y:38:LYS:HE2	28:Y:45:LYS:HE2	1.60	0.83
8:E:6:GLU:HA	8:E:46:THR:HG22	1.58	0.83
12:I:131:THR:HG22	12:I:134:GLU:H	1.44	0.83
1:0:1771:U:H4'	28:Y:20:LEU:HD21	1.61	0.83
1:0:2717:C:H2'	1:0:2718:C:H5"	1.57	0.83
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:C:C2'	1:0:2503:A:H5'	2.09	0.83
18:O:115:SER:N	18:O:118:GLN:HE21	1.76	0.83
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.61	0.83
25:V:122:ARG:HH11	25:V:122:ARG:HG2	1.42	0.83
25:V:88:THR:HG22	25:V:89:ASP:H	1.44	0.83
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.62	0.82
11:H:27:LYS:H	11:H:58:HIS:HD2	1.23	0.82
15:L:106:ASN:HD22	15:L:114:VAL:HG23	1.44	0.82
26:W:76:ARG:HG3	26:W:76:ARG:HH11	1.44	0.82
7:D:37:ALA:O	7:D:40:ILE:HG12	1.80	0.82
4:A:194:MET:HE2	4:A:199:HIS:HB2	1.62	0.82
1:0:2502:C:H2'	1:0:2503:A:H5'	1.62	0.82
2:9:3023:U:H3'	2:9:3024:U:C5'	2.10	0.82
13:J:74:VAL:HG11	13:J:113:ILE:HG12	1.62	0.82
1:0:21:G:H5'	20:Q:2:ILE:HA	1.61	0.82
1:0:1450:C:H4'	1:0:1451:C:OP2	1.78	0.82
28:Y:28:ASP:O	28:Y:31:ILE:HG22	1.79	0.82
15:L:87:MET:HB2	15:L:91:ILE:HD11	1.61	0.81
5:B:27:ASN:H	5:B:27:ASN:HD22	1.25	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.81
6:C:142:ASP:OD1	6:C:237:GLU:HB3	1.81	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.93	0.81
1:0:1603:A:H5'	1:0:1605:G:O4'	1.80	0.81
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.62	0.81
1:0:870:G:C2'	1:0:871:G:H5"	2.11	0.81
22:S:9:LYS:HE3	22:S:13:ARG:NH1	1.95	0.81
1:0:2533:C:H6	1:0:2533:C:H5'	1.46	0.81
13:J:39:GLY:HA2	38:J:4183:HOH:O	1.78	0.80
24:U:1:THR:HG23	24:U:2:VAL:H	1.46	0.80
25:V:137:GLN:HE21	25:V:141:HIS:HE1	1.26	0.80
28:Y:37:HIS:HB2	28:Y:47:LEU:HB2	1.63	0.80
12:I:74:ARG:HB3	12:I:74:ARG:HH11	1.44	0.80
2:9:3056:A:C2'	2:9:3057:A:H5"	2.12	0.80
1:0:450:C:OP1	6:C:184:ARG:NH2	2.15	0.80
20:Q:39:THR:HG22	20:Q:42:GLU:H	1.47	0.79
11:H:45:GLN:HE21	11:H:135:TRP:HE1	1.31	0.79
1:0:2586:U:H3	1:0:2592:G:H22	1.30	0.79
11:H:139:ASP:H	11:H:140:PRO:HD3	1.47	0.79
4:A:36:ASP:OD2	4:A:85:ASP:HB2	1.83	0.79
4:A:194:MET:CE	4:A:199:HIS:HB2	2.13	0.79
1:0:2526:C:O2'	1:0:2527:U:H5'	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:87:LEU:HD12	16:M:186:LEU:HD21	1.65	0.79
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.64	0.79
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.64	0.79
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.63	0.79
2:9:3025:G:H3'	2:9:3026:C:C5'	2.13	0.78
31:2:70:ARG:HG2	31:2:77:ALA:HB2	1.65	0.78
1:0:1201:C:H5"	38:0:7119:HOH:O	1.83	0.78
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.64	0.78
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.64	0.78
1:0:2420:G:O2'	1:0:2421:G:H5'	1.82	0.78
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.19	0.78
4:A:69:LEU:HD21	4:A:120:ARG:HB3	1.65	0.78
15:L:139:PRO:O	15:L:140:ALA:HB3	1.81	0.78
24:U:12:THR:HG22	24:U:15:GLU:CG	2.12	0.78
1:0:2679:G:H2'	1:0:2681:A:OP2	1.82	0.78
1:0:1474:C:H6	1:0:1474:C:H5'	1.49	0.78
1:0:1164:U:H3	1:0:1192:A:H2	1.32	0.77
9:F:46:GLU:O	9:F:73:PRO:HD2	1.85	0.77
1:0:542:A:H5'	1:0:542:A:H8	1.48	0.77
13:J:14:LYS:HB2	13:J:45:PRO:HG2	1.65	0.77
21:R:33:SER:O	21:R:37:VAL:HG23	1.84	0.77
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.85	0.77
6:C:236:THR:HG22	6:C:239:ALA:N	1.98	0.77
1:0:1119:G:H2'	12:I:52:GLN:NE2	1.98	0.77
18:O:115:SER:OG	18:O:118:GLN:HG3	1.84	0.77
26:W:41:PHE:O	26:W:43:VAL:HG23	1.83	0.77
26:W:72:VAL:HG22	26:W:85:VAL:HG12	1.64	0.77
20:Q:8:ALA:HB1	20:Q:13:THR:HG21	1.66	0.77
15:L:164:THR:HG23	15:L:165:SER:N	2.00	0.77
20:Q:44:VAL:O	20:Q:48:GLU:HG3	1.85	0.77
2:9:3025:G:H3'	2:9:3026:C:H5'	1.64	0.77
1:0:1166:A:H1'	1:0:1192:A:C2	2.19	0.76
20:Q:99:ALA:HB1	20:Q:109:MET:CE	2.14	0.76
1:0:240:C:H4'	15:L:146:GLN:NE2	2.00	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.30	0.76
25:V:88:THR:HB	38:V:6679:HOH:O	1.83	0.76
13:J:29:LEU:HB3	13:J:55:VAL:HG11	1.65	0.76
1:0:2094:G:H4'	5:B:245:SER:HB3	1.66	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.52	0.76
25:V:21:LEU:HD22	25:V:26:ILE:HD11	1.67	0.76
1:0:282:C:H1'	1:0:368:C:N4	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:13:MET:HE3	25:V:17:ILE:HG22	1.67	0.76
5:B:238:ASN:ND2	5:B:240:GLY:H	1.81	0.76
7:D:19:GLU:O	7:D:20:LYS:HG2	1.85	0.76
25:V:4:LEU:HD23	25:V:54:PHE:HB3	1.67	0.76
16:M:7:LYS:HE3	19:P:21:ARG:O	1.86	0.76
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.66	0.76
11:H:75:SER:O	11:H:79:ALA:HB2	1.86	0.76
1:0:1751:G:C2'	1:0:1752:G:H5"	2.15	0.76
20:Q:106:GLY:HA2	20:Q:109:MET:HE3	1.67	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.86	0.76
2:9:3069:U:OP1	16:M:4:PRO:HG3	1.86	0.76
12:I:52:GLN:HG3	12:I:53:ILE:N	1.99	0.76
1:0:794:U:H3	1:0:819:A:H61	1.34	0.76
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.50	0.75
1:0:656:G:OP2	17:N:37:ARG:HD2	1.87	0.75
14:K:136:ALA:HB3	38:K:8579:HOH:O	1.86	0.75
1:0:871:G:H8	1:0:871:G:C5'	1.95	0.75
11:H:55:GLN:NE2	11:H:124:ARG:HE	1.85	0.75
1:0:1206:U:H6	1:0:1206:U:H5'	1.50	0.75
18:O:59:ARG:NH2	18:O:66:GLN:HE22	1.85	0.75
15:L:60:ILE:C	15:L:61:ILE:HD12	2.07	0.75
1:0:1116:U:HO2'	1:0:1118:A:H2	0.77	0.75
11:H:162:SER:CB	11:H:163:PRO:HD3	2.16	0.75
1:0:2502:C:H4'	11:H:151:MET:HG2	1.67	0.75
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.68	0.75
1:0:2890:A:H1'	23:T:56:ARG:NH2	2.02	0.75
5:B:125:GLU:O	5:B:129:ARG:HG3	1.86	0.75
6:C:139:VAL:HG13	38:C:8461:HOH:O	1.85	0.75
27:X:187:VAL:HG23	27:X:192:ASP:CB	2.17	0.75
16:M:113:SER:HB2	38:M:8559:HOH:O	1.86	0.74
31:2:25:VAL:HG22	31:2:68:LYS:HG3	1.68	0.74
1:0:21:G:C5'	20:Q:2:ILE:HA	2.17	0.74
10:G:12:ILE:N	10:G:13:PRO:HD3	2.01	0.74
1:0:1120:U:H5"	1:0:1120:U:C6	2.22	0.74
1:0:962:C:H1'	16:M:5:ARG:NH1	2.03	0.74
16:M:11:ARG:HG3	16:M:14:ARG:NH1	2.03	0.74
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.70	0.74
21:R:51:GLN:HE21	21:R:53:ASN:HD21	1.34	0.74
1:0:1160:G:H5'	1:0:1161:A:C5'	2.16	0.74
17:N:32:ARG:O	17:N:32:ARG:HD3	1.87	0.74
7:D:146:LYS:NZ	16:M:107:ASN:HD21	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.52	0.73
1:0:284:C:H4'	1:0:285:A:O5'	1.87	0.73
16:M:86:LEU:HD12	16:M:125:ALA:HB2	1.71	0.73
11:H:47:GLU:HB3	11:H:133:ILE:HD13	1.70	0.73
13:J:62:PRO:HG3	13:J:65:ARG:NH2	2.03	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.70	0.73
1:0:56:G:H5"	24:U:50:ARG:NH1	2.02	0.73
5:B:119:HIS:O	5:B:121:PRO:HD3	1.89	0.73
5:B:297:VAL:HB	38:B:8619:HOH:O	1.88	0.73
1:0:1834:C:H2'	1:0:1840:A:N6	2.03	0.73
15:L:104:ARG:O	15:L:108:LYS:HE2	1.88	0.73
1:0:2507:G:H2'	1:0:2510:C:H42	1.52	0.73
11:H:53:PRO:HG3	11:H:127:GLY:H	1.52	0.73
25:V:13:MET:HE1	25:V:18:GLN:HA	1.69	0.73
1:0:2851:G:O2'	1:0:2852:A:H5'	1.87	0.73
7:D:57:THR:HG23	7:D:63:ILE:HG22	1.71	0.73
1:0:1080:C:H4'	1:0:1081:A:OP1	1.87	0.73
11:H:59:ASN:HD22	11:H:59:ASN:N	1.87	0.72
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.24	0.72
11:H:130:HIS:CD2	11:H:133:ILE:HD11	2.24	0.72
2:9:3092:G:H2'	2:9:3093:A:C8	2.24	0.72
11:H:56:ILE:HG22	11:H:61:LEU:HD22	1.70	0.72
1:0:545:G:C8	1:0:545:G:H5'	2.23	0.72
1:0:541:C:C2'	1:0:542:A:H5"	2.20	0.72
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.72	0.72
16:M:184:ILE:HG22	16:M:185:GLU:HG3	1.70	0.72
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.71	0.72
1:0:603:A:H5"	1:0:604:G:OP1	1.88	0.72
10:G:16:LYS:O	10:G:20:VAL:HG23	1.89	0.72
1:0:447:A:OP1	22:S:2:LYS:HG2	1.90	0.72
16:M:159:TYR:HB3	16:M:162:ASP:HB2	1.72	0.72
20:Q:9:ASP:O	20:Q:13:THR:HB	1.90	0.72
16:M:89:GLY:O	16:M:92:ALA:HB3	1.89	0.72
14:K:143:THR:HG22	14:K:145:LEU:H	1.54	0.72
8:E:23:GLU:HG2	8:E:28:SER:CB	2.20	0.72
8:E:11:VAL:HG12	8:E:12:ASP:N	2.04	0.71
1:0:121:U:OP2	30:1:10:ARG:NH2	2.23	0.71
1:0:289:G:N2	1:0:363:A:H2	1.86	0.71
1:0:1118:A:H3'	1:0:1118:A:C8	2.25	0.71
25:V:21:LEU:HD22	25:V:26:ILE:CD1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:109:LEU:HD13	13:J:113:ILE:HD11	1.72	0.71
7:D:99:ASP:HB3	7:D:103:ASN:H	1.56	0.71
7:D:105:SER:CB	7:D:131:THR:HG23	2.19	0.71
1:0:541:C:H2'	1:0:542:A:H5"	1.71	0.71
1:0:1160:G:C5'	1:0:1161:A:H5'	2.14	0.71
11:H:28:ILE:HA	11:H:62:GLU:OE1	1.90	0.71
25:V:88:THR:HG22	25:V:89:ASP:N	2.05	0.71
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.71	0.71
2:9:3048:C:H4'	16:M:141:ARG:HH21	1.55	0.71
20:Q:14:ALA:HB3	20:Q:147:LEU:HB2	1.72	0.71
1:0:2827:A:H2'	1:0:2828:G:O4'	1.89	0.71
25:V:4:LEU:HD22	25:V:52:VAL:CG2	2.20	0.71
24:U:39:ALA:N	24:U:40:PRO:HD2	2.06	0.71
16:M:144:GLY:O	16:M:147:ILE:HG22	1.90	0.71
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.56	0.71
12:I:93:ARG:HH11	12:I:93:ARG:HB3	1.56	0.71
23:T:9:CYS:HA	23:T:52:THR:HG23	1.72	0.71
11:H:137:ASN:O	11:H:139:ASP:N	2.23	0.71
31:2:17:HIS:O	31:2:18:GLN:HG3	1.90	0.71
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.21	0.71
1:0:1328:A:OP1	27:X:169:ARG:HD2	1.90	0.70
11:H:55:GLN:HE21	11:H:124:ARG:NE	1.89	0.70
7:D:64:ARG:HG2	7:D:67:ASP:HB3	1.73	0.70
26:W:78:GLU:HG2	26:W:79:GLU:H	1.56	0.70
25:V:88:THR:HG23	25:V:110:GLN:HE21	1.54	0.70
1:0:2256:G:O2'	1:0:2257:G:H5'	1.89	0.70
1:0:1185:U:H2'	1:0:1186:C:C6	2.27	0.70
15:L:34:GLU:HB3	15:L:35:PRO:HD2	1.74	0.70
1:0:31:C:H4'	38:S:7242:HOH:O	1.90	0.70
28:Y:40:PRO:HD3	28:Y:47:LEU:HD11	1.73	0.70
11:H:35:ASN:ND2	11:H:80:ASN:HA	2.07	0.70
1:0:2716:G:H5"	5:B:206:THR:HG21	1.72	0.70
1:0:1805:G:H2'	1:0:1806:G:H8	1.56	0.70
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.74	0.70
27:X:189:ASN:C	27:X:189:ASN:HD22	1.95	0.70
20:Q:18:LEU:HB2	20:Q:143:VAL:HG12	1.72	0.70
1:0:1535:G:H2'	1:0:1536:C:C6	2.27	0.70
1:0:1684:A:H1'	30:1:43:ARG:HH22	1.55	0.70
29:Z:25:LYS:HD2	30:1:49:GLU:H	1.55	0.70
16:M:138:ASP:O	16:M:140:GLN:N	2.23	0.70
7:D:27:ILE:HG22	7:D:28:GLY:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:58:GLU:HA	9:F:61:MET:HG3	1.72	0.70
23:T:52:THR:HG22	23:T:54:THR:H	1.57	0.70
1:0:371:U:H2'	1:0:372:A:H8	1.57	0.70
23:T:39:ASN:ND2	23:T:44:ARG:HH11	1.89	0.70
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.24	0.70
26:W:71:ARG:HB3	26:W:88:GLU:OE1	1.92	0.69
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.73	0.69
6:C:115:LEU:O	6:C:118:THR:HB	1.92	0.69
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.26	0.69
1:0:1165:G:H4'	1:0:1174:A:O2'	1.91	0.69
4:A:51:ARG:HB2	38:A:8617:HOH:O	1.91	0.69
15:L:139:PRO:O	15:L:140:ALA:CB	2.39	0.69
16:M:132:ASN:O	16:M:135:VAL:HG12	1.92	0.69
5:B:177:HIS:O	5:B:181:ILE:HG13	1.93	0.69
16:M:48:VAL:CG1	16:M:55:ASP:HB3	2.22	0.69
16:M:119:GLN:O	16:M:123:ILE:HG13	1.93	0.69
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.07	0.69
6:C:236:THR:CG2	6:C:239:ALA:H	2.01	0.69
14:K:133:VAL:HA	38:K:8579:HOH:O	1.91	0.69
11:H:45:GLN:HG3	11:H:135:TRP:NE1	2.08	0.69
26:W:15:ARG:NH1	26:W:15:ARG:HB3	2.06	0.69
5:B:55:ASN:HB3	5:B:63:GLU:HA	1.73	0.69
1:0:236:A:H4'	1:0:237:G:H5'	1.75	0.69
1:0:1926:G:H2'	1:0:1927:A:H8	1.58	0.69
1:0:1130:U:H2'	1:0:1131:G:O4'	1.93	0.69
20:Q:39:THR:HG23	20:Q:107:GLU:O	1.93	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.22	0.69
1:0:1942:A:H3'	38:0:8223:HOH:O	1.92	0.69
15:L:35:PRO:HG2	15:L:38:VAL:HG23	1.75	0.68
1:0:560:C:H42	1:0:597:A:H61	1.41	0.68
5:B:321:PRO:HA	38:B:8672:HOH:O	1.92	0.68
22:S:32:ARG:NH1	22:S:38:ARG:HH12	1.90	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.57	0.68
1:0:2908:A:H2'	1:0:2909:G:O4'	1.94	0.68
24:U:12:THR:CG2	24:U:15:GLU:HG3	2.14	0.68
1:0:285:A:H2'	1:0:286:U:O4'	1.94	0.68
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.57	0.68
17:N:47:ARG:HA	17:N:50:ARG:NH1	2.08	0.68
4:A:131:HIS:O	4:A:132:ASP:HB2	1.92	0.68
1:0:1790:C:H2'	1:0:1791:U:H6	1.59	0.68
22:S:71:VAL:HG11	22:S:90:PRO:CB	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:187:VAL:CG2	27:X:192:ASP:HB2	2.23	0.68
1:0:2414:A:H2'	1:0:2415:A:C8	2.29	0.68
1:0:188:C:H5"	15:L:163:LEU:HD21	1.76	0.68
1:0:2346:C:O2'	7:D:52:THR:HG21	1.93	0.68
15:L:164:THR:CG2	15:L:165:SER:N	2.56	0.68
26:W:72:VAL:HG22	26:W:85:VAL:CG1	2.24	0.68
16:M:164:ASP:CG	16:M:167:ASP:HA	2.14	0.68
6:C:219:ASN:O	6:C:222:ASP:OD1	2.12	0.68
16:M:169:PRO:O	16:M:172:PHE:HB3	1.93	0.68
22:S:47:THR:HB	22:S:100:ASP:HB3	1.75	0.68
7:D:20:LYS:HA	7:D:75:LEU:O	1.93	0.68
8:E:37:ASP:OD1	12:I:125:SER:HB3	1.94	0.68
15:L:164:THR:HG22	15:L:167:GLY:N	2.02	0.68
1:0:1450:C:O2'	1:0:1494:A:H5'	1.93	0.68
15:L:12:TRP:CE2	15:L:20:ILE:HD11	2.28	0.68
5:B:258:GLY:H	5:B:260:HIS:CE1	2.11	0.68
15:L:37:VAL:HG21	15:L:108:LYS:HG3	1.75	0.67
13:J:74:VAL:HG13	13:J:113:ILE:HG23	1.76	0.67
1:0:1209:C:H2'	1:0:1210:G:H8	1.56	0.67
17:N:47:ARG:HA	17:N:50:ARG:HH12	1.59	0.67
6:C:1:MET:HG2	6:C:2:GLN:H	1.58	0.67
5:B:41:PHE:HA	5:B:79:MET:HE2	1.76	0.67
5:B:168:GLY:H	5:B:174:ARG:HD3	1.57	0.67
1:0:1244:U:OP1	12:I:18:ILE:HD13	1.94	0.67
1:0:1191:A:H3'	1:0:1192:A:H5"	1.76	0.67
15:L:55:LYS:O	15:L:60:ILE:HD12	1.95	0.67
1:0:2768:A:H2'	1:0:2769:C:O4'	1.93	0.67
7:D:50:VAL:O	7:D:71:ALA:HA	1.95	0.67
12:I:133:GLY:O	12:I:137:GLU:HG3	1.95	0.67
1:0:2274:A:H1'	15:L:86:MET:SD	2.34	0.67
14:K:67:ARG:O	14:K:71:GLU:HG3	1.94	0.67
17:N:44:ASN:OD1	17:N:65:LEU:HB2	1.95	0.67
1:0:288:A:H61	1:0:364:C:H42	1.42	0.67
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.77	0.67
4:A:192:VAL:HB	38:A:8604:HOH:O	1.94	0.67
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.67
1:0:2897:C:H2'	1:0:2898:G:H8	1.59	0.67
15:L:65:VAL:HG21	15:L:105:ALA:HB2	1.75	0.67
22:S:50:VAL:HG12	22:S:56:ALA:HA	1.76	0.67
1:0:2769:C:O2'	1:0:2770:G:H5'	1.94	0.67
24:U:64:GLY:O	24:U:65:ASP:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:GLN:HG2	5:B:255:GLY:N	2.08	0.67
14:K:73:VAL:HG23	14:K:74:THR:H	1.60	0.67
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.59	0.67
5:B:24:PRO:HG2	5:B:204:GLY:HA2	1.76	0.67
1:0:2265:U:H2'	1:0:2266:A:C8	2.30	0.67
1:0:1930:A:H2'	1:0:1931:A:C8	2.30	0.67
1:0:1008:C:H5"	11:H:16:ARG:HH12	1.59	0.67
28:Y:53:GLY:HA2	28:Y:67:GLY:O	1.94	0.67
1:0:1299:G:O6	14:K:6:ARG:HD3	1.95	0.67
9:F:107:VAL:O	9:F:111:ILE:HG13	1.95	0.67
1:0:820:G:OP2	4:A:171:LYS:NZ	2.27	0.67
2:9:3023:U:C3'	2:9:3024:U:H5"	2.20	0.66
25:V:6:GLN:HB2	25:V:26:ILE:CD1	2.25	0.66
1:0:559:U:H5'	1:0:559:U:H6	1.59	0.66
17:N:73:ASP:HA	17:N:92:VAL:O	1.95	0.66
25:V:122:ARG:NH2	25:V:154:ARG:OXT	2.26	0.66
12:I:19:MET:CE	12:I:132:LEU:HD11	2.25	0.66
1:0:2256:G:C2'	1:0:2257:G:H5'	2.25	0.66
1:0:1926:G:H2'	1:0:1927:A:C8	2.29	0.66
12:I:117:ASP:O	12:I:119:THR:HG23	1.96	0.66
6:C:233:THR:HG22	6:C:234:VAL:H	1.60	0.66
1:0:2769:C:H2'	1:0:2770:G:O4'	1.95	0.66
11:H:26:LYS:HD2	11:H:28:ILE:CD1	2.25	0.66
7:D:64:ARG:CG	7:D:67:ASP:HB3	2.26	0.66
20:Q:18:LEU:HB2	20:Q:143:VAL:CG1	2.26	0.66
2:9:3039:U:H1'	2:9:3044:A:H61	1.61	0.66
27:X:203:VAL:HG12	27:X:228:VAL:HG22	1.78	0.66
1:0:2421:G:H3'	1:0:2422:U:H5"	1.76	0.66
11:H:47:GLU:HB3	11:H:133:ILE:CD1	2.26	0.66
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.78	0.66
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.61	0.66
23:T:14:GLU:O	23:T:17:THR:HB	1.95	0.66
28:Y:30:GLU:O	28:Y:33:HIS:HB3	1.95	0.66
11:H:150:LYS:HB2	11:H:157:ILE:HD12	1.78	0.66
1:0:2506:A:O2'	1:0:2507:G:O5'	2.14	0.66
7:D:135:VAL:HG22	7:D:136:ARG:H	1.61	0.66
1:0:2594:C:O2'	1:0:2595:U:H5'	1.95	0.66
5:B:162:MET:CE	5:B:308:LEU:HD21	2.22	0.66
11:H:33:MET:HB2	11:H:83:PHE:HB3	1.77	0.66
13:J:81:ARG:HB2	13:J:87:ARG:NH1	2.11	0.66
28:Y:11:THR:OG1	28:Y:23:ARG:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:238:ASN:HD22	5:B:240:GLY:N	1.87	0.65
5:B:195:ARG:HD2	5:B:324:ASP:OD1	1.96	0.65
15:L:72:SER:HB2	15:L:93:ARG:HG2	1.77	0.65
5:B:280:VAL:CG1	5:B:334:SER:HA	2.27	0.65
1:0:2269:C:C2'	1:0:2270:G:H5'	2.26	0.65
1:0:1641:A:H2'	1:0:1642:A:H5'	1.78	0.65
1:0:2578:G:H5'	1:0:2578:G:H8	1.61	0.65
5:B:175:LEU:HD23	5:B:175:LEU:C	2.17	0.65
1:0:1771:U:C4'	28:Y:20:LEU:HD21	2.26	0.65
8:E:11:VAL:HG12	8:E:12:ASP:H	1.61	0.65
28:Y:38:LYS:HE2	28:Y:45:LYS:CE	2.27	0.65
31:2:55:VAL:O	31:2:56:PRO:O	2.15	0.65
1:0:2271:G:H5'	38:A:8579:HOH:O	1.95	0.65
11:H:13:ALA:HA	11:H:91:HIS:HE1	1.62	0.65
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.65
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.78	0.65
21:R:37:VAL:O	21:R:41:VAL:HG23	1.96	0.65
5:B:168:GLY:N	5:B:174:ARG:HD3	2.11	0.65
1:0:1505:U:H5'	1:0:1505:U:H6	1.60	0.65
16:M:154:LEU:O	16:M:155:GLU:HB3	1.96	0.65
1:0:877:G:H5'	1:0:878:G:OP1	1.96	0.65
1:0:111:C:O2'	29:Z:20:ARG:HG2	1.96	0.65
16:M:163:PHE:HE1	16:M:171:HIS:HD1	1.44	0.65
20:Q:29:LYS:HD3	38:Q:8542:HOH:O	1.96	0.65
2:9:3054:A:O2'	2:9:3055:U:H5'	1.97	0.65
1:0:544:G:H2'	1:0:545:G:H5"	1.79	0.65
11:H:140:PRO:HA	11:H:142:VAL:HG12	1.78	0.65
15:L:37:VAL:HG21	15:L:108:LYS:CG	2.27	0.65
1:0:1234:U:N3	5:B:244:PRO:HB3	2.12	0.65
1:0:2717:C:O2'	1:0:2718:C:H5"	1.97	0.64
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.77	0.64
12:I:19:MET:HE3	12:I:132:LEU:HD11	1.78	0.64
1:0:2878:U:H2'	1:0:2879:A:O4'	1.97	0.64
29:Z:28:HIS:CE1	29:Z:31:LYS:HE2	2.32	0.64
2:9:3006:C:OP1	16:M:37:ARG:NH1	2.29	0.64
28:Y:29:VAL:O	28:Y:33:HIS:HB2	1.97	0.64
23:T:52:THR:HG22	23:T:54:THR:N	2.13	0.64
14:K:54:PRO:HG2	14:K:57:VAL:HG21	1.78	0.64
6:C:235:PHE:HE2	6:C:243:VAL:HG21	1.62	0.64
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.64
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:36:PRO:HA	5:B:168:GLY:CA	2.27	0.64
1:0:184:G:H5"	15:L:153:THR:HG22	1.78	0.64
26:W:25:ARG:HD3	26:W:64:ALA:O	1.97	0.64
2:9:3028:U:H5"	16:M:40:ASN:HD21	1.63	0.64
28:Y:33:HIS:CE1	28:Y:49:ARG:HD2	2.33	0.64
1:0:2094:G:C4'	5:B:245:SER:HB3	2.27	0.64
24:U:49:LEU:O	24:U:53:ILE:HG13	1.97	0.64
2:9:3049:G:O2'	2:9:3050:G:H5'	1.96	0.64
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.96	0.64
13:J:74:VAL:CG1	13:J:113:ILE:HG12	2.26	0.64
12:I:74:ARG:CB	12:I:74:ARG:HH11	2.10	0.64
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.64
1:0:1803:C:H2'	1:0:1804:A:C8	2.33	0.64
20:Q:25:PHE:CE2	20:Q:29:LYS:HE2	2.32	0.64
4:A:140:LEU:HB3	4:A:141:PRO:HD2	1.77	0.64
1:0:407:A:H2'	1:0:408:A:C8	2.33	0.64
21:R:57:THR:HG22	21:R:59:ASP:N	2.12	0.64
17:N:32:ARG:HE	17:N:35:LYS:HD2	1.63	0.64
20:Q:18:LEU:HD12	20:Q:143:VAL:HG11	1.80	0.64
11:H:44:ALA:HA	11:H:163:PRO:O	1.98	0.64
14:K:104:ASP:O	14:K:105:TYR:HB3	1.96	0.64
22:S:101:LEU:HD13	22:S:112:LEU:HD11	1.79	0.64
23:T:52:THR:CG2	23:T:54:THR:HB	2.28	0.64
1:0:2613:G:O2'	1:0:2614:C:H5'	1.98	0.64
11:H:27:LYS:N	11:H:58:HIS:HD2	1.94	0.64
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.28	0.64
12:I:27:ALA:HB1	12:I:87:LEU:HD21	1.80	0.64
14:K:143:THR:HG22	14:K:144:ASP:N	2.13	0.63
1:0:1972:U:H2'	1:0:1973:A:H5'	1.80	0.63
1:0:157:G:H4'	15:L:95:LYS:HE3	1.80	0.63
7:D:25:MET:CE	7:D:41:LEU:HG	2.27	0.63
4:A:48:ASP:HB3	38:A:8617:HOH:O	1.97	0.63
13:J:55:VAL:HG12	13:J:56:SER:H	1.62	0.63
11:H:14:TYR:H	11:H:91:HIS:CE1	2.15	0.63
12:I:107:ASN:ND2	12:I:109:TYR:H	1.96	0.63
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.63
15:L:87:MET:HB3	31:2:46:ILE:HG21	1.80	0.63
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.28	0.63
23:T:14:GLU:OE1	23:T:15:PRO:HD2	1.98	0.63
1:0:1595:G:O2'	1:0:1596:U:H5'	1.99	0.63
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:183:ASP:OD2	16:M:186:LEU:HD12	1.99	0.63
22:S:49:GLU:OE2	22:S:97:ARG:HD2	1.98	0.63
11:H:84:ARG:NH2	11:H:135:TRP:HH2	1.96	0.63
11:H:147:ARG:HA	11:H:150:LYS:NZ	2.14	0.63
1:0:2690:U:O2'	8:E:111:LYS:HE3	1.98	0.63
14:K:24:ALA:HB2	14:K:30:ARG:HD2	1.81	0.63
26:W:30:MET:HE1	26:W:55:ASN:HA	1.79	0.63
10:G:64:ASN:N	10:G:64:ASN:HD22	1.94	0.63
12:I:45:VAL:HG21	12:I:129:PHE:CD1	2.34	0.63
26:W:15:ARG:HH11	26:W:15:ARG:CB	2.10	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.99	0.63
10:G:64:ASN:O	10:G:68:GLU:HG3	1.98	0.63
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.81	0.63
1:0:960:G:H2'	1:0:960:G:N3	2.14	0.63
1:0:136:C:H2'	1:0:137:U:O4'	1.98	0.63
15:L:52:LEU:HD13	15:L:116:ASN:HB3	1.80	0.63
11:H:26:LYS:HD3	11:H:89:PRO:HG3	1.80	0.63
1:0:1474:C:C6	1:0:1474:C:H5'	2.33	0.63
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.63	0.63
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.64	0.63
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.67	0.63
13:J:10:GLN:H	13:J:10:GLN:HE21	0.75	0.62
14:K:114:VAL:HG11	38:K:8579:HOH:O	1.99	0.62
4:A:94:LEU:N	4:A:94:LEU:HD23	2.14	0.62
11:H:13:ALA:HA	11:H:91:HIS:CE1	2.33	0.62
32:0:9500:SLD:C6S	3:4:76:A:H5"	2.29	0.62
1:0:1741:U:H5'	1:0:1742:A:OP1	1.99	0.62
1:0:553:G:P	27:X:204:ARG:HH22	2.22	0.62
4:A:164:ARG:HB2	28:Y:68:CYS:SG	2.39	0.62
1:0:2070:G:H2'	1:0:2072:G:OP1	2.00	0.62
1:0:2265:U:H2'	1:0:2266:A:H8	1.64	0.62
2:9:3040:C:N4	7:D:51:ARG:HB2	2.13	0.62
21:R:57:THR:HG22	21:R:59:ASP:H	1.65	0.62
27:X:186:ARG:HG2	27:X:186:ARG:HH11	1.64	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
1:0:1667:A:H8	1:0:1667:A:H5'	1.64	0.62
2:9:3051:A:H5'	16:M:160:SER:HB3	1.81	0.62
5:B:56:ASP:HB3	5:B:322:ARG:HH21	1.65	0.62
1:0:2780:C:H2'	1:0:2781:U:C6	2.34	0.62
1:0:731:U:H2'	1:0:732:C:C6	2.35	0.62
31:2:65:THR:HG23	31:2:67:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:62:TYR:CE2	28:Y:64:ILE:HG23	2.34	0.62
1:0:1636:G:O2'	1:0:1637:A:H5'	1.98	0.62
1:0:2256:G:H2'	1:0:2257:G:H5'	1.82	0.62
22:S:32:ARG:NH1	22:S:38:ARG:NH1	2.47	0.62
25:V:68:THR:HG23	25:V:69:ARG:HG2	1.79	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.62
1:0:2456:A:H2'	1:0:2457:U:C6	2.34	0.62
2:9:3006:C:H5"	16:M:37:ARG:HH12	1.63	0.62
25:V:137:GLN:HE21	25:V:141:HIS:CE1	2.13	0.62
14:K:138:GLY:HA3	38:K:8558:HOH:O	2.00	0.62
1:0:2269:C:O2'	1:0:2270:G:H5'	2.00	0.62
1:0:2054:A:N3	20:Q:128:ARG:NH2	2.47	0.62
11:H:48:LEU:HG	11:H:157:ILE:HG21	1.82	0.62
1:0:2421:G:H3'	1:0:2422:U:C5'	2.27	0.62
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.14	0.62
18:O:76:GLY:O	18:O:79:SER:N	2.32	0.62
29:Z:21:ARG:HD2	29:Z:39:PHE:HB2	1.82	0.62
1:0:702:G:O2'	1:0:703:G:H5'	2.00	0.62
1:0:638:C:H2'	1:0:639:A:C8	2.35	0.62
1:0:2505:G:O2'	1:0:2506:A:H5'	2.00	0.61
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.00	0.61
1:0:558:C:O2'	1:0:559:U:H5"	1.99	0.61
2:9:3030:C:OP1	7:D:137:PRO:O	2.18	0.61
13:J:98:VAL:HG13	13:J:102:GLU:HA	1.82	0.61
18:O:7:LYS:HD3	18:O:21:VAL:CG2	2.30	0.61
11:H:29:ALA:HB3	11:H:65:ARG:NH1	2.09	0.61
28:Y:30:GLU:HA	28:Y:33:HIS:HB3	1.81	0.61
22:S:9:LYS:CE	22:S:13:ARG:NH1	2.62	0.61
27:X:112:GLU:OE1	27:X:112:GLU:HA	2.00	0.61
4:A:121:ALA:O	4:A:124:VAL:HG22	1.99	0.61
20:Q:40:ALA:O	20:Q:44:VAL:HG23	2.01	0.61
2:9:3044:A:O4'	7:D:76:ARG:NE	2.33	0.61
9:F:96:ALA:HA	38:F:3111:HOH:O	2.00	0.61
1:0:470:U:O2'	29:Z:16:HIS:HD2	1.82	0.61
1:0:2375:G:H2'	1:0:2376:C:C6	2.35	0.61
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.24	0.61
1:0:2533:C:C6	1:0:2533:C:H5'	2.33	0.61
16:M:91:ARG:HG3	16:M:186:LEU:HD23	1.81	0.61
1:0:1850:U:H2'	1:0:1851:G:H8	1.65	0.61
16:M:48:VAL:HG11	16:M:55:ASP:HB3	1.82	0.61
15:L:48:ARG:HH11	15:L:52:LEU:HD21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2795:C:O2'	1:0:2796:U:H5'	2.00	0.61
23:T:11:THR:HG22	23:T:53:ASP:OD2	2.01	0.61
1:0:1909:A:H2'	1:0:1910:A:C8	2.35	0.61
1:0:281:U:H2'	1:0:282:C:O4'	2.01	0.61
1:0:696:C:O2'	1:0:697:G:H5'	2.00	0.61
1:0:1250:C:O2'	1:0:1251:C:H5'	2.01	0.61
12:I:74:ARG:O	12:I:78:ILE:HG12	2.00	0.61
1:0:669:G:O2'	1:0:670:G:H5'	2.00	0.61
1:0:1422:U:H2'	1:0:1423:C:C6	2.35	0.61
1:0:2502:C:C4'	11:H:151:MET:HG2	2.30	0.61
1:0:1882:C:H2'	1:0:1883:U:H6	1.64	0.61
16:M:152:GLU:C	16:M:154:LEU:H	2.03	0.61
2:9:3013:A:O2'	2:9:3014:G:H5"	2.00	0.61
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.83	0.61
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.19	0.61
27:X:200:THR:HG22	27:X:201:GLU:HG3	1.83	0.61
9:F:56:PRO:HG2	15:L:44:THR:HA	1.82	0.61
1:0:2840:A:OP1	5:B:211:THR:HG23	2.01	0.61
5:B:145:HIS:HD2	5:B:146:THR:O	1.84	0.61
1:0:657:G:OP1	6:C:27:ARG:NH2	2.28	0.61
1:0:1170:U:O2'	1:0:1172:G:N7	2.32	0.61
25:V:84:VAL:HG12	38:V:6679:HOH:O	1.99	0.61
10:G:71:LEU:C	10:G:73:ASP:H	2.04	0.61
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.81	0.61
25:V:122:ARG:NH1	25:V:152:ALA:O	2.34	0.61
4:A:199:HIS:HD2	4:A:201:PHE:HB2	1.66	0.61
24:U:39:ALA:C	24:U:41:GLU:H	2.04	0.61
26:W:9:VAL:HG22	26:W:88:GLU:OE2	2.01	0.60
1:0:1666:C:O2'	1:0:1667:A:H5"	2.00	0.60
2:9:3025:G:C3'	2:9:3026:C:H5'	2.31	0.60
9:F:56:PRO:CG	15:L:44:THR:HA	2.32	0.60
1:0:1666:C:C2'	1:0:1667:A:H5'	2.31	0.60
6:C:27:ARG:HD2	17:N:5:PRO:HD2	1.81	0.60
4:A:27:LEU:HD21	4:A:55:VAL:HG21	1.83	0.60
1:0:1393:A:H2'	1:0:1394:C:C6	2.36	0.60
1:0:1003:U:HO2'	11:H:90:PHE:HE1	1.49	0.60
1:0:1119:G:H22	1:0:1246:A:H2	1.48	0.60
31:2:42:ARG:HH11	31:2:42:ARG:HG3	1.65	0.60
12:I:75:PRO:HG2	12:I:105:LEU:HD21	1.82	0.60
1:0:777:U:O2'	29:Z:11:LYS:HG2	2.01	0.60
20:Q:106:GLY:HA2	20:Q:109:MET:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:95:GLU:HB3	11:H:119:VAL:HG11	1.82	0.60
12:I:52:GLN:HG3	12:I:53:ILE:H	1.64	0.60
23:T:49:LEU:HG	38:T:3805:HOH:O	2.00	0.60
1:0:645:U:OP2	14:K:4:LYS:HE2	2.00	0.60
1:0:241:A:C2	1:0:378:A:H4'	2.36	0.60
1:0:2001:G:O2'	1:0:2002:C:H5'	2.01	0.60
28:Y:30:GLU:HA	28:Y:33:HIS:CB	2.32	0.60
1:0:1158:G:O2'	1:0:1159:G:H5'	2.01	0.60
31:2:60:LYS:HG3	31:2:61:PRO:HD2	1.84	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.37	0.60
12:I:45:VAL:HG23	12:I:130:VAL:O	2.01	0.60
1:0:2266:A:H2'	1:0:2267:G:C8	2.36	0.60
13:J:28:GLU:HG2	13:J:58:THR:HB	1.84	0.60
1:0:2028:U:H2'	1:0:2029:C:C6	2.36	0.60
6:C:118:THR:O	6:C:136:VAL:HG13	2.01	0.60
11:H:27:LYS:H	11:H:58:HIS:CD2	2.13	0.60
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.13	0.60
1:0:2415:A:N3	16:M:26:LEU:HD13	2.17	0.60
4:A:164:ARG:HA	28:Y:69:TYR:CE1	2.36	0.60
1:0:2598:U:O2	1:0:2600:A:H8	1.83	0.60
20:Q:18:LEU:HG	20:Q:91:LEU:HD13	1.84	0.60
16:M:165:ALA:HB1	38:M:8526:HOH:O	2.02	0.60
1:0:2241:C:H2'	1:0:2242:U:C6	2.37	0.60
1:0:256:C:H2'	1:0:257:G:O4'	2.02	0.60
7:D:44:ILE:HG23	7:D:45:THR:HG23	1.83	0.60
11:H:139:ASP:N	11:H:140:PRO:CD	2.65	0.60
18:O:59:ARG:HH22	18:O:66:GLN:HE22	1.48	0.60
7:D:135:VAL:HG22	7:D:136:ARG:N	2.17	0.60
1:0:2779:G:H21	8:E:143:GLN:NE2	2.00	0.60
1:0:2720:C:O2	13:J:87:ARG:NH2	2.35	0.60
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.17	0.60
1:0:29:C:O2'	1:0:30:U:H5'	2.02	0.60
15:L:74:ARG:HG3	15:L:74:ARG:HH11	1.66	0.59
25:V:64:THR:O	25:V:68:THR:HG22	2.02	0.59
1:0:2320:U:H4'	1:0:2321:A:O4'	2.02	0.59
11:H:31:PHE:CD2	11:H:85:ILE:HG23	2.37	0.59
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.31	0.59
1:0:2361:A:H2'	1:0:2362:A:C8	2.37	0.59
1:0:2256:G:H2'	1:0:2257:G:C5'	2.31	0.59
20:Q:61:GLN:NE2	38:Q:8542:HOH:O	2.35	0.59
15:L:48:ARG:NH1	15:L:52:LEU:HD21	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:51:VAL:HG13	5:B:53:LEU:HD13	1.83	0.59
7:D:95:THR:O	7:D:97:GLN:N	2.31	0.59
25:V:149:LEU:HG	25:V:153:MET:CE	2.32	0.59
1:0:902:G:N7	14:K:18:HIS:HD2	1.99	0.59
9:F:58:GLU:OE1	15:L:27:ARG:NH2	2.34	0.59
1:0:1790:C:H2'	1:0:1791:U:C6	2.37	0.59
2:9:3014:G:H8	2:9:3014:G:H5'	1.67	0.59
14:K:35:ARG:O	14:K:40:PHE:HA	2.02	0.59
8:E:11:VAL:HG13	8:E:23:GLU:O	2.03	0.59
26:W:76:ARG:O	26:W:77:PHE:HB3	2.01	0.59
10:G:12:ILE:N	10:G:13:PRO:CD	2.64	0.59
31:2:84:ARG:HD3	38:2:8554:HOH:O	2.02	0.59
30:1:40:ARG:HG2	30:1:40:ARG:HH11	1.67	0.59
1:0:2507:G:H2'	1:0:2510:C:N4	2.17	0.59
11:H:127:GLY:O	11:H:128:ALA:HB3	2.03	0.59
6:C:1:MET:HG2	6:C:2:GLN:NE2	2.16	0.59
13:J:115:ARG:HG3	13:J:116:GLU:N	2.18	0.59
16:M:155:GLU:O	16:M:156:GLU:HG3	2.02	0.59
1:0:1461:U:H2'	1:0:1462:C:C6	2.37	0.59
1:0:947:U:H2'	1:0:948:G:C8	2.37	0.59
15:L:138:HIS:ND1	15:L:139:PRO:O	2.31	0.59
26:W:43:VAL:HG12	26:W:44:ASP:N	2.17	0.59
7:D:86:THR:O	7:D:90:LEU:HG	2.02	0.59
27:X:235:GLU:CD	27:X:235:GLU:H	2.03	0.59
1:0:303:C:O2'	1:0:304:G:H5'	2.03	0.59
1:0:2356:A:H2'	1:0:2357:G:O4'	2.03	0.59
1:0:2413:A:N7	16:M:109:PRO:HB3	2.17	0.59
20:Q:12:THR:HG22	20:Q:149:GLU:OE1	2.03	0.59
11:H:46:VAL:HG12	11:H:146:TRP:HZ3	1.68	0.59
4:A:194:MET:HE2	4:A:199:HIS:CB	2.32	0.59
16:M:151:ASP:O	16:M:154:LEU:HB2	2.01	0.59
14:K:54:PRO:HG2	14:K:57:VAL:CG2	2.32	0.59
1:0:449:A:N7	6:C:43:LYS:HG2	2.18	0.59
16:M:33:ARG:NH1	16:M:103:ASP:OD2	2.26	0.59
16:M:164:ASP:OD2	16:M:167:ASP:HA	2.02	0.59
2:9:3039:U:H1'	2:9:3044:A:N6	2.17	0.59
1:0:1855:G:H8	4:A:144:GLU:OE2	1.85	0.59
7:D:25:MET:CE	7:D:37:ALA:HB1	2.31	0.59
25:V:110:GLN:NE2	25:V:110:GLN:HA	2.18	0.59
26:W:76:ARG:HG3	26:W:76:ARG:NH1	2.16	0.59
23:T:52:THR:HG22	23:T:54:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:H2'	1:0:1553:C:C6	2.38	0.59
30:1:41:HIS:HD2	30:1:44:ARG:H	1.51	0.58
1:0:282:C:O2'	1:0:283:U:H5'	2.03	0.58
6:C:233:THR:HG22	6:C:234:VAL:N	2.17	0.58
1:0:2363:G:O2'	19:P:11:ARG:HG3	2.03	0.58
1:0:95:A:H5"	1:0:97:G:O4'	2.03	0.58
9:F:91:VAL:HG12	9:F:92:GLY:H	1.64	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:338:C:H4'	6:C:174:ILE:CD1	2.32	0.58
14:K:149:ARG:O	14:K:150:GLN:HB2	2.03	0.58
16:M:143:ARG:HA	16:M:172:PHE:CD2	2.38	0.58
1:0:694:A:H2'	1:0:695:C:H5'	1.84	0.58
4:A:110:SER:HA	4:A:118:PHE:HE1	1.68	0.58
17:N:14:LEU:HG	17:N:102:ILE:HD11	1.85	0.58
2:9:3055:U:H4'	2:9:3056:A:C8	2.37	0.58
16:M:25:ARG:HA	16:M:28:LYS:HG3	1.84	0.58
27:X:200:THR:HG22	27:X:201:GLU:CG	2.32	0.58
7:D:94:ALA:HB3	7:D:174:VAL:CA	2.33	0.58
1:0:625:U:H5"	1:0:1044:C:N4	2.18	0.58
15:L:74:ARG:NH1	15:L:74:ARG:HG3	2.17	0.58
1:0:292:G:H2'	1:0:358:G:N2	2.17	0.58
7:D:99:ASP:HA	38:D:5675:HOH:O	2.04	0.58
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.85	0.58
9:F:110:GLU:HA	9:F:113:ASP:OD2	2.03	0.58
15:L:80:GLY:O	15:L:81:ARG:HD2	2.04	0.58
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.68	0.58
5:B:144:THR:HG22	5:B:145:HIS:N	2.18	0.58
24:U:56:ILE:O	24:U:60:GLN:HG3	2.03	0.58
17:N:87:THR:O	17:N:91:GLN:HG3	2.04	0.58
18:O:9:LEU:O	18:O:13:VAL:HG12	2.03	0.58
11:H:166:ASN:HD22	11:H:166:ASN:N	1.99	0.58
18:O:115:SER:H	18:O:118:GLN:NE2	1.82	0.58
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.86	0.58
14:K:145:LEU:O	14:K:148:GLU:HG3	2.03	0.58
1:0:1643:C:O2'	1:0:1644:C:H5'	2.04	0.58
15:L:37:VAL:HG13	15:L:63:VAL:HG11	1.86	0.58
25:V:122:ARG:HH11	25:V:122:ARG:CG	2.14	0.58
1:0:21:G:H4'	20:Q:2:ILE:HG22	1.84	0.58
5:B:96:PRO:HG2	38:B:8648:HOH:O	2.03	0.58
25:V:65:VAL:HG12	25:V:116:LEU:HD13	1.86	0.58
1:0:2300:A:H4'	1:0:2301:A:O5'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1164:U:C4'	1:0:1165:G:OP1	2.48	0.58
1:0:1864:C:OP1	15:L:75:THR:HG23	2.03	0.58
1:0:812:A:H2'	1:0:813:C:C6	2.39	0.58
14:K:93:VAL:HG12	14:K:97:VAL:HG23	1.85	0.58
31:2:11:CYS:HB2	31:2:20:HIS:CE1	2.38	0.58
23:T:17:THR:HG22	23:T:18:GLY:N	2.18	0.58
1:0:2894:C:O2'	1:0:2895:C:H5'	2.04	0.58
1:0:862:U:H2'	1:0:863:G:H8	1.68	0.58
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.85	0.58
1:0:1444:G:O2'	1:0:1445:G:H5'	2.02	0.58
1:0:2668:G:H2'	1:0:2669:U:C6	2.38	0.58
1:0:544:G:C2'	1:0:545:G:H5"	2.34	0.57
11:H:46:VAL:O	11:H:146:TRP:HH2	1.87	0.57
7:D:19:GLU:O	7:D:133:ASN:HB3	2.03	0.57
12:I:39:VAL:HG12	12:I:40:ASN:ND2	2.18	0.57
8:E:132:THR:HG23	8:E:132:THR:O	2.03	0.57
22:S:73:HIS:CD2	22:S:88:PRO:HG3	2.38	0.57
1:0:10:U:HO2'	1:0:11:A:H8	1.50	0.57
16:M:97:VAL:HG12	16:M:127:LEU:HD11	1.86	0.57
2:9:3048:C:H4'	16:M:141:ARG:NH2	2.17	0.57
1:0:1804:A:H2'	1:0:1805:G:C8	2.39	0.57
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.67	0.57
13:J:72:VAL:HG11	13:J:121:PHE:CD1	2.39	0.57
1:0:566:A:H2'	1:0:567:U:O4'	2.04	0.57
21:R:6:LYS:HB2	21:R:27:ALA:O	2.04	0.57
11:H:47:GLU:CB	11:H:133:ILE:HD13	2.35	0.57
11:H:26:LYS:HE3	11:H:28:ILE:HB	1.86	0.57
1:0:820:G:C6	4:A:171:LYS:HB2	2.39	0.57
17:N:77:ALA:HB1	17:N:98:LEU:HD12	1.86	0.57
4:A:33:GLU:O	4:A:34:ASP:HB2	2.03	0.57
23:T:13:ILE:HG12	23:T:32:CYS:HB3	1.85	0.57
1:0:1441:G:O2'	1:0:1442:A:H5'	2.03	0.57
1:0:2756:U:H3	1:0:2896:A:H2	1.53	0.57
13:J:55:VAL:HG12	13:J:56:SER:N	2.19	0.57
18:O:13:VAL:HG11	18:O:40:VAL:HG11	1.86	0.57
1:0:1496:G:H5'	1:0:1572:A:H1'	1.86	0.57
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.04	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57
12:I:39:VAL:HG13	12:I:106:GLY:O	2.03	0.57
9:F:117:GLU:C	9:F:119:ARG:H	2.08	0.57
16:M:78:MET:HB2	16:M:79:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:44:GLY:O	24:U:48:GLU:HG2	2.04	0.57
11:H:71:TYR:C	11:H:73:GLN:H	2.08	0.57
1:0:1783:A:O2'	1:0:1784:U:H5'	2.04	0.57
1:0:297:U:H2'	1:0:298:C:H6	1.69	0.57
11:H:53:PRO:HA	11:H:125:VAL:O	2.05	0.57
2:9:3028:U:H2'	2:9:3029:C:C6	2.40	0.57
27:X:99:ALA:HB2	27:X:233:TYR:CZ	2.40	0.57
1:0:832:U:H2'	1:0:833:G:C8	2.39	0.57
28:Y:19:GLY:O	28:Y:23:ARG:HG2	2.05	0.57
13:J:99:ASP:OD1	13:J:101:ASN:N	2.36	0.57
1:0:1827:G:H2'	1:0:1828:G:C8	2.39	0.57
15:L:186:SER:O	15:L:189:VAL:HG12	2.04	0.57
25:V:38:THR:HG22	25:V:39:ASP:N	2.20	0.57
24:U:11:MET:HB3	24:U:15:GLU:HB2	1.87	0.57
11:H:83:PHE:HZ	11:H:146:TRP:HE1	1.47	0.57
25:V:151:GLU:O	25:V:154:ARG:HB3	2.04	0.57
4:A:199:HIS:CD2	4:A:201:PHE:H	2.23	0.57
1:0:797:A:H4'	28:Y:10:ARG:N	2.19	0.57
1:0:962:C:H1'	16:M:5:ARG:HH12	1.69	0.57
1:0:1667:A:H2'	1:0:1668:U:C6	2.40	0.57
12:I:107:ASN:HD21	12:I:109:TYR:HB2	1.70	0.57
1:0:1333:U:H2'	1:0:1334:C:C6	2.40	0.57
28:Y:50:ALA:HB3	28:Y:54:ILE:HG22	1.85	0.57
28:Y:57:CYS:SG	28:Y:59:HIS:HB3	2.45	0.57
11:H:49:VAL:O	11:H:157:ILE:HG23	2.05	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.30	0.57
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.34	0.57
1:0:1205:U:C2'	1:0:1206:U:H5"	2.35	0.57
1:0:1803:C:H2'	1:0:1804:A:H8	1.68	0.57
1:0:1189:A:H3'	38:0:8560:HOH:O	2.05	0.57
5:B:140:LEU:HA	38:B:8592:HOH:O	2.04	0.57
38:0:6828:HOH:O	11:H:4:ALA:HB3	2.05	0.57
4:A:87:GLU:HB3	38:A:8635:HOH:O	2.04	0.57
1:0:170:U:H2'	1:0:171:C:H5'	1.87	0.57
28:Y:10:ARG:HA	38:Y:8416:HOH:O	2.03	0.57
1:0:371:U:H2'	1:0:372:A:C8	2.40	0.57
1:0:1234:U:C4	5:B:244:PRO:HB3	2.40	0.57
1:0:2456:A:H2'	1:0:2457:U:H6	1.69	0.57
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.23	0.57
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.04	0.57
9:F:19:ALA:O	9:F:22:VAL:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2780:C:H2'	1:0:2781:U:H6	1.68	0.56
18:O:80:ARG:HG2	18:O:87:ARG:CZ	2.35	0.56
1:0:2729:C:O2'	1:0:2730:G:H5'	2.05	0.56
1:0:12:U:H2'	1:0:13:G:H5'	1.86	0.56
1:0:290:C:O2'	1:0:291:C:H5'	2.05	0.56
29:Z:25:LYS:HD2	30:1:49:GLU:N	2.19	0.56
10:G:23:ILE:O	10:G:27:ILE:HG13	2.04	0.56
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.56
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.87	0.56
2:9:3023:U:H6	2:9:3023:U:H5"	1.69	0.56
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.35	0.56
11:H:35:ASN:HD21	11:H:80:ASN:HA	1.69	0.56
24:U:39:ALA:N	24:U:40:PRO:CD	2.67	0.56
26:W:78:GLU:HG2	26:W:79:GLU:N	2.18	0.56
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.19	0.56
22:S:28:SER:O	22:S:32:ARG:HG3	2.05	0.56
17:N:47:ARG:HH11	17:N:47:ARG:HG3	1.70	0.56
16:M:143:ARG:NH1	16:M:173:ASP:OD2	2.36	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.39	0.56
1:0:431:G:P	15:L:48:ARG:HH12	2.28	0.56
1:0:1352:A:N1	6:C:48:SER:HB3	2.20	0.56
1:0:1829:A:H2'	1:0:1830:C:H5'	1.88	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
15:L:172:GLY:O	15:L:183:VAL:HG11	2.04	0.56
1:0:2404:G:O5'	19:P:68:GLY:HA3	2.04	0.56
1:0:392:U:O2'	15:L:182:LYS:HE2	2.05	0.56
14:K:90:ARG:NH2	14:K:121:ILE:HD11	2.21	0.56
20:Q:82:GLU:HG3	20:Q:83:LYS:N	2.20	0.56
21:R:52:VAL:HG22	21:R:66:VAL:HG22	1.88	0.56
12:I:26:VAL:HG13	12:I:36:VAL:HG11	1.88	0.56
2:9:3055:U:H4'	2:9:3056:A:H8	1.71	0.56
25:V:21:LEU:HD21	25:V:48:VAL:HG11	1.88	0.56
16:M:71:TRP:HE3	16:M:175:LEU:HD22	1.71	0.56
9:F:47:LEU:HB2	9:F:108:LEU:HD11	1.88	0.56
7:D:146:LYS:HZ1	16:M:107:ASN:HD21	1.51	0.56
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.87	0.56
1:0:2269:C:H2'	1:0:2270:G:H5'	1.86	0.56
24:U:58:THR:O	24:U:62:GLU:HG3	2.05	0.56
15:L:155:HIS:CE1	15:L:158:ARG:HE	2.23	0.56
1:0:64:G:H2'	1:0:65:C:C6	2.40	0.56
1:0:2011:A:H4'	1:0:2012:U:O5'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:H2'	1:0:559:U:H5'	1.86	0.56
2:9:3028:U:H5"	16:M:40:ASN:ND2	2.20	0.56
1:0:960:G:H4'	38:0:8921:HOH:O	2.05	0.56
19:P:64:GLU:HG3	19:P:74:ASP:OD2	2.05	0.56
1:0:1139:U:H2'	1:0:1140:C:C6	2.40	0.56
1:0:445:U:H2'	1:0:446:G:H8	1.69	0.56
2:9:3025:G:H5"	2:9:3026:C:C6	2.40	0.56
26:W:37:LEU:CD1	26:W:85:VAL:HG21	2.32	0.56
12:I:74:ARG:NH1	12:I:76:ASP:HB2	2.20	0.56
5:B:175:LEU:O	5:B:175:LEU:HD23	2.05	0.56
1:0:732:C:H2'	1:0:733:U:C6	2.40	0.56
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.06	0.56
11:H:97:LYS:HD3	11:H:117:LYS:HD3	1.86	0.56
1:0:2364:A:H5"	19:P:15:LYS:HD3	1.87	0.56
1:0:1669:A:H2'	1:0:1670:G:C8	2.41	0.56
18:O:16:VAL:HG12	18:O:17:GLY:N	2.20	0.56
4:A:51:ARG:NH1	4:A:120:ARG:O	2.38	0.56
1:0:2768:A:O2'	1:0:2769:C:H5'	2.05	0.56
2:9:3029:C:H2'	2:9:3030:C:H5'	1.87	0.56
1:0:2054:A:C2	20:Q:128:ARG:NH2	2.74	0.56
1:0:862:U:H2'	1:0:863:G:C8	2.39	0.56
38:0:6414:HOH:O	5:B:298:LYS:HD3	2.06	0.56
1:0:1586:G:O2'	1:0:1587:U:H5'	2.06	0.56
7:D:25:MET:SD	7:D:40:ILE:HD11	2.46	0.56
7:D:69:ILE:O	7:D:69:ILE:HG22	2.05	0.56
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.73	0.56
1:0:2310:G:OP2	11:H:114:PRO:HD2	2.05	0.56
15:L:134:ILE:O	15:L:136:PRO:HD3	2.05	0.56
5:B:82:VAL:HG12	5:B:82:VAL:O	2.06	0.56
1:0:2909:G:O2'	1:0:2910:A:H5'	2.06	0.56
1:0:2119:C:O2'	1:0:2120:U:H5'	2.06	0.56
12:I:27:ALA:HB1	12:I:87:LEU:CD2	2.36	0.56
7:D:10:PHE:CG	7:D:11:HIS:N	2.73	0.56
1:0:2426:G:H1'	38:0:6980:HOH:O	2.05	0.56
1:0:2435:U:OP1	31:2:28:GLY:HA3	2.06	0.56
1:0:1154:A:H2'	1:0:1155:G:C8	2.40	0.56
1:0:1453:G:H2'	1:0:1454:U:O4'	2.06	0.56
6:C:20:ASP:O	6:C:23:GLU:HB2	2.06	0.56
11:H:157:ILE:HG22	11:H:158:ASN:N	2.21	0.56
1:0:1733:A:H4'	5:B:212:GLN:HA	1.88	0.56
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:81:ARG:HB2	13:J:87:ARG:HH11	1.70	0.56
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.05	0.56
1:0:485:A:N3	1:0:487:G:H5"	2.21	0.56
26:W:66:THR:HG23	26:W:67:PRO:HD2	1.88	0.56
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.86	0.56
12:I:99:GLU:HA	38:I:7377:HOH:O	2.06	0.56
20:Q:104:PHE:HB2	20:Q:109:MET:HE1	1.88	0.55
23:T:44:ARG:HB3	38:T:3805:HOH:O	2.06	0.55
1:0:1882:C:H2'	1:0:1883:U:C6	2.42	0.55
4:A:192:VAL:HG12	4:A:192:VAL:O	2.05	0.55
16:M:77:ASN:OD1	16:M:79:PRO:HD2	2.05	0.55
2:9:3023:U:H4'	2:9:3024:U:OP2	2.05	0.55
30:1:18:ASN:ND2	30:1:40:ARG:H	2.04	0.55
17:N:53:GLN:HG2	17:N:56:GLU:OE1	2.07	0.55
1:0:1657:A:H2'	1:0:1658:A:C8	2.41	0.55
11:H:46:VAL:HG21	38:H:8387:HOH:O	2.05	0.55
25:V:21:LEU:HD21	25:V:48:VAL:CG1	2.36	0.55
1:0:596:C:H2'	1:0:597:A:C8	2.41	0.55
5:B:280:VAL:HG13	5:B:334:SER:HA	1.88	0.55
18:O:7:LYS:HD3	18:O:21:VAL:HG21	1.87	0.55
38:0:7746:HOH:O	15:L:178:LYS:HB2	2.06	0.55
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.36	0.55
9:F:61:MET:HB3	15:L:19:GLN:OE1	2.05	0.55
14:K:66:VAL:HG23	14:K:67:ARG:N	2.21	0.55
25:V:149:LEU:HG	25:V:153:MET:HE2	1.87	0.55
1:0:671:A:O2'	1:0:672:G:H2'	2.07	0.55
1:0:1223:G:O2'	1:0:1224:G:H5'	2.06	0.55
31:2:3:MET:O	31:2:90:PHE:HA	2.05	0.55
27:X:103:THR:HG22	27:X:104:GLU:OE2	2.07	0.55
6:C:168:ARG:NH2	6:C:190:ALA:O	2.39	0.55
9:F:56:PRO:HG2	15:L:43:PRO:O	2.06	0.55
1:0:542:A:H2'	1:0:543:G:O4'	2.07	0.55
21:R:32:ALA:HA	21:R:36:GLU:OE1	2.06	0.55
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.88	0.55
28:Y:56:MET:HA	28:Y:62:TYR:O	2.06	0.55
1:0:319:A:H4'	1:0:338:C:C4	2.41	0.55
26:W:31:ILE:O	26:W:35:GLU:HG3	2.06	0.55
1:0:1789:G:O6	18:O:73:HIS:HE1	1.89	0.55
1:0:793:A:H5"	18:O:83:LYS:HG2	1.89	0.55
28:Y:42:CYS:SG	28:Y:44:PHE:HB2	2.47	0.55
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.36	0.55
1:0:1249:U:H2'	1:0:1250:C:C6	2.41	0.55
1:0:67:A:H5"	1:0:69:A:C8	2.41	0.55
6:C:124:VAL:HA	6:C:230:GLY:O	2.07	0.55
9:F:37:THR:O	9:F:41:GLU:HG3	2.07	0.55
1:0:420:U:H2'	1:0:421:C:C6	2.42	0.55
1:0:2715:G:O2'	5:B:262:ARG:HD2	2.06	0.55
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.37	0.55
15:L:12:TRP:O	15:L:15:PRO:HD3	2.07	0.55
15:L:47:ASP:CG	15:L:48:ARG:H	2.09	0.55
22:S:71:VAL:HG13	22:S:91:LEU:O	2.07	0.55
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.87	0.55
4:A:36:ASP:HB2	4:A:84:VAL:N	2.22	0.55
1:0:432:G:O2'	1:0:433:C:H5'	2.07	0.55
10:G:71:LEU:O	10:G:73:ASP:N	2.40	0.55
15:L:134:ILE:HG23	15:L:141:ILE:HD13	1.89	0.55
8:E:7:ILE:HG22	8:E:45:ASP:O	2.07	0.55
11:H:31:PHE:HA	11:H:85:ILE:CG2	2.37	0.55
4:A:179:MET:HG2	4:A:186:TRP:CG	2.42	0.55
13:J:74:VAL:HG12	13:J:75:ARG:HG3	1.89	0.55
28:Y:27:ALA:HA	38:Y:8416:HOH:O	2.07	0.55
2:9:3114:G:O6	16:M:11:ARG:HD3	2.06	0.55
9:F:91:VAL:CG1	9:F:92:GLY:N	2.70	0.55
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.88	0.55
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.88	0.55
15:L:149:TRP:O	15:L:152:ARG:HG2	2.07	0.55
6:C:218:VAL:N	38:C:8434:HOH:O	2.40	0.55
1:0:1165:G:H1'	1:0:1174:A:H1'	1.89	0.54
4:A:170:VAL:HG13	28:Y:22:ILE:HG21	1.89	0.54
1:0:1942:A:H2'	1:0:1943:C:H6	1.72	0.54
1:0:596:C:H2'	1:0:597:A:H8	1.72	0.54
1:0:2600:A:H2'	1:0:2601:A:O4'	2.07	0.54
1:0:832:U:H2'	1:0:833:G:H8	1.72	0.54
21:R:11:THR:H	21:R:14:ALA:HB3	1.71	0.54
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.89	0.54
13:J:75:ARG:HG2	13:J:90:PHE:CD2	2.42	0.54
1:0:1943:C:O4'	4:A:212:PRO:HA	2.08	0.54
1:0:2777:G:O2'	1:0:2778:A:H5'	2.07	0.54
1:0:398:U:H2'	1:0:399:C:C6	2.43	0.54
25:V:125:HIS:CD2	25:V:127:GLY:H	2.25	0.54
1:0:2502:C:H2'	1:0:2503:A:C5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2718:C:H6	1:0:2718:C:H5'	1.71	0.54
1:0:506:G:N2	1:0:509:A:H5'	2.19	0.54
1:0:2072:G:C6	1:0:2533:C:H1'	2.42	0.54
1:0:2769:C:C2'	1:0:2770:G:H5'	2.37	0.54
24:U:57:LYS:HA	24:U:60:GLN:HE21	1.71	0.54
1:0:825:U:H5"	1:0:826:U:OP1	2.07	0.54
11:H:3:GLY:HA2	11:H:57:ARG:NH1	2.23	0.54
1:0:1377:C:H5'	1:0:1377:C:H6	1.71	0.54
1:0:2885:A:H2'	1:0:2886:C:H6	1.71	0.54
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.89	0.54
25:V:90:TYR:CE2	25:V:99:ALA:HB2	2.41	0.54
1:0:2419:U:H5"	1:0:2420:G:H5'	1.89	0.54
21:R:57:THR:C	21:R:59:ASP:H	2.11	0.54
6:C:40:ALA:CB	6:C:100:LEU:HD12	2.37	0.54
2:9:3064:C:C2'	2:9:3065:A:H5'	2.37	0.54
14:K:65:ASP:CG	14:K:111:ALA:HB3	2.28	0.54
1:0:263:U:O4'	9:F:59:ILE:HD13	2.07	0.54
1:0:1119:G:N2	1:0:1246:A:H2	2.05	0.54
9:F:28:ALA:HB3	9:F:99:THR:O	2.07	0.54
14:K:73:VAL:HG23	14:K:74:THR:N	2.22	0.54
25:V:125:HIS:HD2	25:V:127:GLY:H	1.55	0.54
26:W:21:PRO:HG2	26:W:24:LYS:HD3	1.90	0.54
1:0:2050:G:H5"	20:Q:80:TYR:O	2.07	0.54
1:0:2766:A:O2'	1:0:2767:C:H5'	2.07	0.54
2:9:3076:G:C3'	2:9:3077:A:H5"	2.28	0.54
31:2:69:TYR:HB2	31:2:78:HIS:CE1	2.43	0.54
1:0:1666:C:O2'	1:0:1667:A:C5'	2.55	0.54
1:0:2897:C:H2'	1:0:2898:G:C8	2.41	0.54
1:0:2676:C:H4'	12:I:70:PHE:CE1	2.42	0.54
1:0:100:C:H4'	22:S:16:LEU:HB2	1.90	0.54
4:A:42:VAL:HG21	4:A:74:VAL:CG1	2.38	0.54
2:9:3056:A:H1'	7:D:14:ARG:HG2	1.90	0.54
6:C:16:VAL:HG12	6:C:17:ASP:N	2.22	0.54
1:0:282:C:H1'	1:0:368:C:H42	1.70	0.54
11:H:31:PHE:HD2	11:H:85:ILE:O	1.90	0.54
1:0:1331:A:OP2	27:X:142:SER:OG	2.23	0.54
1:0:263:U:C4	9:F:54:VAL:HG13	2.42	0.54
1:0:660:A:H4'	1:0:661:G:O5'	2.08	0.54
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.90	0.54
5:B:305:ASP:O	5:B:306:LYS:HB2	2.08	0.54
5:B:248:ARG:O	5:B:251:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:48:LYS:HG2	38:Y:8435:HOH:O	2.08	0.54
1:0:2112:A:H2'	1:0:2113:G:C8	2.41	0.54
18:O:29:GLY:O	18:O:32:ALA:HB3	2.07	0.54
2:9:3006:C:C5'	16:M:37:ARG:NH1	2.67	0.54
9:F:28:ALA:CB	9:F:99:THR:HG23	2.37	0.54
30:1:39:ARG:HG2	38:1:3143:HOH:O	2.06	0.54
1:0:2379:G:H4'	1:0:2380:A:H5"	1.90	0.54
7:D:140:ARG:O	7:D:144:ARG:HG2	2.07	0.54
16:M:34:LEU:HD22	16:M:129:ILE:HD13	1.88	0.54
1:0:947:U:H2'	1:0:948:G:H8	1.70	0.54
20:Q:98:ASN:N	20:Q:98:ASN:HD22	2.04	0.54
4:A:53:ALA:HB3	38:A:8617:HOH:O	2.08	0.54
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.54
16:M:154:LEU:HD11	38:M:8526:HOH:O	2.08	0.54
1:0:60:A:O2'	1:0:61:G:H5'	2.08	0.54
1:0:2437:A:H2'	1:0:2438:G:C8	2.42	0.54
1:0:512:G:O3'	1:0:513:A:H8	1.91	0.54
16:M:34:LEU:HA	16:M:47:LEU:HD23	1.89	0.53
1:0:249:G:O2'	1:0:250:C:H5'	2.08	0.53
29:Z:28:HIS:HD2	29:Z:30:LYS:H	1.56	0.53
13:J:28:GLU:OE2	13:J:58:THR:HG21	2.08	0.53
5:B:52:VAL:O	5:B:53:LEU:HD12	2.06	0.53
1:0:1123:A:C2	1:0:1129:C:H4'	2.43	0.53
1:0:168:C:O2'	1:0:169:A:H5'	2.08	0.53
1:0:415:A:O2'	1:0:416:G:H5'	2.09	0.53
16:M:139:TRP:HA	16:M:139:TRP:CE3	2.42	0.53
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.89	0.53
15:L:87:MET:HB2	15:L:91:ILE:CD1	2.36	0.53
31:2:56:PRO:HA	38:2:8553:HOH:O	2.07	0.53
1:0:639:A:H2'	1:0:640:G:C8	2.43	0.53
7:D:94:ALA:HB3	7:D:174:VAL:HA	1.89	0.53
38:9:8461:HOH:O	19:P:25:PRO:HB2	2.08	0.53
1:0:316:A:N3	1:0:336:G:O2'	2.39	0.53
1:0:352:A:H2'	1:0:353:G:C8	2.43	0.53
9:F:52:GLU:HG3	9:F:77:VAL:O	2.09	0.53
28:Y:30:GLU:HB2	38:Y:8416:HOH:O	2.07	0.53
1:0:447:A:O2'	1:0:448:G:H5'	2.08	0.53
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.38	0.53
1:0:1884:G:O6	4:A:190:ARG:HD2	2.07	0.53
1:0:1666:C:H2'	1:0:1667:A:H8	1.73	0.53
14:K:61:ALA:HA	38:K:8569:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2791:U:H1'	1:0:2792:A:H5"	1.91	0.53
22:S:19:ARG:NH1	22:S:68:ASP:O	2.41	0.53
1:0:381:G:H5"	38:0:5237:HOH:O	2.06	0.53
1:0:2276:U:H2'	1:0:2277:U:C6	2.43	0.53
1:0:1528:A:H2'	1:0:1529:G:O4'	2.08	0.53
1:0:1182:C:H1'	1:0:1192:A:H8	1.73	0.53
9:F:63:ILE:HB	9:F:64:PRO:CD	2.33	0.53
1:0:797:A:C4'	28:Y:10:ARG:N	2.72	0.53
16:M:11:ARG:HG3	16:M:14:ARG:HH12	1.72	0.53
1:0:1805:G:H2'	1:0:1806:G:C8	2.40	0.53
13:J:98:VAL:CG1	13:J:102:GLU:HA	2.38	0.53
1:0:1825:U:O2'	1:0:1826:C:H5'	2.08	0.53
18:O:131:PHE:CD1	18:O:137:LEU:HD13	2.43	0.53
13:J:34:VAL:HG22	13:J:47:ALA:HB2	1.90	0.53
1:0:2243:C:HO2'	1:0:2244:A:H8	1.56	0.53
7:D:59:GLY:O	7:D:61:PHE:N	2.35	0.53
1:0:1471:A:H2'	1:0:1472:C:C6	2.43	0.53
22:S:37:GLN:OE1	22:S:118:SER:HA	2.09	0.53
1:0:810:G:H2'	1:0:811:C:C6	2.43	0.53
6:C:127:ARG:HG2	6:C:127:ARG:NH1	2.20	0.53
1:0:2781:U:O2'	1:0:2782:G:H5'	2.08	0.53
31:2:65:THR:HB	31:2:83:TRP:H	1.73	0.53
1:0:1516:C:H2'	1:0:1517:U:C6	2.44	0.53
1:0:2247:C:O2'	1:0:2248:C:H5'	2.07	0.53
25:V:52:VAL:HG22	25:V:53:ALA:H	1.74	0.53
1:0:2353:A:O2'	16:M:7:LYS:HB3	2.08	0.53
14:K:133:VAL:HG13	38:K:8558:HOH:O	2.09	0.53
7:D:57:THR:HG23	7:D:63:ILE:CG2	2.38	0.53
20:Q:18:LEU:HD12	20:Q:143:VAL:CG1	2.38	0.53
1:0:111:C:O2'	1:0:112:G:H5'	2.07	0.53
1:0:861:A:H2'	1:0:862:U:C6	2.43	0.53
1:0:462:A:C2	30:1:37:HIS:HB3	2.43	0.53
1:0:1934:A:C8	1:0:1935:C:C5	2.96	0.53
25:V:81:ASP:OD1	25:V:92:ASP:HB2	2.09	0.53
1:0:1058:A:H2'	1:0:1060:C:H5"	1.91	0.53
15:L:32:ARG:HH21	15:L:123:ASP:HB3	1.74	0.53
7:D:41:LEU:CA	7:D:44:ILE:HG22	2.37	0.53
1:0:280:C:H2'	1:0:281:U:O4'	2.09	0.53
16:M:167:ASP:O	16:M:168:LEU:HD23	2.08	0.53
1:0:2721:U:H4'	13:J:87:ARG:HG3	1.91	0.53
1:0:120:A:H2'	1:0:120:A:N3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.53
1:0:1701:A:H4'	1:0:1702:U:H5"	1.89	0.53
7:D:23:VAL:HG23	7:D:41:LEU:HD22	1.89	0.53
1:0:2712:G:H5'	38:J:4183:HOH:O	2.09	0.53
16:M:71:TRP:CE3	16:M:175:LEU:HD22	2.43	0.53
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.90	0.53
1:0:703:G:O2'	1:0:704:C:H5'	2.09	0.53
38:0:4718:HOH:O	15:L:189:VAL:HG21	2.08	0.53
25:V:108:ARG:HE	25:V:114:PRO:HG3	1.74	0.53
20:Q:118:LYS:HE3	20:Q:139:PRO:HB3	1.91	0.53
12:I:46:ILE:HG12	12:I:53:ILE:HD13	1.91	0.53
24:U:39:ALA:O	24:U:41:GLU:N	2.42	0.53
20:Q:29:LYS:HB3	38:Q:8533:HOH:O	2.08	0.53
1:0:661:G:C5	1:0:686:A:C2	2.96	0.53
1:0:1304:U:H2'	1:0:1305:C:C6	2.44	0.53
1:0:394:G:H1	15:L:181:GLU:CD	2.12	0.53
2:9:3060:C:O2'	2:9:3061:C:H5'	2.08	0.53
25:V:10:GLU:HG3	25:V:11:VAL:N	2.24	0.53
11:H:147:ARG:HA	11:H:150:LYS:HZ3	1.73	0.53
1:0:1878:G:O2'	1:0:1879:U:P	2.67	0.53
2:9:3041:C:O4'	7:D:50:VAL:HG23	2.08	0.53
5:B:87:TYR:HD1	38:B:8592:HOH:O	1.91	0.53
22:S:35:TYR:CG	22:S:112:LEU:HD22	2.43	0.53
7:D:95:THR:C	7:D:97:GLN:H	2.13	0.53
1:0:1515:A:H2'	1:0:1516:C:C6	2.43	0.53
1:0:324:G:O2'	1:0:325:U:H5'	2.09	0.53
1:0:1714:C:O2'	1:0:1715:C:H5'	2.08	0.53
15:L:87:MET:CB	31:2:46:ILE:HG21	2.38	0.52
6:C:175:LYS:HD3	6:C:184:ARG:O	2.09	0.52
1:0:1850:U:H2'	1:0:1851:G:C8	2.44	0.52
1:0:1829:A:H5"	38:0:4035:HOH:O	2.09	0.52
6:C:130:GLU:HG2	6:C:168:ARG:HD3	1.91	0.52
25:V:1:MET:N	25:V:37:GLU:HG3	2.24	0.52
1:0:2812:A:C2	1:0:2814:A:N6	2.72	0.52
1:0:470:U:O2'	29:Z:16:HIS:CD2	2.61	0.52
1:0:695:C:O2'	1:0:696:C:H5'	2.08	0.52
1:0:949:U:O2'	19:P:40:HIS:HE1	1.92	0.52
1:0:858:U:H2'	1:0:859:C:H6	1.74	0.52
1:0:1899:C:O2'	1:0:1900:A:H5'	2.09	0.52
1:0:2115:U:H2'	1:0:2116:U:C6	2.44	0.52
11:H:26:LYS:CD	11:H:28:ILE:HB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:31:ILE:HG23	28:Y:32:LYS:N	2.25	0.52
4:A:88:ILE:O	4:A:88:ILE:HG22	2.09	0.52
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.09	0.52
1:0:1821:A:O2'	1:0:1822:A:H5'	2.09	0.52
7:D:154:LYS:H	7:D:154:LYS:CD	2.17	0.52
1:0:1206:U:C6	1:0:1206:U:H5'	2.37	0.52
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.38	0.52
16:M:151:ASP:OD1	16:M:154:LEU:HD13	2.10	0.52
1:0:1634:G:H2'	1:0:1635:U:C6	2.44	0.52
1:0:2468:A:H61	31:2:48:ASN:HD21	1.58	0.52
1:0:1568:G:O2'	1:0:1569:U:H5'	2.08	0.52
1:0:1055:G:OP2	11:H:94:ARG:NH1	2.43	0.52
1:0:332:G:O2'	1:0:333:G:H5'	2.10	0.52
1:0:1638:U:O2'	1:0:1639:U:H5'	2.09	0.52
7:D:23:VAL:HG23	7:D:23:VAL:O	2.09	0.52
1:0:2346:C:O5'	1:0:2346:C:H6	1.92	0.52
25:V:65:VAL:CG1	25:V:116:LEU:HD13	2.38	0.52
2:9:3064:C:H2'	2:9:3065:A:H5'	1.91	0.52
1:0:858:U:H2'	1:0:859:C:C6	2.43	0.52
9:F:49:PHE:O	9:F:95:ALA:HA	2.09	0.52
1:0:621:C:H5'	27:X:132:ASP:OD2	2.10	0.52
1:0:1268:C:H2'	1:0:1269:G:H8	1.75	0.52
5:B:162:MET:HE3	5:B:308:LEU:CD2	2.31	0.52
1:0:1191:A:C3'	1:0:1192:A:H5"	2.38	0.52
4:A:192:VAL:O	4:A:207:GLN:HG2	2.10	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.52
1:0:2326:U:H4'	1:0:2412:G:H4'	1.90	0.52
1:0:221:G:H2'	1:0:222:A:C8	2.44	0.52
1:0:1787:C:H4'	1:0:2883:A:O4'	2.10	0.52
1:0:330:C:H5	6:C:170:ASP:OD2	1.92	0.52
1:0:240:C:O2	1:0:240:C:H2'	2.10	0.52
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.45	0.52
1:0:2266:A:OP2	15:L:90:ARG:NH2	2.42	0.52
1:0:1513:C:O2'	1:0:1514:C:H5'	2.10	0.52
1:0:1456:C:H2'	1:0:1457:U:C6	2.44	0.52
6:C:236:THR:O	6:C:239:ALA:N	2.43	0.52
22:S:71:VAL:HG12	22:S:72:ILE:N	2.23	0.52
1:0:1134:G:OP2	11:H:156:THR:HG23	2.09	0.52
22:S:9:LYS:HE3	22:S:13:ARG:HH11	1.70	0.52
8:E:15:GLN:HG2	8:E:19:ASP:O	2.10	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:52:LEU:HD13	15:L:116:ASN:CG	2.30	0.52
25:V:38:THR:HG22	25:V:39:ASP:H	1.74	0.52
1:0:1730:G:H5'	1:0:1731:C:C5	2.45	0.52
1:0:269:G:O3'	1:0:274:G:H4'	2.09	0.52
16:M:62:HIS:HB3	16:M:65:ASP:OD1	2.09	0.52
1:0:289:G:O2'	1:0:290:C:H5'	2.10	0.52
8:E:15:GLN:HB2	8:E:20:ILE:HG23	1.92	0.52
1:0:1878:G:O2'	1:0:1879:U:C6	2.60	0.52
5:B:36:PRO:HA	5:B:168:GLY:HA2	1.92	0.52
1:0:2269:C:H2'	1:0:2270:G:C5'	2.40	0.52
1:0:105:G:O2'	1:0:106:A:H5'	2.10	0.52
1:0:1497:G:H4'	1:0:1627:G:O2'	2.10	0.52
1:0:226:A:H1'	1:0:393:G:C5	2.45	0.52
1:0:2903:C:O2'	1:0:2904:U:H5'	2.10	0.52
11:H:47:GLU:HG2	11:H:133:ILE:HD12	1.91	0.52
1:0:155:C:O2'	1:0:156:C:H5'	2.10	0.52
11:H:59:ASN:ND2	11:H:59:ASN:N	2.56	0.52
1:0:542:A:H5'	1:0:542:A:C8	2.37	0.52
7:D:38:GLU:OE2	7:D:51:ARG:CZ	2.57	0.52
15:L:47:ASP:CG	15:L:48:ARG:N	2.64	0.52
1:0:1527:A:H1'	1:0:1528:A:C8	2.45	0.52
17:N:84:THR:CG2	17:N:88:LYS:HE3	2.40	0.52
9:F:30:LYS:HB2	9:F:97:ALA:HB3	1.91	0.52
16:M:180:LEU:O	16:M:181:ASP:HB3	2.08	0.52
1:0:1345:A:H2'	1:0:1346:U:C6	2.45	0.52
1:0:175:G:H2'	15:L:192:ALA:HB3	1.91	0.52
22:S:63:ILE:HD11	22:S:75:GLU:HB2	1.91	0.52
1:0:189:A:OP1	15:L:171:ARG:NH2	2.43	0.51
19:P:26:PRO:O	19:P:30:VAL:HG23	2.10	0.51
1:0:1634:G:H2'	1:0:1635:U:H6	1.74	0.51
13:J:98:VAL:HG13	13:J:99:ASP:N	2.24	0.51
1:0:255:A:H2'	1:0:256:C:C6	2.45	0.51
25:V:26:ILE:HG13	25:V:26:ILE:O	2.10	0.51
22:S:9:LYS:HB2	38:S:7242:HOH:O	2.10	0.51
25:V:13:MET:CE	25:V:17:ILE:HG22	2.39	0.51
5:B:63:GLU:HG3	5:B:63:GLU:O	2.10	0.51
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.10	0.51
1:0:820:G:C5	4:A:171:LYS:HB2	2.46	0.51
15:L:52:LEU:HD13	15:L:116:ASN:CB	2.40	0.51
1:0:1909:A:N1	1:0:2128:G:H1'	2.25	0.51
15:L:147:LEU:O	15:L:149:TRP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:42:LYS:NZ	19:P:43:ILE:O	2.42	0.51
27:X:178:HIS:CG	27:X:179:PRO:HD2	2.46	0.51
25:V:73:LEU:O	25:V:74:GLU:HG3	2.11	0.51
1:0:2531:U:O2'	1:0:2532:A:H5'	2.10	0.51
1:0:2296:C:H5	19:P:3:SER:HG	1.58	0.51
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.40	0.51
1:0:1820:G:C6	1:0:2030:A:C2	2.98	0.51
5:B:62:ARG:HA	5:B:65:MET:CE	2.38	0.51
5:B:62:ARG:HA	5:B:65:MET:HE2	1.92	0.51
5:B:304:PRO:CG	5:B:307:ARG:NH1	2.73	0.51
2:9:3007:G:H5'	38:9:8479:HOH:O	2.09	0.51
1:0:2121:G:H1'	38:0:5481:HOH:O	2.10	0.51
1:0:816:G:H5'	1:0:1598:A:H4'	1.93	0.51
17:N:96:VAL:HG13	17:N:100:GLN:HB2	1.93	0.51
7:D:170:TYR:O	7:D:171:ASP:HB3	2.09	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.44	0.51
1:0:419:A:H1'	1:0:1921:A:C2	2.45	0.51
8:E:11:VAL:CG1	8:E:12:ASP:N	2.72	0.51
16:M:115:VAL:HG23	38:M:8559:HOH:O	2.10	0.51
5:B:72:THR:HB	38:B:8619:HOH:O	2.09	0.51
5:B:280:VAL:HG13	5:B:333:GLU:O	2.10	0.51
1:0:958:G:H2'	1:0:959:C:C6	2.45	0.51
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.38	0.51
1:0:1159:G:H21	1:0:1189:A:H8	1.58	0.51
24:U:64:GLY:O	24:U:65:ASP:CB	2.58	0.51
16:M:154:LEU:O	16:M:155:GLU:CB	2.58	0.51
22:S:78:THR:HB	22:S:87:VAL:O	2.11	0.51
19:P:32:GLU:HA	19:P:71:TYR:OH	2.11	0.51
6:C:173:LYS:HB3	6:C:187:ARG:HG3	1.90	0.51
11:H:151:MET:CE	11:H:151:MET:HA	2.41	0.51
15:L:38:VAL:HG12	15:L:38:VAL:O	2.11	0.51
1:0:2346:C:O2'	1:0:2347:C:H5'	2.11	0.51
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.29	0.51
1:0:2241:C:O2'	1:0:2242:U:H5'	2.11	0.51
17:N:96:VAL:CG1	17:N:100:GLN:HB2	2.41	0.51
1:0:39:G:H2'	1:0:40:C:O4'	2.11	0.51
1:0:1385:G:O3'	26:W:49:ARG:NH1	2.43	0.51
12:I:90:LYS:HB2	36:I:8502:CL:CL	2.47	0.51
25:V:4:LEU:CD2	25:V:54:PHE:HB3	2.38	0.51
1:0:506:G:H22	1:0:509:A:H5"	1.73	0.51
16:M:87:LEU:CD1	16:M:186:LEU:HD21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1810:C:OP1	23:T:44:ARG:NE	2.32	0.51
26:W:9:VAL:HG13	26:W:88:GLU:OE2	2.11	0.51
31:2:55:VAL:HG23	31:2:55:VAL:O	2.10	0.51
1:0:184:G:H5"	15:L:153:THR:CG2	2.41	0.51
1:0:2598:U:O2	1:0:2600:A:C8	2.63	0.51
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.44	0.51
1:0:1332:C:O2'	1:0:1333:U:H5'	2.11	0.51
30:1:36:ASN:HB3	30:1:39:ARG:NE	2.25	0.51
5:B:294:TYR:HE2	38:B:8665:HOH:O	1.94	0.51
6:C:109:LEU:O	6:C:109:LEU:HD12	2.10	0.51
1:0:2785:C:H4'	1:0:2786:G:OP2	2.11	0.51
16:M:64:SER:C	16:M:66:LEU:H	2.12	0.51
15:L:27:ARG:NH2	15:L:44:THR:HG23	2.26	0.51
31:2:14:CYS:HB3	31:2:16:GLU:HG2	1.93	0.51
27:X:99:ALA:HB2	27:X:233:TYR:CE2	2.45	0.51
1:0:1333:U:H2'	1:0:1334:C:H6	1.76	0.51
1:0:222:A:H2'	1:0:223:G:O4'	2.10	0.51
1:0:920:C:H5"	1:0:921:G:O5'	2.11	0.51
28:Y:22:ILE:O	28:Y:26:VAL:HG23	2.11	0.51
31:2:69:TYR:O	31:2:77:ALA:HA	2.10	0.51
1:0:1189:A:H1'	1:0:1209:C:O4'	2.11	0.51
1:0:1855:G:H4'	1:0:1856:C:O5'	2.09	0.51
15:L:155:HIS:ND1	15:L:158:ARG:NE	2.54	0.51
1:0:1920:C:O2'	1:0:1921:A:H5'	2.11	0.51
2:9:3045:A:H2'	2:9:3046:C:H6	1.75	0.51
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.46	0.51
11:H:26:LYS:HD3	11:H:89:PRO:CG	2.40	0.51
8:E:11:VAL:CG1	8:E:12:ASP:H	2.24	0.51
1:0:1849:G:H1'	1:0:2011:A:N1	2.26	0.51
1:0:1855:G:O6	4:A:141:PRO:HG2	2.11	0.51
1:0:2676:C:H4'	12:I:70:PHE:HE1	1.76	0.51
1:0:1819:G:H2'	1:0:1820:G:H4'	1.93	0.51
5:B:75:GLU:C	5:B:77:PRO:HD3	2.32	0.51
28:Y:26:VAL:O	28:Y:30:GLU:HG3	2.11	0.50
31:2:70:ARG:HH11	31:2:70:ARG:HG2	1.76	0.50
21:R:33:SER:OG	21:R:36:GLU:HG3	2.12	0.50
25:V:13:MET:HE3	25:V:17:ILE:CG2	2.38	0.50
11:H:85:ILE:O	11:H:85:ILE:HG23	2.11	0.50
11:H:165:GLY:C	11:H:166:ASN:HD22	2.14	0.50
1:0:243:A:H61	1:0:269:G:H1'	1.75	0.50
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:195:C:H2'	1:0:196:G:H5'	1.93	0.50
1:0:2667:G:H1'	1:0:2914:A:N3	2.25	0.50
1:0:2314:G:C2'	1:0:2315:C:H5'	2.41	0.50
26:W:85:VAL:HG12	26:W:86:GLU:N	2.26	0.50
24:U:20:LEU:HD22	24:U:60:GLN:HE22	1.75	0.50
14:K:90:ARG:NH1	14:K:119:THR:HG21	2.26	0.50
6:C:165:ASP:O	6:C:168:ARG:HB3	2.12	0.50
19:P:75:ILE:HD13	19:P:84:ILE:HD11	1.94	0.50
1:0:426:G:H2'	1:0:427:C:O4'	2.12	0.50
1:0:1192:A:O2'	1:0:1193:A:OP1	2.29	0.50
1:0:1197:G:N2	38:0:7119:HOH:O	2.39	0.50
1:0:288:A:H2'	1:0:289:G:C8	2.45	0.50
1:0:283:U:H5	1:0:284:C:N4	2.09	0.50
16:M:24:LEU:HD13	19:P:26:PRO:HB3	1.93	0.50
14:K:125:PHE:CE1	14:K:140:VAL:HG13	2.47	0.50
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.75	0.50
19:P:46:SER:O	19:P:48:PRO:HD3	2.12	0.50
1:0:213:G:N2	1:0:225:G:H2'	2.26	0.50
20:Q:119:VAL:HG12	20:Q:119:VAL:O	2.11	0.50
1:0:2758:G:H2'	1:0:2759:C:C6	2.47	0.50
1:0:182:G:O2'	1:0:183:A:H5'	2.12	0.50
5:B:217:ARG:CD	5:B:257:THR:HG22	2.41	0.50
21:R:51:GLN:HB3	21:R:67:ARG:NH1	2.26	0.50
7:D:86:THR:C	7:D:89:PRO:HD2	2.31	0.50
1:0:1804:A:H2'	1:0:1805:G:H8	1.74	0.50
2:9:3041:C:C6	7:D:50:VAL:HG21	2.47	0.50
13:J:82:ARG:NH2	13:J:115:ARG:HG2	2.26	0.50
11:H:165:GLY:HA3	38:H:8403:HOH:O	2.11	0.50
11:H:166:ASN:N	11:H:166:ASN:ND2	2.60	0.50
1:0:1398:G:O2'	1:0:1399:A:H5'	2.11	0.50
18:O:134:VAL:O	18:O:137:LEU:HB3	2.11	0.50
20:Q:119:VAL:CG2	20:Q:142:ASP:HB2	2.42	0.50
25:V:22:GLU:HG2	25:V:27:HIS:CD2	2.46	0.50
1:0:2862:G:H4'	5:B:336:GLN:O	2.12	0.50
1:0:2540:G:O2'	1:0:2541:U:H5"	2.11	0.50
8:E:107:PHE:CD2	8:E:108:LEU:HD13	2.47	0.50
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.41	0.50
4:A:100:PRO:O	4:A:103:VAL:HG23	2.11	0.50
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.11	0.50
25:V:38:THR:O	25:V:42:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1822:A:O2'	1:0:1823:G:H5'	2.11	0.50
2:9:3002:U:OP2	2:9:3002:U:H4'	2.11	0.50
8:E:16:ASP:O	8:E:17:HIS:HB2	2.11	0.50
31:2:8:ASN:O	31:2:9:THR:HB	2.10	0.50
23:T:33:SER:O	23:T:37:GLU:HG3	2.12	0.50
11:H:86:ARG:HD3	11:H:130:HIS:HD2	1.77	0.50
5:B:207:LYS:HG2	5:B:304:PRO:HB3	1.93	0.50
26:W:9:VAL:HG13	26:W:88:GLU:OE1	2.12	0.50
1:0:1008:C:OP1	11:H:16:ARG:NH2	2.44	0.50
1:0:667:C:H2'	1:0:668:C:H6	1.76	0.50
7:D:97:GLN:O	7:D:97:GLN:HG2	2.11	0.50
1:0:1762:C:O2'	1:0:1763:C:H5'	2.11	0.50
1:0:20:G:H21	20:Q:117:HIS:HD2	1.60	0.50
20:Q:132:ARG:HG2	20:Q:133:ALA:N	2.26	0.50
22:S:71:VAL:CG1	22:S:90:PRO:HB3	2.25	0.50
25:V:122:ARG:NH1	25:V:122:ARG:CG	2.74	0.50
11:H:59:ASN:HD22	11:H:59:ASN:H	1.59	0.50
12:I:19:MET:HE1	12:I:132:LEU:HD21	1.93	0.50
14:K:148:GLU:HA	38:K:8578:HOH:O	2.10	0.50
14:K:104:ASP:HB3	38:K:8569:HOH:O	2.11	0.50
1:0:241:A:N1	1:0:378:A:H4'	2.27	0.50
15:L:166:ALA:HA	15:L:169:ARG:NH1	2.27	0.50
1:0:2626:C:H2'	1:0:2627:G:C8	2.47	0.50
38:0:5742:HOH:O	12:I:47:THR:HB	2.11	0.50
1:0:1538:C:O2'	1:0:1539:U:H5'	2.12	0.50
11:H:130:HIS:CG	11:H:133:ILE:HD11	2.47	0.50
6:C:237:GLU:HB2	38:C:8441:HOH:O	2.11	0.50
28:Y:38:LYS:CE	28:Y:45:LYS:HE2	2.38	0.50
38:0:5524:HOH:O	17:N:35:LYS:HD3	2.12	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.25	0.50
7:D:57:THR:HG23	7:D:63:ILE:CB	2.42	0.50
22:S:48:VAL:HG22	22:S:98:VAL:HA	1.92	0.50
18:O:38:GLU:HA	18:O:41:ARG:NH1	2.27	0.50
1:0:2699:A:H2'	1:0:2700:G:O4'	2.11	0.50
1:0:2251:G:H2'	1:0:2252:A:C8	2.46	0.50
25:V:60:GLU:O	25:V:63:GLU:HB2	2.12	0.50
25:V:63:GLU:HG2	25:V:93:ILE:HG22	1.92	0.50
1:0:151:A:C2	1:0:442:A:C8	3.00	0.50
1:0:2101:A:H2'	6:C:63:SER:OG	2.11	0.50
20:Q:111:ILE:HG23	20:Q:145:LEU:HD11	1.92	0.50
11:H:142:VAL:HG13	38:H:8387:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:38:VAL:C	15:L:63:VAL:HG13	2.33	0.50
4:A:199:HIS:CD2	4:A:201:PHE:HB2	2.47	0.50
13:J:49:LEU:HD21	13:J:74:VAL:O	2.12	0.50
5:B:304:PRO:HD2	5:B:307:ARG:NH1	2.27	0.50
1:0:1171:A:H2'	1:0:1172:G:H5'	1.94	0.50
1:0:1463:A:H2'	1:0:1464:U:C6	2.47	0.50
38:0:4491:HOH:O	15:L:152:ARG:HG3	2.12	0.50
1:0:353:G:H2'	1:0:354:A:C8	2.46	0.50
1:0:352:A:H2'	1:0:353:G:H8	1.75	0.50
22:S:19:ARG:HD3	22:S:67:LEU:O	2.12	0.50
1:0:2541:U:H2'	1:0:2542:C:C6	2.47	0.50
1:0:90:A:H2'	1:0:91:G:O4'	2.12	0.50
1:0:154:C:P	15:L:188:ARG:HH12	2.34	0.50
1:0:281:U:O2'	1:0:282:C:H5'	2.11	0.49
1:0:962:C:H2'	1:0:963:C:H5'	1.94	0.49
12:I:93:ARG:HH11	12:I:93:ARG:CB	2.25	0.49
1:0:2818:A:H2	38:B:8648:HOH:O	1.93	0.49
1:0:694:A:C2'	1:0:695:C:H5'	2.42	0.49
26:W:14:LEU:HD12	26:W:67:PRO:O	2.12	0.49
1:0:354:A:H2'	1:0:355:C:C6	2.47	0.49
18:O:71:LYS:O	18:O:71:LYS:HG3	2.12	0.49
1:0:2416:G:H2'	1:0:2417:C:C6	2.47	0.49
18:O:98:ILE:HD12	18:O:102:ARG:NE	2.27	0.49
1:0:1266:U:H4'	27:X:115:ARG:HH21	1.76	0.49
6:C:166:ILE:HD13	6:C:207:LEU:HD22	1.93	0.49
1:0:1174:A:C5	1:0:1201:C:H4'	2.46	0.49
7:D:40:ILE:HG23	38:D:5583:HOH:O	2.11	0.49
14:K:143:THR:CG2	14:K:144:ASP:N	2.76	0.49
12:I:39:VAL:HG11	12:I:107:ASN:HB2	1.92	0.49
1:0:396:U:OP2	31:2:38:ARG:NH1	2.37	0.49
1:0:2547:C:H2'	1:0:2548:C:H6	1.77	0.49
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.94	0.49
1:0:2911:C:H2'	1:0:2912:C:C6	2.48	0.49
30:1:41:HIS:N	30:1:45:ASN:HD22	2.02	0.49
9:F:27:GLY:HA3	9:F:101:ALA:O	2.12	0.49
1:0:1925:G:O2'	1:0:1926:G:H5'	2.12	0.49
29:Z:8:GLN:HE22	29:Z:11:LYS:NZ	2.11	0.49
1:0:2028:U:H2'	1:0:2029:C:H6	1.78	0.49
1:0:297:U:H2'	1:0:298:C:C6	2.47	0.49
1:0:2587:U:H2'	1:0:2589:U:H5"	1.94	0.49
2:9:3017:G:O2'	2:9:3018:U:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:34:TRP:O	12:I:127:ILE:HD11	2.12	0.49
1:0:1425:G:O2'	1:0:1426:C:H5'	2.12	0.49
6:C:164:ALA:O	6:C:167:ASP:HB2	2.12	0.49
2:9:3023:U:C3'	2:9:3024:U:C5'	2.87	0.49
16:M:159:TYR:HE2	16:M:163:PHE:HE2	1.60	0.49
1:0:962:C:C2'	1:0:963:C:H5'	2.42	0.49
1:0:119:A:H2'	1:0:120:A:H5"	1.95	0.49
1:0:657:G:H2'	1:0:658:C:C6	2.48	0.49
25:V:90:TYR:N	25:V:90:TYR:CD1	2.80	0.49
1:0:1935:C:H2'	1:0:1936:C:H6	1.76	0.49
1:0:214:U:H5'	38:0:7028:HOH:O	2.11	0.49
15:L:137:ASP:C	15:L:142:LYS:HE3	2.33	0.49
1:0:1483:C:O2'	1:0:1484:G:H5'	2.12	0.49
25:V:107:LEU:O	25:V:112:LEU:HB2	2.11	0.49
19:P:72:LYS:HG2	19:P:85:ILE:HD13	1.93	0.49
15:L:87:MET:HG2	31:2:46:ILE:HG21	1.94	0.49
1:0:1834:C:H2'	1:0:1840:A:H62	1.75	0.49
30:1:40:ARG:NH1	30:1:40:ARG:HG2	2.28	0.49
30:1:41:HIS:O	30:1:45:ASN:HB2	2.11	0.49
1:0:21:G:H5"	20:Q:1:GLY:O	2.12	0.49
16:M:110:THR:HB	16:M:113:SER:OG	2.12	0.49
5:B:329:TYR:CE2	23:T:15:PRO:HG2	2.48	0.49
18:O:13:VAL:HG21	18:O:41:ARG:HG2	1.94	0.49
1:0:1902:G:O2'	1:0:1903:U:H5'	2.12	0.49
20:Q:111:ILE:HG23	20:Q:145:LEU:CD1	2.42	0.49
1:0:1213:C:O2'	1:0:1214:G:H5'	2.12	0.49
1:0:1687:C:O2	29:Z:9:GLY:HA2	2.13	0.49
1:0:2478:U:H2'	1:0:2479:A:C8	2.47	0.49
25:V:4:LEU:O	25:V:32:CYS:HA	2.12	0.49
5:B:304:PRO:CD	5:B:307:ARG:NH1	2.76	0.49
1:0:1205:U:H2'	1:0:1206:U:H5"	1.94	0.49
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.74	0.49
16:M:22:GLN:HG2	16:M:26:LEU:HD22	1.95	0.49
12:I:6:PHE:HB3	12:I:109:TYR:OH	2.12	0.49
13:J:6:ALA:HB3	13:J:116:GLU:HG2	1.93	0.49
1:0:853:C:H2'	1:0:854:G:O4'	2.12	0.49
1:0:74:A:H2'	1:0:75:U:C6	2.47	0.49
1:0:2446:G:H2'	1:0:2447:A:H8	1.78	0.49
9:F:26:THR:HG21	9:F:103:ALA:CB	2.43	0.49
1:0:2563:U:H2'	1:0:2565:C:O5'	2.12	0.49
22:S:71:VAL:CG1	22:S:72:ILE:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:62:GLU:HA	38:H:8390:HOH:O	2.12	0.49
38:0:4656:HOH:O	15:L:157:LEU:HD11	2.12	0.49
2:9:3014:G:C8	2:9:3014:G:H5'	2.47	0.49
20:Q:82:GLU:O	20:Q:86:LYS:HG3	2.13	0.49
20:Q:119:VAL:HG21	20:Q:142:ASP:CG	2.33	0.49
1:0:1735:C:O2'	1:0:1736:A:H5'	2.13	0.49
2:9:3035:C:H5"	38:9:8457:HOH:O	2.12	0.49
25:V:115:THR:HG23	38:V:5420:HOH:O	2.12	0.49
1:0:1563:G:O2'	1:0:1564:C:OP2	2.23	0.49
1:0:894:A:C2	6:C:87:ARG:NH2	2.81	0.49
15:L:164:THR:HB	38:L:8519:HOH:O	2.12	0.49
1:0:1134:G:H4'	11:H:151:MET:CE	2.32	0.49
1:0:182:G:H5'	38:0:6059:HOH:O	2.13	0.49
11:H:139:ASP:HA	38:H:8375:HOH:O	2.13	0.49
4:A:99:ILE:O	4:A:131:HIS:HE1	1.96	0.49
2:9:3041:C:H4'	7:D:48:MET:HB2	1.94	0.49
8:E:137:ASP:O	8:E:141:VAL:HG23	2.13	0.49
29:Z:28:HIS:O	29:Z:32:LYS:N	2.40	0.49
6:C:21:VAL:C	6:C:23:GLU:H	2.16	0.49
7:D:58:VAL:HG12	7:D:59:GLY:N	2.27	0.49
25:V:67:ALA:HB2	25:V:93:ILE:HD13	1.93	0.49
11:H:131:ILE:HG23	11:H:132:PHE:CD1	2.48	0.49
1:0:1994:A:P	13:J:66:ARG:HH22	2.36	0.49
1:0:1181:A:O2'	1:0:1182:C:H5'	2.12	0.49
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.13	0.49
12:I:93:ARG:HB3	12:I:93:ARG:NH1	2.24	0.49
6:C:174:ILE:HD13	6:C:185:LYS:HE2	1.94	0.49
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.49
1:0:2377:U:O5'	1:0:2377:U:H6	1.95	0.49
1:0:849:C:O2'	1:0:850:U:H5'	2.12	0.49
1:0:1768:C:H2'	1:0:1769:C:O4'	2.13	0.49
1:0:684:G:H2'	1:0:685:C:C6	2.48	0.49
6:C:84:VAL:O	6:C:85:LYS:HB2	2.13	0.49
1:0:612:U:H2'	1:0:613:C:C6	2.48	0.49
7:D:167:GLU:C	7:D:169:THR:H	2.16	0.49
11:H:149:ALA:C	11:H:151:MET:H	2.15	0.49
1:0:1450:C:C4'	1:0:1451:C:OP2	2.55	0.49
24:U:1:THR:HG23	24:U:2:VAL:N	2.23	0.49
1:0:1942:A:O2'	1:0:1943:C:H5'	2.13	0.49
7:D:99:ASP:CB	7:D:103:ASN:H	2.25	0.49
5:B:274:GLU:HA	5:B:292:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:64:ASN:N	10:G:64:ASN:ND2	2.60	0.49
18:O:13:VAL:HG11	18:O:40:VAL:CG1	2.42	0.49
1:0:1086:A:C6	25:V:11:VAL:HG11	2.47	0.49
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.93	0.49
1:0:1162:G:H2'	1:0:1162:G:N3	2.27	0.49
1:0:682:A:H2'	1:0:683:G:O4'	2.11	0.49
30:1:18:ASN:HD21	30:1:40:ARG:H	1.61	0.48
15:L:37:VAL:CG1	15:L:63:VAL:HG11	2.43	0.48
1:0:2504:A:H2'	1:0:2505:G:O4'	2.13	0.48
18:O:59:ARG:HH22	18:O:66:GLN:NE2	2.11	0.48
1:0:776:A:OP1	29:Z:28:HIS:HE1	1.95	0.48
6:C:235:PHE:CE2	6:C:243:VAL:HG21	2.44	0.48
1:0:2668:G:H2'	1:0:2669:U:H6	1.78	0.48
13:J:34:VAL:HB	38:J:7169:HOH:O	2.12	0.48
4:A:200:PRO:HD3	38:A:8522:HOH:O	2.12	0.48
8:E:54:ASP:OD1	8:E:54:ASP:N	2.46	0.48
1:0:1203:G:O2'	1:0:1204:C:H5'	2.13	0.48
1:0:887:G:H2'	1:0:888:U:C6	2.48	0.48
1:0:1808:C:O2'	1:0:1809:G:H5'	2.13	0.48
1:0:2406:U:O2'	1:0:2407:G:H5'	2.13	0.48
15:L:164:THR:HG23	15:L:165:SER:H	1.75	0.48
16:M:72:GLU:HB3	16:M:171:HIS:HE1	1.78	0.48
2:9:3042:C:O2	7:D:76:ARG:NH1	2.46	0.48
7:D:93:LEU:HB3	7:D:97:GLN:OE1	2.13	0.48
1:0:1778:A:H2'	1:0:1779:A:H5'	1.94	0.48
15:L:172:GLY:C	15:L:183:VAL:HG11	2.34	0.48
1:0:2296:C:H2'	1:0:2297:U:H6	1.78	0.48
1:0:1375:A:O2'	1:0:1376:G:H5'	2.12	0.48
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.48	0.48
25:V:88:THR:CG2	25:V:89:ASP:H	2.21	0.48
7:D:146:LYS:HE2	16:M:107:ASN:ND2	2.28	0.48
1:0:1535:G:H2'	1:0:1536:C:H6	1.78	0.48
1:0:1210:G:O2'	1:0:1211:G:H5'	2.14	0.48
1:0:2791:U:C1'	1:0:2792:A:H5"	2.43	0.48
19:P:32:GLU:O	19:P:93:ARG:NH2	2.45	0.48
2:9:3004:G:O2'	16:M:44:ARG:NH2	2.46	0.48
27:X:126:PRO:HG2	27:X:128:PHE:CE1	2.47	0.48
13:J:49:LEU:HA	13:J:73:VAL:HG12	1.95	0.48
1:0:1189:A:O2'	1:0:1208:C:H2'	2.12	0.48
1:0:821:U:H2'	1:0:822:C:H6	1.78	0.48
1:0:120:A:H5'	29:Z:20:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:32:GLY:N	38:F:3111:HOH:O	2.45	0.48
1:0:1829:A:C2'	1:0:1830:C:H5'	2.43	0.48
25:V:11:VAL:O	25:V:12:ASN:HB2	2.14	0.48
1:0:2089:A:O2'	1:0:2090:G:H5'	2.13	0.48
1:0:1015:C:H2'	1:0:1016:U:C6	2.48	0.48
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.43	0.48
31:2:70:ARG:NH1	31:2:70:ARG:HG2	2.28	0.48
23:T:52:THR:HG21	23:T:54:THR:HB	1.95	0.48
1:0:678:G:OP2	6:C:107:ARG:NH2	2.46	0.48
26:W:30:MET:CE	26:W:58:ALA:HB3	2.44	0.48
1:0:638:C:H2'	1:0:639:A:H8	1.77	0.48
14:K:40:PHE:CD1	14:K:41:HIS:N	2.82	0.48
9:F:117:GLU:C	9:F:119:ARG:N	2.67	0.48
4:A:179:MET:HA	4:A:179:MET:CE	2.43	0.48
24:U:55:ARG:O	24:U:59:ILE:HG12	2.14	0.48
20:Q:114:VAL:HA	20:Q:144:GLU:O	2.13	0.48
1:0:344:C:H2'	1:0:345:G:O4'	2.13	0.48
1:0:2387:U:H2'	1:0:2388:C:C6	2.48	0.48
2:9:3023:U:C6	2:9:3023:U:H5"	2.49	0.48
2:9:3026:C:O2'	2:9:3027:C:H5'	2.14	0.48
1:0:1166:A:N3	1:0:1166:A:H2'	2.28	0.48
1:0:2502:C:O2'	1:0:2503:A:H5'	2.13	0.48
11:H:157:ILE:CG2	11:H:158:ASN:N	2.77	0.48
1:0:182:G:O3'	15:L:157:LEU:CD1	2.62	0.48
15:L:108:LYS:HD3	15:L:108:LYS:N	2.28	0.48
25:V:122:ARG:HG2	25:V:152:ALA:O	2.14	0.48
26:W:43:VAL:CG1	26:W:44:ASP:N	2.75	0.48
1:0:1882:C:O2'	1:0:2012:U:OP2	2.32	0.48
19:P:30:VAL:O	19:P:30:VAL:HG12	2.13	0.48
1:0:1422:U:H2'	1:0:1423:C:H6	1.77	0.48
7:D:95:THR:CG2	7:D:174:VAL:HG22	2.43	0.48
2:9:3063:C:O2'	2:9:3064:C:H5'	2.14	0.48
18:O:94:TRP:CZ2	18:O:98:ILE:HG13	2.48	0.48
27:X:117:LEU:HD12	27:X:174:VAL:HG11	1.95	0.48
5:B:215:VAL:HA	5:B:220:VAL:HG22	1.94	0.48
7:D:56:ARG:N	38:D:6752:HOH:O	2.46	0.48
26:W:51:ASP:OD2	26:W:52:PRO:HD2	2.14	0.48
1:0:229:G:O2'	1:0:230:C:H5'	2.13	0.48
21:R:50:GLU:OE2	21:R:69:SER:HB3	2.14	0.48
1:0:707:C:C2	1:0:708:A:C8	3.02	0.48
22:S:40:VAL:HG22	22:S:41:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2858:U:H2'	1:0:2859:C:C6	2.48	0.48
11:H:163:PRO:O	11:H:164:ALA:HB2	2.14	0.48
1:0:2348:C:H2'	1:0:2349:G:H8	1.78	0.48
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.29	0.48
10:G:71:LEU:C	10:G:73:ASP:N	2.66	0.48
5:B:146:THR:O	5:B:148:PRO:HD3	2.14	0.48
1:0:2821:C:H4'	5:B:116:PRO:HB3	1.95	0.48
1:0:1321:A:H2'	1:0:1322:G:C8	2.49	0.48
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.49	0.48
21:R:73:ASP:OD1	21:R:75:GLN:HB2	2.14	0.48
5:B:179:LEU:O	5:B:183:GLU:HG2	2.13	0.48
1:0:272:A:H5'	1:0:273:G:OP2	2.13	0.48
6:C:51:TYR:CE2	29:Z:53:LYS:HB3	2.48	0.48
24:U:12:THR:HG23	24:U:14:ALA:H	1.78	0.48
18:O:115:SER:O	18:O:117:SER:N	2.46	0.48
11:H:75:SER:C	11:H:79:ALA:HB2	2.34	0.48
5:B:279:THR:HG22	5:B:280:VAL:N	2.29	0.48
5:B:87:TYR:O	5:B:138:GLY:N	2.39	0.48
1:0:1972:U:C2'	1:0:1973:A:H5'	2.43	0.48
1:0:1900:A:H2'	1:0:1901:G:H8	1.78	0.48
38:0:3375:HOH:O	15:L:94:LYS:HE2	2.13	0.48
4:A:135:VAL:HG11	4:A:147:ARG:NH2	2.29	0.48
23:T:5:GLU:CG	23:T:10:GLY:O	2.61	0.48
1:0:1905:U:H2'	1:0:1906:C:H6	1.79	0.48
1:0:906:C:OP2	27:X:147:ARG:NH2	2.46	0.48
1:0:549:A:O2'	1:0:550:C:H5'	2.14	0.48
27:X:187:VAL:HG12	27:X:205:ILE:HA	1.96	0.48
31:2:69:TYR:CB	31:2:78:HIS:CE1	2.97	0.48
1:0:1154:A:H2'	1:0:1155:G:H8	1.77	0.48
8:E:80:TRP:O	8:E:134:SER:HA	2.13	0.48
1:0:1903:U:O2'	1:0:1904:A:N7	2.46	0.48
1:0:1218:U:H2'	1:0:1219:U:H6	1.79	0.48
1:0:466:A:H2'	1:0:467:G:O4'	2.13	0.48
1:0:1114:A:O2'	1:0:1115:U:H5'	2.12	0.48
1:0:1308:A:H2'	1:0:1309:U:H6	1.78	0.48
5:B:147:VAL:HG12	5:B:150:ALA:H	1.78	0.48
26:W:85:VAL:HG12	26:W:86:GLU:H	1.78	0.48
14:K:144:ASP:O	14:K:147:GLU:HB2	2.13	0.48
5:B:168:GLY:H	5:B:174:ARG:HH11	1.62	0.48
1:0:1652:C:O4'	4:A:164:ARG:HG3	2.14	0.48
1:0:1462:C:H2'	1:0:1463:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1573:A:H2'	1:0:1574:C:O4'	2.14	0.48
1:0:1268:C:H2'	1:0:1269:G:C8	2.49	0.48
5:B:81:ALA:O	5:B:186:GLY:HA3	2.13	0.48
1:0:598:C:H2'	1:0:599:G:H8	1.78	0.48
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.48
1:0:2015:A:H2'	1:0:2016:U:O4'	2.13	0.48
29:Z:5:THR:HB	29:Z:6:PRO:CD	2.44	0.48
6:C:236:THR:O	6:C:237:GLU:C	2.52	0.47
5:B:43:GLY:O	5:B:308:LEU:HD12	2.13	0.47
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.44	0.47
11:H:26:LYS:HG2	11:H:28:ILE:N	2.19	0.47
8:E:7:ILE:HD11	8:E:11:VAL:C	2.34	0.47
31:2:16:GLU:HG3	31:2:18:GLN:HE21	1.79	0.47
38:9:8479:HOH:O	16:M:18:THR:HG21	2.14	0.47
1:0:1298:U:H2'	1:0:1299:G:C8	2.49	0.47
14:K:24:ALA:CB	14:K:30:ARG:HD2	2.44	0.47
13:J:101:ASN:HB2	13:J:103:ASP:OD2	2.14	0.47
1:0:396:U:O2'	1:0:418:C:H4'	2.13	0.47
5:B:76:THR:N	5:B:77:PRO:HD3	2.28	0.47
22:S:41:ARG:NH1	22:S:42:VAL:O	2.47	0.47
1:0:1289:C:H3'	38:0:7289:HOH:O	2.14	0.47
1:0:2044:G:OP1	26:W:23:HIS:HE1	1.97	0.47
12:I:103:VAL:HG12	38:I:5907:HOH:O	2.13	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.14	0.47
1:0:2523:U:O2'	1:0:2524:G:H5'	2.13	0.47
6:C:132:ASP:HB3	38:C:8371:HOH:O	2.14	0.47
1:0:2735:U:H2'	1:0:2736:U:C6	2.49	0.47
11:H:72:VAL:HG11	11:H:81:TYR:CZ	2.49	0.47
6:C:236:THR:H	6:C:239:ALA:HB3	1.78	0.47
1:0:2503:A:OP1	11:H:147:ARG:NH2	2.44	0.47
8:E:7:ILE:CG2	8:E:45:ASP:O	2.62	0.47
9:F:28:ALA:HB3	9:F:99:THR:HG23	1.95	0.47
14:K:53:ARG:NH2	14:K:57:VAL:HG12	2.29	0.47
1:0:2539:U:C4	32:0:9500:SLD:H7	2.49	0.47
14:K:38:HIS:CD2	14:K:39:GLU:HG3	2.49	0.47
11:H:69:ASN:O	11:H:72:VAL:HG12	2.14	0.47
1:0:1717:A:H5"	18:O:54:LYS:HB2	1.96	0.47
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.14	0.47
11:H:39:GLY:O	11:H:41:THR:N	2.47	0.47
6:C:240:LEU:HD23	6:C:240:LEU:O	2.13	0.47
1:0:157:G:H4'	15:L:95:LYS:CE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:88:THR:CG2	25:V:110:GLN:NE2	2.72	0.47
25:V:119:HIS:CB	38:V:4276:HOH:O	2.62	0.47
5:B:211:THR:HA	5:B:255:GLY:O	2.14	0.47
4:A:164:ARG:HA	28:Y:69:TYR:HE1	1.78	0.47
4:A:65:ARG:C	4:A:66:ARG:HG3	2.35	0.47
1:0:1701:A:H5'	38:0:7166:HOH:O	2.13	0.47
1:0:1266:U:O2'	1:0:1267:C:H5'	2.14	0.47
4:A:114:ASP:HB2	4:A:117:LYS:HE2	1.96	0.47
1:0:1761:U:H5'	18:O:81:LYS:O	2.14	0.47
1:0:711:G:H1'	38:0:7966:HOH:O	2.13	0.47
11:H:26:LYS:HD2	11:H:28:ILE:CG1	2.45	0.47
2:9:3114:G:H2'	2:9:3115:C:C6	2.49	0.47
1:0:1851:G:O2'	1:0:1852:A:H5'	2.14	0.47
25:V:41:TYR:CD2	25:V:44:MET:HE3	2.49	0.47
1:0:310:U:H2'	1:0:311:C:C6	2.49	0.47
15:L:64:ARG:HD2	38:L:8587:HOH:O	2.13	0.47
11:H:140:PRO:HB3	38:H:8387:HOH:O	2.14	0.47
1:0:1603:A:H5'	1:0:1605:G:C4'	2.45	0.47
2:9:3047:A:C2	2:9:3048:C:C2	3.02	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
4:A:99:ILE:O	4:A:131:HIS:CE1	2.68	0.47
1:0:2266:A:H2'	1:0:2267:G:H8	1.77	0.47
1:0:431:G:O2'	1:0:432:G:H5'	2.13	0.47
1:0:2362:A:H2'	1:0:2363:G:C8	2.50	0.47
14:K:124:ASP:OD1	14:K:125:PHE:N	2.47	0.47
1:0:1782:G:O2'	1:0:1783:A:H5'	2.15	0.47
1:0:2437:A:H2'	1:0:2438:G:H8	1.79	0.47
11:H:81:TYR:C	11:H:81:TYR:CD1	2.86	0.47
1:0:1594:C:OP2	18:O:120:ARG:HD2	2.15	0.47
22:S:24:ARG:HH21	22:S:39:ASN:ND2	2.12	0.47
1:0:2473:U:O3'	1:0:2474:A:H3'	2.13	0.47
7:D:153:THR:O	7:D:156:ARG:HB2	2.14	0.47
1:0:288:A:H2'	1:0:289:G:H8	1.80	0.47
1:0:1592:G:O2'	1:0:1593:C:O5'	2.32	0.47
4:A:36:ASP:CB	4:A:85:ASP:H	2.27	0.47
5:B:82:VAL:HG12	5:B:101:TRP:CE3	2.48	0.47
1:0:1927:A:O2'	1:0:1928:C:H5'	2.14	0.47
5:B:320:GLN:HG3	5:B:321:PRO:HD2	1.96	0.47
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.27	0.47
15:L:182:LYS:HD2	15:L:193:LYS:HB2	1.96	0.47
7:D:11:HIS:C	7:D:13:MET:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:24:ARG:HH21	22:S:39:ASN:HD22	1.60	0.47
17:N:39:THR:O	17:N:115:ARG:NH2	2.47	0.47
1:0:1593:C:H5'	18:O:116:SER:O	2.14	0.47
11:H:35:ASN:ND2	11:H:79:ALA:O	2.46	0.47
4:A:95:PRO:HA	4:A:153:ARG:HA	1.97	0.47
5:B:175:LEU:O	5:B:178:ALA:HB3	2.14	0.47
16:M:154:LEU:HD11	16:M:157:PRO:HA	1.97	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.43	0.47
1:0:1741:U:O2'	1:0:2723:G:H4'	2.15	0.47
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.45	0.47
1:0:945:U:H2'	1:0:946:C:C6	2.50	0.47
27:X:234:VAL:HG12	27:X:235:GLU:N	2.29	0.47
1:0:319:A:H4'	1:0:338:C:C5	2.50	0.47
1:0:1624:A:H5'	1:0:1626:A:O4'	2.15	0.47
31:2:7:PHE:HD1	31:2:8:ASN:O	1.97	0.47
1:0:2388:C:O2'	1:0:2389:U:H5'	2.15	0.47
1:0:941:G:C5	1:0:942:U:C4	3.03	0.47
1:0:1872:C:H5	4:A:20:SER:HB3	1.80	0.47
1:0:326:G:O2'	1:0:327:A:H5'	2.14	0.47
26:W:27:ASP:N	26:W:27:ASP:OD2	2.41	0.47
1:0:1792:C:H2'	1:0:1793:C:H6	1.78	0.47
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.47	0.47
1:0:183:A:H5'	15:L:157:LEU:HD12	1.97	0.47
9:F:100:ASP:O	9:F:101:ALA:O	2.33	0.47
1:0:2897:C:O2'	1:0:2898:G:H5'	2.15	0.47
1:0:2898:G:O2'	1:0:2899:A:H5'	2.15	0.47
1:0:1299:G:N7	14:K:6:ARG:NH1	2.62	0.47
1:0:820:G:H5'	1:0:821:U:H5'	1.97	0.47
22:S:48:VAL:CG2	22:S:98:VAL:HA	2.45	0.47
1:0:946:C:H2'	1:0:947:U:C6	2.49	0.47
14:K:90:ARG:HH11	14:K:119:THR:HG21	1.80	0.47
1:0:2435:U:H1'	38:0:6323:HOH:O	2.13	0.47
1:0:2112:A:H2'	1:0:2113:G:H8	1.79	0.47
1:0:1921:A:C6	1:0:1922:A:C2	3.03	0.47
1:0:1307:A:H2'	1:0:1308:A:C8	2.50	0.47
1:0:474:C:O3'	6:C:73:LEU:CD2	2.62	0.47
6:C:242:GLU:HG3	38:C:8390:HOH:O	2.14	0.47
16:M:61:ALA:HB3	16:M:88:ALA:HB2	1.97	0.47
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.97	0.47
13:J:49:LEU:HA	13:J:73:VAL:CG1	2.45	0.47
5:B:177:HIS:NE2	5:B:181:ILE:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:57:VAL:O	14:K:57:VAL:HG12	2.15	0.47
12:I:39:VAL:CG1	12:I:107:ASN:HB2	2.44	0.47
1:0:553:G:O4'	1:0:1325:G:H5'	2.15	0.47
1:0:65:C:O2'	1:0:66:G:H5'	2.15	0.47
11:H:72:VAL:CG1	11:H:81:TYR:CZ	2.98	0.47
38:0:5858:HOH:O	2:9:3103:A:H4'	2.14	0.47
1:0:2687:G:O2'	1:0:2688:U:H5'	2.15	0.47
7:D:166:ILE:HB	38:D:6326:HOH:O	2.15	0.47
31:2:70:ARG:CG	31:2:77:ALA:HB2	2.40	0.47
9:F:99:THR:HG23	9:F:99:THR:O	2.14	0.47
5:B:175:LEU:C	5:B:175:LEU:CD2	2.83	0.47
10:G:67:LEU:O	10:G:71:LEU:HG	2.14	0.47
23:T:6:CYS:C	23:T:8:TYR:H	2.18	0.47
1:0:2729:C:H2'	1:0:2730:G:H8	1.79	0.47
1:0:1701:A:H4'	1:0:1702:U:C5'	2.44	0.47
1:0:2326:U:H4'	1:0:2412:G:C4'	2.45	0.47
16:M:42:HIS:CG	16:M:62:HIS:HE1	2.33	0.47
1:0:1217:G:H2'	1:0:1218:U:C6	2.50	0.47
1:0:2858:U:H2'	1:0:2859:C:H6	1.80	0.47
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.97	0.47
7:D:91:ALA:HB1	38:D:5198:HOH:O	2.13	0.47
1:0:1800:G:O2'	1:0:1801:A:H5'	2.14	0.47
1:0:1181:A:H2'	1:0:1182:C:O4'	2.14	0.46
1:0:289:G:N1	1:0:363:A:C2	2.78	0.46
13:J:75:ARG:O	13:J:93:ASN:HA	2.15	0.46
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.97	0.46
31:2:42:ARG:HH11	31:2:42:ARG:CG	2.27	0.46
30:1:19:SER:O	30:1:36:ASN:ND2	2.47	0.46
16:M:139:TRP:CH2	16:M:176:ARG:NH1	2.83	0.46
1:0:581:G:O2'	1:0:582:C:H5'	2.15	0.46
1:0:1584:C:O2'	1:0:1585:C:H5'	2.15	0.46
1:0:383:A:H4'	38:0:6225:HOH:O	2.15	0.46
28:Y:81:LYS:O	28:Y:82:ALA:C	2.53	0.46
1:0:317:A:OP1	22:S:52:ARG:O	2.32	0.46
11:H:162:SER:CB	11:H:163:PRO:CD	2.78	0.46
7:D:21:VAL:HG13	7:D:131:THR:O	2.14	0.46
16:M:100:ALA:O	16:M:129:ILE:HG23	2.15	0.46
1:0:1942:A:H1'	38:A:8564:HOH:O	2.15	0.46
21:R:51:GLN:NE2	21:R:53:ASN:HD21	2.06	0.46
5:B:85:ARG:NH1	38:B:8648:HOH:O	2.47	0.46
9:F:110:GLU:HG2	38:F:6926:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:98:ASN:ND2	20:Q:98:ASN:N	2.64	0.46
1:0:1269:G:H2'	1:0:1270:U:C6	2.50	0.46
1:0:1787:C:O2'	1:0:1788:U:H5'	2.15	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.46
1:0:665:A:H2'	1:0:666:A:C8	2.51	0.46
11:H:109:ASP:HB2	38:H:8349:HOH:O	2.15	0.46
22:S:30:ASP:O	22:S:33:GLU:HB3	2.15	0.46
1:0:1252:A:H2'	1:0:1253:C:O4'	2.15	0.46
1:0:2004:U:H4'	38:0:6205:HOH:O	2.16	0.46
6:C:127:ARG:HH21	6:C:225:PRO:HG2	1.70	0.46
1:0:1246:A:O2'	1:0:1247:A:H3'	2.15	0.46
5:B:55:ASN:HB3	5:B:64:GLY:H	1.80	0.46
5:B:274:GLU:HG3	5:B:275:GLY:N	2.30	0.46
4:A:55:VAL:HG22	4:A:68:ILE:O	2.15	0.46
9:F:113:ASP:O	9:F:117:GLU:HG3	2.16	0.46
21:R:14:ALA:HA	21:R:25:GLN:NE2	2.29	0.46
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.45	0.46
1:0:958:G:O2'	1:0:959:C:H5'	2.16	0.46
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.96	0.46
1:0:482:G:H4'	1:0:508:A:N1	2.30	0.46
1:0:1600:G:H8	1:0:1600:G:OP2	1.98	0.46
17:N:26:TRP:HB2	38:N:3062:HOH:O	2.15	0.46
2:9:3095:C:O2'	2:9:3096:C:H5'	2.16	0.46
11:H:137:ASN:O	11:H:138:PRO:C	2.53	0.46
16:M:74:PRO:HG2	16:M:159:TYR:CZ	2.51	0.46
7:D:67:ASP:O	7:D:69:ILE:HG13	2.16	0.46
6:C:107:ARG:CB	6:C:107:ARG:HH11	2.27	0.46
5:B:7:ARG:HB2	5:B:7:ARG:CZ	2.46	0.46
23:T:14:GLU:OE1	23:T:15:PRO:CD	2.63	0.46
1:0:1677:U:OP2	30:1:8:LYS:NZ	2.44	0.46
13:J:50:GLY:O	13:J:120:ARG:NH1	2.43	0.46
1:0:1773:G:C2'	1:0:1774:G:H5'	2.46	0.46
21:R:29:ASP:OD1	21:R:31:ARG:HG3	2.16	0.46
27:X:107:PRO:HB3	27:X:182:PHE:CD2	2.51	0.46
1:0:138:U:H5"	1:0:139:C:OP2	2.16	0.46
1:0:259:G:O2'	1:0:260:C:H5'	2.15	0.46
1:0:2311:A:O2'	1:0:2312:G:H5'	2.15	0.46
1:0:366:U:H2'	1:0:367:G:O4'	2.15	0.46
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.45	0.46
12:I:77:GLY:O	12:I:78:ILE:C	2.54	0.46
16:M:73:ALA:HB1	16:M:74:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:69:TYR:HE1	31:2:80:ARG:HB2	1.79	0.46
10:G:12:ILE:HG13	38:G:6833:HOH:O	2.15	0.46
5:B:79:MET:HE1	38:B:8639:HOH:O	2.14	0.46
29:Z:28:HIS:ND1	29:Z:31:LYS:HE2	2.29	0.46
1:0:170:U:H2'	1:0:171:C:C5'	2.45	0.46
7:D:11:HIS:O	7:D:12:GLU:HB3	2.15	0.46
16:M:139:TRP:HA	16:M:139:TRP:HE3	1.81	0.46
1:0:212:A:O4'	1:0:214:U:C6	2.68	0.46
1:0:2332:A:H5'	1:0:2333:G:OP2	2.15	0.46
1:0:2748:G:H1'	38:0:8782:HOH:O	2.15	0.46
15:L:87:MET:HB3	31:2:46:ILE:CD1	2.24	0.46
15:L:67:ILE:CD1	15:L:104:ARG:HD2	2.46	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.46
17:N:14:LEU:CG	17:N:102:ILE:HD11	2.45	0.46
5:B:147:VAL:O	5:B:150:ALA:HB3	2.15	0.46
1:0:200:U:H2'	38:0:4388:HOH:O	2.15	0.46
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.46
1:0:745:G:O6	17:N:68:GLY:HA3	2.15	0.46
1:0:1064:U:H2'	1:0:1065:G:C8	2.51	0.46
1:0:2825:C:H4'	1:0:2826:G:O5'	2.15	0.46
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.51	0.46
1:0:724:G:O2'	1:0:725:C:H5'	2.15	0.46
1:0:2761:A:C4	1:0:2763:G:C8	3.04	0.46
1:0:1118:A:H62	1:0:1244:U:H3	1.63	0.46
7:D:49:PRO:HG3	38:D:5828:HOH:O	2.15	0.46
4:A:199:HIS:HD2	4:A:201:PHE:H	1.61	0.46
16:M:83:LEU:HD13	16:M:175:LEU:HD23	1.98	0.46
8:E:107:PHE:CE1	8:E:152:THR:HB	2.51	0.46
14:K:120:LEU:HD12	14:K:133:VAL:HG21	1.97	0.46
8:E:68:HIS:O	8:E:72:MET:HG3	2.16	0.46
22:S:73:HIS:CD2	22:S:88:PRO:CG	2.99	0.46
18:O:105:LEU:CD2	18:O:137:LEU:HD21	2.45	0.46
1:0:2786:G:H2'	38:0:8861:HOH:O	2.15	0.46
7:D:91:ALA:HB2	7:D:106:PHE:CD2	2.51	0.46
25:V:59:GLN:NE2	25:V:97:ALA:HB3	2.30	0.46
1:0:2034:U:H2'	1:0:2035:C:H6	1.80	0.46
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.46
12:I:19:MET:HE1	12:I:132:LEU:HD11	1.97	0.46
1:0:1878:G:O2'	1:0:1879:U:OP2	2.34	0.46
1:0:1300:G:H1'	38:0:5591:HOH:O	2.15	0.46
1:0:2578:G:C8	1:0:2578:G:H5'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:15:THR:HG22	11:H:91:HIS:HA	1.98	0.46
27:X:184:GLU:OE1	27:X:204:ARG:NH1	2.49	0.46
1:0:445:U:H2'	1:0:446:G:C8	2.51	0.46
1:0:399:C:H5'	15:L:179:GLY:O	2.16	0.46
1:0:1735:C:H2'	1:0:1736:A:H8	1.80	0.46
1:0:2035:C:O2'	1:0:2036:C:H5'	2.16	0.46
12:I:135:ILE:O	12:I:139:LEU:HG	2.15	0.46
1:0:2365:G:H4'	19:P:45:PRO:O	2.15	0.46
13:J:62:PRO:CG	13:J:65:ARG:HH21	2.14	0.46
15:L:104:ARG:O	15:L:108:LYS:HG2	2.15	0.46
9:F:58:GLU:CD	15:L:27:ARG:HH22	2.18	0.46
16:M:67:ALA:C	16:M:69:TYR:H	2.20	0.46
16:M:71:TRP:N	38:M:8539:HOH:O	2.49	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.46	0.46
1:0:2899:A:O2'	1:0:2900:G:H5'	2.16	0.46
5:B:279:THR:CG2	5:B:280:VAL:N	2.79	0.46
1:0:1003:U:O2	11:H:90:PHE:CZ	2.69	0.46
1:0:926:A:O2'	14:K:41:HIS:CD2	2.69	0.46
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.98	0.46
16:M:62:HIS:O	16:M:65:ASP:OD1	2.34	0.46
1:0:1773:G:H2'	1:0:1774:G:H5'	1.98	0.46
1:0:47:G:N3	1:0:114:A:C2	2.84	0.46
1:0:299:U:O2'	1:0:300:C:H5'	2.16	0.46
26:W:18:ARG:HA	38:W:5356:HOH:O	2.16	0.46
1:0:2453:G:H3'	38:0:6807:HOH:O	2.15	0.46
1:0:903:U:OP2	14:K:11:ARG:NH1	2.44	0.46
4:A:4:ILE:HG22	4:A:198:ASP:O	2.16	0.46
1:0:453:A:H4'	1:0:455:A:N7	2.31	0.46
15:L:84:LYS:O	15:L:87:MET:HG2	2.16	0.46
30:1:41:HIS:H	30:1:45:ASN:ND2	2.04	0.46
16:M:67:ALA:C	16:M:69:TYR:N	2.69	0.46
16:M:91:ARG:HG3	16:M:186:LEU:CD2	2.44	0.46
1:0:2781:U:H2'	1:0:2782:G:H5'	1.97	0.46
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.46
1:0:2698:G:H2'	1:0:2699:A:C8	2.51	0.46
9:F:26:THR:HB	9:F:102:GLY:HA3	1.98	0.46
1:0:1557:G:O2'	1:0:1558:C:H5'	2.16	0.46
1:0:101:C:H2'	1:0:102:A:H8	1.81	0.46
25:V:34:LEU:CD1	25:V:100:LEU:HD13	2.46	0.46
7:D:60:GLU:O	7:D:62:ASP:N	2.49	0.46
1:0:232:A:H4'	38:0:6972:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:156:C:H5"	15:L:171:ARG:CD	2.25	0.45
11:H:150:LYS:CB	11:H:157:ILE:HD12	2.46	0.45
1:0:1593:C:OP1	18:O:117:SER:HB3	2.16	0.45
11:H:58:HIS:HA	11:H:61:LEU:HD23	1.98	0.45
31:2:69:TYR:CE1	31:2:80:ARG:HB2	2.50	0.45
27:X:186:ARG:NH1	27:X:186:ARG:HG2	2.30	0.45
9:F:110:GLU:O	9:F:114:LYS:HG3	2.15	0.45
1:0:1335:C:OP2	27:X:207:SER:CB	2.64	0.45
1:0:1512:G:O2'	1:0:1513:C:H5'	2.16	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.84	0.45
22:S:15:PRO:O	22:S:19:ARG:HG3	2.16	0.45
1:0:1305:C:O2'	1:0:1306:U:H5'	2.15	0.45
1:0:1626:A:H2'	1:0:1627:G:O4'	2.16	0.45
23:T:34:SER:HA	23:T:37:GLU:OE1	2.16	0.45
6:C:197:SER:OG	6:C:242:GLU:OE2	2.32	0.45
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.84	0.45
1:0:128:A:O2'	1:0:129:A:H5'	2.16	0.45
1:0:1116:U:C2'	1:0:1118:A:H2	2.27	0.45
25:V:4:LEU:HA	25:V:4:LEU:HD23	1.74	0.45
25:V:122:ARG:NH1	25:V:122:ARG:HG2	2.20	0.45
12:I:19:MET:HE2	12:I:78:ILE:HG22	1.97	0.45
1:0:1206:U:H2'	1:0:1207:A:O4'	2.16	0.45
1:0:963:C:H2'	1:0:964:G:C8	2.50	0.45
1:0:2256:G:C2'	1:0:2257:G:C5'	2.93	0.45
4:A:192:VAL:CG1	4:A:192:VAL:O	2.64	0.45
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.51	0.45
1:0:553:G:H5'	38:0:4440:HOH:O	2.16	0.45
1:0:1421:C:O2'	1:0:1422:U:H5'	2.16	0.45
5:B:146:THR:O	5:B:159:PRO:HB3	2.16	0.45
1:0:1171:A:C2'	1:0:1172:G:H5'	2.46	0.45
1:0:2546:U:H5	5:B:2:GLN:HE22	1.63	0.45
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.81	0.45
1:0:2885:A:H2'	1:0:2886:C:C6	2.51	0.45
16:M:139:TRP:HH2	16:M:176:ARG:HH11	1.62	0.45
1:0:1058:A:H2'	1:0:1060:C:C5'	2.47	0.45
2:9:3061:C:H2'	2:9:3062:A:H8	1.82	0.45
1:0:2314:G:O2'	1:0:2315:C:H5'	2.16	0.45
11:H:34:GLY:HA3	11:H:81:TYR:O	2.16	0.45
12:I:51:GLU:O	12:I:55:GLU:HG3	2.16	0.45
1:0:689:G:O2'	1:0:690:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:31:ILE:HG12	18:O:43:LEU:HD13	1.98	0.45
8:E:77:THR:OG1	8:E:78:GLU:N	2.48	0.45
1:0:1917:G:H2'	1:0:1918:U:C6	2.51	0.45
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.46	0.45
11:H:59:ASN:H	11:H:59:ASN:ND2	2.14	0.45
20:Q:39:THR:CG2	20:Q:42:GLU:HG3	2.46	0.45
16:M:73:ALA:HB1	16:M:74:PRO:HD2	1.98	0.45
1:0:251:C:O2'	1:0:252:C:H5'	2.16	0.45
9:F:101:ALA:HB2	9:F:108:LEU:HD22	1.97	0.45
9:F:99:THR:O	9:F:100:ASP:HB2	2.15	0.45
16:M:184:ILE:HG22	16:M:185:GLU:N	2.30	0.45
29:Z:25:LYS:O	29:Z:25:LYS:HG2	2.17	0.45
1:0:697:G:H4'	1:0:730:G:O3'	2.17	0.45
1:0:2547:C:H2'	1:0:2548:C:C6	2.51	0.45
1:0:2355:G:H5"	1:0:2356:A:OP2	2.16	0.45
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.29	0.45
1:0:170:U:C2'	1:0:171:C:H5'	2.47	0.45
1:0:709:G:O2'	17:N:25:VAL:HG12	2.16	0.45
1:0:2453:G:H4'	14:K:50:GLY:C	2.37	0.45
17:N:21:SER:OG	17:N:106:PRO:HB2	2.17	0.45
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.65	0.45
1:0:489:A:C8	22:S:82:THR:HG22	2.51	0.45
1:0:1940:C:H5"	4:A:234:GLY:HA3	1.97	0.45
1:0:2630:G:O6	4:A:206:ARG:NH2	2.49	0.45
1:0:869:G:OP1	15:L:79:LYS:HE2	2.16	0.45
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.97	0.45
1:0:2846:C:OP1	5:B:158:LYS:HD3	2.16	0.45
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.45
2:9:3026:C:H2'	2:9:3027:C:H6	1.81	0.45
11:H:151:MET:HE3	11:H:151:MET:HA	1.97	0.45
16:M:182:GLY:O	16:M:183:ASP:O	2.34	0.45
5:B:304:PRO:HD2	5:B:307:ARG:CD	2.40	0.45
1:0:249:G:H1'	1:0:265:U:O2	2.17	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.91	0.45
1:0:283:U:H5"	1:0:284:C:P	2.56	0.45
16:M:115:VAL:HG23	16:M:116:PHE:H	1.81	0.45
21:R:51:GLN:HB3	21:R:67:ARG:HH12	1.82	0.45
7:D:57:THR:HG23	7:D:63:ILE:HA	1.99	0.45
14:K:97:VAL:HG12	14:K:98:GLU:O	2.16	0.45
1:0:711:G:C2	1:0:718:C:C2	3.05	0.45
27:X:107:PRO:HB3	27:X:182:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:70:ILE:O	26:W:70:ILE:HG23	2.16	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.79	0.45
1:0:1381:A:N3	1:0:1382:G:H1'	2.32	0.45
1:0:295:C:H2'	1:0:296:G:O4'	2.16	0.45
7:D:73:VAL:HG21	38:D:5828:HOH:O	2.15	0.45
1:0:31:C:H2'	38:0:8568:HOH:O	2.15	0.45
16:M:115:VAL:O	16:M:118:ILE:HB	2.17	0.45
4:A:161:GLY:O	28:Y:68:CYS:SG	2.75	0.45
4:A:57:ALA:HA	4:A:67:LEU:HD23	1.98	0.45
1:0:2000:G:O2'	1:0:2001:G:H5'	2.17	0.45
7:D:95:THR:HG21	7:D:174:VAL:HG22	1.99	0.45
1:0:1517:U:C2	1:0:1670:G:N2	2.84	0.45
19:P:75:ILE:CD1	19:P:84:ILE:HD11	2.46	0.45
7:D:35:ALA:HB2	38:D:5858:HOH:O	2.16	0.45
1:0:583:G:H2'	1:0:584:U:C6	2.51	0.45
25:V:130:HIS:O	25:V:136:GLY:HA3	2.17	0.45
1:0:539:G:H2'	1:0:540:A:C8	2.52	0.45
2:9:3117:G:H2'	2:9:3118:C:C6	2.51	0.45
27:X:189:ASN:C	27:X:189:ASN:ND2	2.67	0.45
9:F:99:THR:HA	38:F:3461:HOH:O	2.17	0.45
18:O:59:ARG:HG2	18:O:59:ARG:HH11	1.82	0.45
1:0:1184:C:H1'	38:0:8953:HOH:O	2.16	0.45
1:0:2716:G:C5'	5:B:206:THR:HG21	2.45	0.45
1:0:2346:C:H4'	7:D:52:THR:HG22	1.99	0.45
5:B:137:LEU:HD11	5:B:140:LEU:HD21	1.99	0.45
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.97	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.36	0.45
1:0:1500:U:P	18:O:41:ARG:HH22	2.39	0.45
16:M:77:ASN:OD1	16:M:80:SER:HB2	2.17	0.45
18:O:16:VAL:CG1	18:O:20:ARG:HB2	2.47	0.45
5:B:248:ARG:O	5:B:251:VAL:CG1	2.65	0.45
1:0:1735:C:H2'	1:0:1736:A:C8	2.51	0.45
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.46	0.45
11:H:112:ARG:O	11:H:113:ALA:C	2.55	0.45
27:X:172:THR:HG22	27:X:173:ALA:N	2.32	0.45
13:J:118:ALA:HA	13:J:125:ALA:HB2	1.99	0.45
25:V:54:PHE:CZ	25:V:140:LYS:HB2	2.52	0.45
30:1:40:ARG:HG3	30:1:45:ASN:CB	2.46	0.45
15:L:37:VAL:CG2	15:L:108:LYS:HG3	2.45	0.45
16:M:161:GLY:O	16:M:162:ASP:C	2.54	0.45
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.51	0.45
22:S:96:VAL:HG13	22:S:97:ARG:N	2.32	0.45
1:0:668:C:H2'	1:0:669:G:H8	1.80	0.45
10:G:27:ILE:HD12	10:G:70:ALA:HB1	1.98	0.45
29:Z:8:GLN:HE22	29:Z:11:LYS:HZ2	1.63	0.45
1:0:338:C:H4'	6:C:174:ILE:HD11	1.97	0.45
1:0:338:C:H4'	6:C:174:ILE:HD12	1.99	0.45
1:0:243:A:H61	1:0:269:G:C1'	2.29	0.45
1:0:958:G:H2'	1:0:959:C:H6	1.80	0.45
1:0:1813:U:O2'	18:O:81:LYS:HE3	2.17	0.45
27:X:106:THR:HG23	27:X:107:PRO:HD2	1.99	0.45
27:X:141:THR:HG23	38:X:8599:HOH:O	2.16	0.45
13:J:22:ASP:OD1	13:J:22:ASP:C	2.55	0.45
1:0:514:G:OP1	1:0:514:G:H2'	2.16	0.45
1:0:1565:C:O4'	1:0:2738:G:H1'	2.16	0.45
1:0:1416:G:C2'	1:0:1417:G:H5'	2.46	0.45
4:A:69:LEU:CD2	4:A:120:ARG:HB3	2.41	0.45
2:9:3047:A:H2'	2:9:3048:C:C6	2.51	0.45
5:B:144:THR:CG2	5:B:145:HIS:N	2.79	0.45
1:0:64:G:H2'	1:0:65:C:H6	1.80	0.45
1:0:2625:C:O2'	1:0:2626:C:H5'	2.16	0.45
20:Q:113:HIS:O	20:Q:145:LEU:HD12	2.17	0.45
1:0:1600:G:H4'	38:0:6539:HOH:O	2.17	0.45
9:F:20:LEU:O	9:F:23:ALA:HB3	2.16	0.45
6:C:126:ASP:C	6:C:128:GLY:N	2.70	0.45
1:0:1156:C:O2'	1:0:1157:C:H5'	2.17	0.45
15:L:99:ARG:HD2	15:L:167:GLY:HA2	1.98	0.45
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.45
11:H:136:VAL:HG22	11:H:137:ASN:O	2.16	0.45
20:Q:39:THR:HG22	20:Q:42:GLU:HG3	1.98	0.45
1:0:2421:G:H4'	38:0:5686:HOH:O	2.17	0.45
31:2:11:CYS:HB2	31:2:20:HIS:NE2	2.32	0.45
12:I:17:CYS:HA	12:I:119:THR:O	2.17	0.45
5:B:7:ARG:CG	5:B:7:ARG:HH11	2.23	0.45
21:R:58:MET:SD	30:1:8:LYS:HE3	2.57	0.45
1:0:1973:A:H2'	1:0:1974:G:O4'	2.17	0.45
15:L:59:GLY:HA3	15:L:141:ILE:HD12	1.99	0.45
20:Q:66:VAL:HG22	20:Q:79:ARG:CZ	2.47	0.45
25:V:40:ALA:O	25:V:44:MET:HG3	2.16	0.45
8:E:162:PHE:CD1	8:E:162:PHE:N	2.84	0.45
1:0:740:G:O2'	1:0:741:C:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:953:G:H5'	38:0:8786:HOH:O	2.17	0.45
5:B:38:VAL:HG22	5:B:142:LEU:HD12	1.99	0.45
1:0:1613:C:H2'	1:0:1614:G:O4'	2.17	0.45
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.45
22:S:44:ALA:HA	22:S:62:VAL:HG12	1.99	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.45
1:0:1134:G:C4'	11:H:151:MET:HE1	2.35	0.45
5:B:195:ARG:N	5:B:198:GLU:OE1	2.45	0.45
6:C:104:ASP:O	6:C:108:GLN:HG3	2.17	0.45
1:0:1470:A:OP1	15:L:93:ARG:HD2	2.17	0.45
15:L:113:ARG:NH2	15:L:156:ARG:HG2	2.31	0.45
17:N:14:LEU:CD2	17:N:102:ILE:HD11	2.47	0.45
1:0:1514:C:H2'	1:0:1515:A:H8	1.81	0.45
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.99	0.45
1:0:538:C:H5"	1:0:539:G:C8	2.52	0.45
1:0:1758:U:H2'	1:0:1759:A:O4'	2.17	0.45
6:C:76:ARG:HD2	38:C:8444:HOH:O	2.17	0.45
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.45
6:C:140:VAL:HB	38:C:8463:HOH:O	2.16	0.45
1:0:1523:G:H2'	1:0:1524:U:C6	2.52	0.45
27:X:219:GLU:HG3	27:X:220:GLU:N	2.31	0.45
16:M:34:LEU:HD13	16:M:47:LEU:HD21	1.99	0.44
12:I:19:MET:HE2	12:I:79:PHE:HA	1.98	0.44
23:T:46:ALA:HB1	23:T:52:THR:HG21	2.00	0.44
17:N:47:ARG:HG3	17:N:47:ARG:NH1	2.32	0.44
5:B:7:ARG:CG	5:B:7:ARG:NH1	2.80	0.44
26:W:30:MET:HE2	26:W:58:ALA:HB3	1.98	0.44
17:N:77:ALA:HA	17:N:96:VAL:O	2.17	0.44
1:0:169:A:H1'	31:2:48:ASN:ND2	2.31	0.44
22:S:24:ARG:NH2	22:S:39:ASN:HD22	2.15	0.44
2:9:3031:C:O2'	2:9:3032:G:H5'	2.17	0.44
1:0:653:C:H2'	1:0:654:A:C8	2.51	0.44
1:0:2561:C:OP1	8:E:153:ARG:NH2	2.50	0.44
16:M:47:LEU:HD13	16:M:97:VAL:HG11	1.98	0.44
28:Y:31:ILE:CG2	28:Y:32:LYS:N	2.80	0.44
16:M:72:GLU:H	16:M:171:HIS:CE1	2.35	0.44
4:A:101:GLU:HG2	38:A:8580:HOH:O	2.17	0.44
4:A:132:ASP:OD1	4:A:133:ARG:N	2.50	0.44
1:0:1384:C:H5'	26:W:30:MET:HG2	1.99	0.44
18:O:7:LYS:CD	18:O:21:VAL:CG2	2.95	0.44
1:0:658:C:O2'	1:0:662:U:OP1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:149:LEU:HG	25:V:153:MET:HE1	2.00	0.44
1:0:812:A:H2'	1:0:813:C:H6	1.80	0.44
17:N:96:VAL:HA	38:N:4258:HOH:O	2.17	0.44
1:0:1937:U:O2'	1:0:1938:G:H5'	2.17	0.44
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.99	0.44
1:0:2709:G:H4'	13:J:3:ALA:CB	2.47	0.44
5:B:98:THR:HG22	5:B:99:GLU:H	1.83	0.44
19:P:77:ASP:N	19:P:80:LYS:O	2.49	0.44
1:0:1611:G:O2'	1:0:1612:A:H5'	2.18	0.44
1:0:2106:C:H2'	1:0:2107:U:C6	2.53	0.44
1:0:1548:U:O2'	1:0:1549:C:H5'	2.17	0.44
6:C:223:LEU:HA	6:C:223:LEU:HD12	1.87	0.44
14:K:144:ASP:HA	14:K:147:GLU:HG3	1.99	0.44
7:D:64:ARG:O	7:D:67:ASP:OD2	2.36	0.44
23:T:17:THR:CG2	23:T:18:GLY:N	2.81	0.44
14:K:125:PHE:CZ	14:K:140:VAL:HG13	2.52	0.44
1:0:1857:A:N6	1:0:2247:C:H1'	2.32	0.44
26:W:23:HIS:HB2	38:W:7830:HOH:O	2.16	0.44
16:M:58:LEU:HD12	16:M:58:LEU:N	2.32	0.44
13:J:21:ALA:O	13:J:96:VAL:HG22	2.17	0.44
1:0:1894:C:C2	1:0:1939:U:C4	3.05	0.44
1:0:349:U:O2'	1:0:350:C:H5'	2.18	0.44
1:0:2481:G:C3'	1:0:2482:G:H5"	2.46	0.44
15:L:88:VAL:HG12	15:L:89:ASN:N	2.32	0.44
16:M:37:ARG:NE	38:M:8534:HOH:O	2.50	0.44
18:O:115:SER:C	18:O:117:SER:H	2.20	0.44
11:H:139:ASP:O	11:H:139:ASP:CG	2.56	0.44
26:W:78:GLU:CG	26:W:79:GLU:H	2.26	0.44
1:0:1184:C:O2'	1:0:1185:U:P	2.76	0.44
1:0:2415:A:C2	16:M:25:ARG:HB3	2.52	0.44
1:0:731:U:H2'	1:0:732:C:H6	1.80	0.44
8:E:69:ILE:O	8:E:72:MET:HB2	2.16	0.44
11:H:117:LYS:O	11:H:119:VAL:HG13	2.18	0.44
18:O:10:ALA:HA	18:O:13:VAL:CG1	2.48	0.44
1:0:1872:C:O2	4:A:25:ALA:HA	2.18	0.44
1:0:653:C:H5"	38:N:7674:HOH:O	2.16	0.44
1:0:1372:A:H3'	38:0:8863:HOH:O	2.18	0.44
1:0:81:G:N3	1:0:98:A:C2	2.85	0.44
9:F:34:ASN:O	9:F:38:LYS:HG3	2.16	0.44
1:0:328:U:O4'	6:C:202:THR:HG22	2.17	0.44
16:M:32:PRO:HD2	16:M:99:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2755:G:H1'	38:0:5590:HOH:O	2.18	0.44
11:H:86:ARG:HG2	11:H:86:ARG:H	1.44	0.44
1:0:1164:U:N3	1:0:1192:A:H2	2.07	0.44
1:0:363:A:O2'	1:0:364:C:H5'	2.18	0.44
25:V:110:GLN:HE21	25:V:110:GLN:HA	1.82	0.44
25:V:80:ASP:O	25:V:84:VAL:HG23	2.17	0.44
1:0:821:U:H5"	38:0:4004:HOH:O	2.17	0.44
32:0:9500:SLD:N4S	3:4:75:C:OP2	2.50	0.44
5:B:52:VAL:C	5:B:53:LEU:HD12	2.38	0.44
1:0:1463:A:H2'	1:0:1464:U:H6	1.82	0.44
13:J:34:VAL:CG2	13:J:47:ALA:HB2	2.48	0.44
1:0:2912:C:O2'	1:0:2913:A:H5'	2.18	0.44
1:0:113:A:OP2	1:0:114:A:H2'	2.18	0.44
2:9:3088:G:OP1	25:V:130:HIS:NE2	2.40	0.44
18:O:109:ARG:NH1	18:O:119:TYR:CE2	2.85	0.44
1:0:1746:A:O4'	1:0:1747:A:C2	2.70	0.44
14:K:101:ASP:C	14:K:103:ALA:H	2.20	0.44
1:0:622:G:P	27:X:148:GLY:HA3	2.57	0.44
13:J:10:GLN:NE2	13:J:10:GLN:N	2.31	0.44
1:0:2509:A:OP2	1:0:2510:C:H5	2.01	0.44
13:J:113:ILE:HD12	13:J:128:ALA:HB2	2.00	0.44
28:Y:30:GLU:HB3	28:Y:34:LYS:HE3	1.99	0.44
26:W:43:VAL:CG1	26:W:47:ALA:HB3	2.47	0.44
1:0:283:U:H5	1:0:284:C:H42	1.65	0.44
25:V:13:MET:HE1	25:V:18:GLN:CA	2.43	0.44
1:0:1299:G:N2	38:0:5591:HOH:O	2.50	0.44
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.44
1:0:1514:C:O2'	1:0:1515:A:H5'	2.18	0.44
1:0:2091:G:O3'	5:B:235:ARG:HD3	2.17	0.44
1:0:101:C:H2'	1:0:102:A:C8	2.53	0.44
1:0:1019:C:O2	19:P:94:GLN:NE2	2.51	0.44
1:0:659:A:H5"	38:N:6799:HOH:O	2.17	0.44
1:0:2815:G:N7	12:I:80:LYS:NZ	2.64	0.44
1:0:152:A:O2'	1:0:153:C:H5'	2.18	0.44
1:0:1432:U:H5'	38:0:3181:HOH:O	2.17	0.44
25:V:7:LEU:HD12	25:V:53:ALA:HB2	2.00	0.44
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.46	0.44
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.90	0.44
4:A:56:ALA:O	4:A:68:ILE:N	2.49	0.44
1:0:377:C:O2'	1:0:378:A:H5'	2.18	0.44
7:D:173:GLU:O	7:D:174:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:72:VAL:HG13	11:H:72:VAL:O	2.17	0.44
2:9:3078:G:N2	2:9:3103:A:OP2	2.48	0.44
1:0:2064:U:H2'	1:0:2065:C:H6	1.83	0.44
1:0:1759:A:N3	1:0:1818:C:H2'	2.33	0.44
1:0:1283:G:O2'	1:0:1284:G:H5'	2.18	0.44
15:L:40:ILE:O	15:L:40:ILE:HG13	2.18	0.44
1:0:818:A:O2'	28:Y:13:ARG:HD3	2.17	0.44
1:0:130:C:O2'	1:0:131:A:N7	2.50	0.44
1:0:1118:A:H8	1:0:1119:G:H5"	1.82	0.44
1:0:1180:U:H2'	1:0:1181:A:O4'	2.18	0.44
1:0:1201:C:H2'	1:0:1202:A:H5'	1.99	0.44
11:H:26:LYS:CG	11:H:28:ILE:H	2.20	0.44
1:0:2896:A:OP1	26:W:15:ARG:NH1	2.51	0.44
25:V:7:LEU:CD1	25:V:53:ALA:HB2	2.48	0.44
1:0:541:C:O2'	1:0:542:A:H5"	2.18	0.44
10:G:12:ILE:HA	38:G:8806:HOH:O	2.18	0.44
15:L:153:THR:O	15:L:156:ARG:HG3	2.17	0.44
12:I:107:ASN:HD22	12:I:107:ASN:C	2.20	0.44
27:X:184:GLU:OE2	27:X:204:ARG:HD2	2.17	0.44
5:B:148:PRO:HD2	38:B:8593:HOH:O	2.18	0.44
14:K:121:ILE:HG12	14:K:141:GLU:HB2	1.99	0.44
1:0:60:A:H5'	30:1:19:SER:HG	1.83	0.44
1:0:1901:G:O2'	1:0:1902:G:H5'	2.18	0.44
1:0:2252:A:H2'	1:0:2253:G:O4'	2.18	0.44
1:0:612:U:H2'	1:0:613:C:H6	1.83	0.44
1:0:2868:C:H2'	1:0:2869:G:O4'	2.18	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.53	0.44
1:0:2834:G:C4	1:0:2847:G:N2	2.85	0.44
1:0:2401:A:H5'	38:0:3467:HOH:O	2.17	0.44
1:0:1072:G:OP2	27:X:154:ARG:NH2	2.51	0.44
2:9:3053:G:O2'	2:9:3054:A:H5'	2.18	0.44
11:H:84:ARG:CZ	11:H:135:TRP:CH2	3.00	0.44
7:D:27:ILE:CG2	7:D:28:GLY:H	2.18	0.44
25:V:122:ARG:CG	25:V:152:ALA:O	2.66	0.44
16:M:104:ILE:O	16:M:107:ASN:HB2	2.17	0.44
7:D:136:ARG:HD2	7:D:155:HIS:O	2.18	0.44
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.18	0.44
5:B:41:PHE:CE1	5:B:79:MET:HG3	2.53	0.44
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.33	0.44
24:U:23:LEU:HD22	24:U:49:LEU:HD23	2.00	0.44
1:0:308:U:H5'	22:S:97:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:56:MET:CE	28:Y:63:LYS:HE3	2.48	0.44
8:E:69:ILE:HA	8:E:72:MET:CE	2.48	0.44
25:V:5:VAL:HG11	25:V:153:MET:CE	2.48	0.44
1:0:1936:C:O2'	1:0:1937:U:H5'	2.18	0.44
38:J:408:HOH:O	23:T:37:GLU:HB3	2.17	0.44
9:F:26:THR:HB	9:F:102:GLY:O	2.17	0.44
1:0:823:U:H2'	1:0:824:G:O4'	2.17	0.44
38:0:7167:HOH:O	27:X:158:LYS:HD3	2.17	0.44
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.18	0.44
1:0:2872:U:H2'	1:0:2873:C:H6	1.83	0.44
6:C:156:LEU:HD12	6:C:156:LEU:O	2.18	0.44
1:0:2807:U:OP2	5:B:28:SER:OG	2.28	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.44
15:L:87:MET:HG3	15:L:87:MET:H	1.35	0.43
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.00	0.43
12:I:19:MET:HE1	12:I:132:LEU:CD2	2.47	0.43
1:0:1852:A:H2'	1:0:1853:C:H6	1.83	0.43
2:9:3039:U:H3'	2:9:3040:C:H5"	1.99	0.43
1:0:2595:U:O2'	1:0:2596:A:H5'	2.18	0.43
13:J:81:ARG:HD3	13:J:87:ARG:NH1	2.33	0.43
1:0:1505:U:C6	1:0:1505:U:H5'	2.48	0.43
1:0:861:A:H2'	1:0:862:U:H6	1.83	0.43
1:0:60:A:H5'	30:1:19:SER:OG	2.18	0.43
7:D:55:LYS:O	7:D:56:ARG:HB2	2.18	0.43
1:0:2004:U:C2'	1:0:2005:G:OP1	2.66	0.43
1:0:102:A:H2'	1:0:103:U:C6	2.53	0.43
16:M:114:LYS:O	16:M:117:ALA:HB3	2.18	0.43
1:0:1052:G:H2'	1:0:1052:G:N3	2.33	0.43
1:0:2719:A:C2	5:B:70:PRO:HG3	2.53	0.43
1:0:2880:A:H2'	1:0:2881:C:O4'	2.18	0.43
13:J:78:LYS:HA	13:J:79:PRO:HD3	1.85	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.05	0.43
20:Q:50:VAL:O	20:Q:53:GLY:N	2.51	0.43
9:F:8:VAL:HG13	9:F:12:LEU:HD13	1.99	0.43
1:0:1537:C:H1'	38:0:7461:HOH:O	2.18	0.43
9:F:115:VAL:O	9:F:118:LEU:N	2.51	0.43
4:A:36:ASP:CA	4:A:83:GLY:HA3	2.47	0.43
9:F:104:ALA:O	9:F:108:LEU:HB3	2.18	0.43
4:A:95:PRO:HG2	4:A:98:GLU:HG2	2.00	0.43
1:0:305:A:C5	1:0:329:A:C2	3.06	0.43
7:D:77:ASP:HB3	7:D:78:GLU:H	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:212:ARG:HD2	38:X:8610:HOH:O	2.17	0.43
1:0:1116:U:O2'	1:0:1118:A:C2	2.44	0.43
16:M:37:ARG:HA	16:M:37:ARG:HD3	1.83	0.43
11:H:26:LYS:CE	11:H:28:ILE:HB	2.47	0.43
1:0:2502:C:H4'	11:H:151:MET:CG	2.43	0.43
18:O:114:LEU:HA	18:O:118:GLN:NE2	2.34	0.43
16:M:49:THR:CG2	16:M:56:ASP:HB2	2.36	0.43
25:V:122:ARG:NH2	38:V:4276:HOH:O	2.49	0.43
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.83	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.99	0.43
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.81	0.43
19:P:40:HIS:HD2	19:P:60:THR:OG1	2.01	0.43
1:0:1114:A:H2'	1:0:1115:U:H6	1.83	0.43
1:0:1278:A:P	17:N:19:ARG:HH22	2.41	0.43
1:0:1486:A:C5	30:1:2:LYS:HG3	2.53	0.43
1:0:2529:G:O2'	1:0:2530:C:H5'	2.18	0.43
12:I:97:ALA:O	12:I:101:VAL:HG23	2.17	0.43
8:E:101:GLU:HB2	8:E:116:THR:O	2.17	0.43
1:0:602:A:O2'	1:0:605:C:H4'	2.19	0.43
11:H:47:GLU:HG2	11:H:133:ILE:CD1	2.49	0.43
15:L:95:LYS:HG2	15:L:99:ARG:HB3	1.99	0.43
18:O:103:THR:HA	18:O:106:ARG:HH12	1.81	0.43
8:E:7:ILE:HD11	8:E:11:VAL:O	2.19	0.43
11:H:58:HIS:CE1	11:H:59:ASN:ND2	2.86	0.43
1:0:2694:A:C4'	8:E:91:PHE:HE1	2.23	0.43
1:0:1805:G:O2'	1:0:1806:G:H5'	2.18	0.43
1:0:235:C:O2'	1:0:236:A:H2'	2.18	0.43
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.53	0.43
1:0:695:C:H2'	1:0:696:C:C6	2.53	0.43
27:X:100:ARG:HE	27:X:234:VAL:HG21	1.81	0.43
1:0:2434:A:O3'	31:2:28:GLY:HA3	2.19	0.43
5:B:62:ARG:HG2	5:B:65:MET:HE3	2.00	0.43
1:0:2758:G:O2'	1:0:2759:C:H5'	2.19	0.43
4:A:109:GLU:HG2	4:A:116:GLY:N	2.33	0.43
15:L:85:ARG:C	15:L:87:MET:HG3	2.39	0.43
16:M:47:LEU:CD1	16:M:97:VAL:HG11	2.48	0.43
18:O:103:THR:O	18:O:106:ARG:HB3	2.18	0.43
31:2:69:TYR:CE1	31:2:80:ARG:HD2	2.53	0.43
5:B:55:ASN:CB	5:B:63:GLU:HA	2.46	0.43
27:X:203:VAL:CG1	27:X:228:VAL:HG22	2.46	0.43
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:56:ASN:O	30:1:8:LYS:HE2	2.18	0.43
1:0:1461:U:H2'	1:0:1462:C:H6	1.80	0.43
1:0:2244:A:H5"	15:L:29:GLN:OE1	2.19	0.43
7:D:60:GLU:C	7:D:62:ASP:N	2.72	0.43
27:X:144:ARG:NE	38:X:8621:HOH:O	2.50	0.43
1:0:400:C:O2'	1:0:401:C:H5'	2.19	0.43
10:G:18:GLU:O	10:G:21:ASP:HB2	2.18	0.43
1:0:1244:U:H4'	1:0:1246:A:O4'	2.19	0.43
15:L:55:LYS:HB2	15:L:60:ILE:CD1	2.49	0.43
15:L:61:ILE:N	15:L:61:ILE:HD12	2.33	0.43
26:W:9:VAL:HG13	26:W:88:GLU:CD	2.38	0.43
5:B:180:ASP:O	5:B:181:ILE:C	2.57	0.43
38:0:5481:HOH:O	15:L:86:MET:HE3	2.18	0.43
27:X:200:THR:HG22	27:X:201:GLU:HG2	2.00	0.43
1:0:2296:C:H2'	1:0:2297:U:C6	2.53	0.43
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.54	0.43
1:0:1114:A:H2'	1:0:1115:U:C6	2.54	0.43
1:0:1276:U:H3'	17:N:19:ARG:HH11	1.83	0.43
7:D:128:LEU:C	7:D:128:LEU:HD23	2.39	0.43
16:M:15:GLU:O	16:M:17:ARG:HG3	2.19	0.43
28:Y:58:GLY:HA3	38:Y:8442:HOH:O	2.19	0.43
11:H:28:ILE:HG23	38:H:8390:HOH:O	2.17	0.43
27:X:189:ASN:ND2	27:X:192:ASP:H	2.16	0.43
8:E:22:VAL:O	8:E:28:SER:HA	2.19	0.43
1:0:797:A:H5'	28:Y:10:ARG:HG2	2.00	0.43
10:G:12:ILE:HG22	10:G:12:ILE:O	2.19	0.43
13:J:87:ARG:HB2	23:T:19:THR:HG23	2.01	0.43
1:0:353:G:H2'	1:0:354:A:H8	1.82	0.43
9:F:49:PHE:CD1	9:F:49:PHE:N	2.87	0.43
1:0:473:A:O2'	1:0:474:C:H5'	2.19	0.43
27:X:151:SER:HB3	27:X:154:ARG:HB3	2.00	0.43
1:0:883:U:O2	1:0:883:U:H2'	2.18	0.43
1:0:1755:A:H2'	1:0:1756:G:O4'	2.18	0.43
22:S:3:GLN:HA	22:S:4:PRO:HD3	1.89	0.43
7:D:21:VAL:HA	7:D:131:THR:O	2.18	0.43
13:J:90:PHE:CD1	13:J:90:PHE:N	2.87	0.43
16:M:143:ARG:HA	16:M:172:PHE:CE2	2.54	0.43
22:S:87:VAL:HB	22:S:88:PRO:HD2	2.00	0.43
15:L:184:ARG:NH1	15:L:184:ARG:HB2	2.34	0.43
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.43
12:I:4:ALA:O	12:I:5:GLU:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:50:GLY:HA3	19:P:87:THR:OG1	2.19	0.43
1:0:999:C:O2'	1:0:1000:C:H5'	2.19	0.43
1:0:2670:G:O2'	1:0:2671:U:H5'	2.18	0.43
1:0:2661:U:H3	1:0:2812:A:H62	1.67	0.43
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.49	0.43
25:V:26:ILE:CG1	25:V:26:ILE:O	2.66	0.43
28:Y:32:LYS:HB3	28:Y:32:LYS:HE2	1.90	0.43
1:0:264:G:H1'	1:0:265:U:H5	1.82	0.43
13:J:29:LEU:HB3	13:J:55:VAL:CG1	2.42	0.43
1:0:1205:U:H2'	1:0:1206:U:C5'	2.49	0.43
7:D:146:LYS:CE	16:M:107:ASN:ND2	2.81	0.43
1:0:559:U:O2'	1:0:560:C:H5'	2.19	0.43
1:0:1008:C:H2'	1:0:1009:U:C6	2.53	0.43
1:0:111:C:H2'	1:0:112:G:O4'	2.19	0.43
1:0:2538:A:H4'	1:0:2539:U:OP1	2.19	0.43
1:0:2054:A:H2	20:Q:128:ARG:HH22	1.61	0.43
18:O:16:VAL:CG1	18:O:17:GLY:N	2.82	0.43
1:0:685:C:O2	1:0:748:C:H4'	2.18	0.43
26:W:26:ALA:O	26:W:27:ASP:C	2.57	0.43
13:J:125:ALA:C	13:J:127:ALA:H	2.21	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.43
1:0:2106:C:H1'	1:0:2484:U:O2	2.19	0.43
38:0:3070:HOH:O	5:B:214:PRO:HD2	2.19	0.43
1:0:2060:A:H2'	1:0:2061:C:C6	2.54	0.43
1:0:1566:C:O2'	1:0:1567:A:H5'	2.19	0.43
21:R:42:GLU:HG2	21:R:49:VAL:HG23	2.01	0.43
15:L:122:GLU:HB2	15:L:126:HIS:O	2.19	0.43
2:9:3056:A:O2'	7:D:14:ARG:HD3	2.19	0.43
1:0:250:C:O2'	1:0:251:C:H5'	2.18	0.43
1:0:1853:C:H5'	4:A:228:ILE:O	2.18	0.43
4:A:103:VAL:HA	4:A:104:PRO:HD3	1.84	0.43
1:0:1008:C:O2'	1:0:1009:U:H5'	2.19	0.43
9:F:36:THR:OG1	38:F:3111:HOH:O	2.22	0.43
16:M:108:SER:HA	16:M:109:PRO:HD3	1.80	0.43
1:0:392:U:H4'	15:L:193:LYS:HB3	2.00	0.43
11:H:111:MET:O	11:H:114:PRO:HD3	2.19	0.43
1:0:1377:C:H5'	1:0:1377:C:C6	2.51	0.43
1:0:354:A:H2'	1:0:355:C:H6	1.83	0.43
19:P:93:ARG:HG3	19:P:93:ARG:NH1	2.34	0.43
1:0:2684:A:H2'	1:0:2685:C:C6	2.54	0.43
1:0:1947:G:N2	1:0:1966:U:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:97:ALA:HB2	4:A:150:PRO:HB2	2.01	0.43
18:O:135:ALA:HB1	18:O:139:ARG:HH12	1.84	0.43
15:L:71:SER:HB2	15:L:92:THR:HG22	2.00	0.43
24:U:12:THR:HG23	24:U:14:ALA:N	2.34	0.42
38:0:4117:HOH:O	15:L:87:MET:HE1	2.19	0.42
5:B:205:VAL:O	5:B:307:ARG:CD	2.67	0.42
20:Q:89:LEU:HD23	20:Q:89:LEU:HA	1.79	0.42
14:K:133:VAL:HB	38:K:8562:HOH:O	2.19	0.42
1:0:1329:A:N1	36:0:8513:CL:CL	2.88	0.42
1:0:1667:A:C8	1:0:1667:A:H5'	2.50	0.42
6:C:138:VAL:O	6:C:234:VAL:HA	2.19	0.42
1:0:2688:U:H2'	1:0:2689:A:C8	2.54	0.42
1:0:152:A:H2'	1:0:153:C:C6	2.54	0.42
6:C:7:ASP:C	6:C:9:ASP:H	2.22	0.42
1:0:123:U:H2'	1:0:124:C:C6	2.54	0.42
7:D:151:ILE:HA	7:D:152:PRO:HD3	1.89	0.42
5:B:238:ASN:ND2	5:B:240:GLY:N	2.54	0.42
15:L:35:PRO:HD2	15:L:38:VAL:CG2	2.48	0.42
25:V:154:ARG:HB3	25:V:154:ARG:HE	1.50	0.42
28:Y:27:ALA:O	28:Y:28:ASP:C	2.57	0.42
2:9:3007:G:H4'	16:M:55:ASP:OD2	2.18	0.42
1:0:2840:A:H3'	38:0:8528:HOH:O	2.18	0.42
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.00	0.42
21:R:57:THR:CG2	21:R:58:MET:N	2.82	0.42
12:I:6:PHE:O	12:I:8:ALA:N	2.52	0.42
1:0:2730:G:O2'	1:0:2731:G:H5'	2.19	0.42
1:0:61:G:C2	1:0:62:C:C2	3.07	0.42
1:0:2708:G:H2'	1:0:2709:G:O4'	2.19	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.54	0.42
31:2:5:ARG:HG3	31:2:5:ARG:O	2.20	0.42
1:0:843:A:C2	1:0:846:A:C8	3.08	0.42
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.34	0.42
1:0:2544:G:H2'	1:0:2545:U:O4'	2.18	0.42
25:V:29:VAL:O	25:V:30:ASN:HB2	2.18	0.42
38:0:4962:HOH:O	6:C:149:LYS:HE3	2.18	0.42
6:C:178:GLN:O	6:C:179:GLY:C	2.58	0.42
16:M:34:LEU:HD22	16:M:129:ILE:CD1	2.49	0.42
1:0:2896:A:N3	1:0:2896:A:H2'	2.34	0.42
11:H:46:VAL:CG1	11:H:146:TRP:HZ3	2.32	0.42
7:D:133:ASN:HD22	7:D:133:ASN:HA	1.66	0.42
38:0:7645:HOH:O	16:M:4:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:39:ALA:C	24:U:41:GLU:N	2.72	0.42
1:0:1328:A:N7	1:0:1329:A:C5	2.87	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.47	0.42
1:0:2347:C:H2'	1:0:2348:C:H6	1.85	0.42
1:0:776:A:H1'	1:0:779:U:O4	2.19	0.42
1:0:639:A:H2'	1:0:640:G:H8	1.83	0.42
1:0:1139:U:H2'	1:0:1140:C:H6	1.84	0.42
13:J:9:THR:HG22	13:J:78:LYS:HG2	2.01	0.42
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.19	0.42
38:9:8411:HOH:O	7:D:68:PRO:HG3	2.20	0.42
1:0:525:G:H2'	1:0:526:U:O4'	2.18	0.42
1:0:1433:G:O2'	1:0:1434:A:H5'	2.19	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.42
7:D:166:ILE:O	7:D:169:THR:N	2.51	0.42
16:M:175:LEU:HD12	16:M:175:LEU:HA	1.75	0.42
1:0:2353:A:H4'	1:0:2354:A:O5'	2.19	0.42
29:Z:25:LYS:CD	30:1:49:GLU:H	2.28	0.42
1:0:2011:A:H5'	1:0:2013:G:H1'	2.00	0.42
16:M:152:GLU:C	16:M:154:LEU:N	2.72	0.42
1:0:1635:U:O2'	1:0:1636:G:H5'	2.19	0.42
11:H:31:PHE:HE2	11:H:87:LYS:O	2.02	0.42
27:X:235:GLU:N	27:X:235:GLU:CD	2.71	0.42
1:0:565:A:H2'	1:0:566:A:C8	2.54	0.42
11:H:71:TYR:C	11:H:73:GLN:N	2.71	0.42
1:0:1669:A:H2'	1:0:1670:G:H8	1.84	0.42
38:0:5879:HOH:O	11:H:57:ARG:HG3	2.19	0.42
6:C:40:ALA:HB3	6:C:100:LEU:HD12	2.02	0.42
1:0:675:U:O2'	6:C:42:ARG:NH1	2.52	0.42
1:0:1649:G:O2'	1:0:1650:C:H5'	2.18	0.42
1:0:301:G:O2'	1:0:302:A:H5'	2.19	0.42
1:0:1028:U:H5'	1:0:1031:G:O4'	2.19	0.42
5:B:152:PRO:HD2	38:B:8645:HOH:O	2.18	0.42
12:I:142:ASN:O	12:I:144:THR:N	2.52	0.42
1:0:2053:G:H4'	20:Q:136:TRP:CE2	2.55	0.42
5:B:33:ASP:HB3	5:B:34:GLY:H	1.71	0.42
1:0:2039:A:H4'	1:0:2760:C:O2'	2.20	0.42
12:I:45:VAL:HG22	12:I:46:ILE:N	2.34	0.42
11:H:48:LEU:CG	11:H:157:ILE:HG21	2.48	0.42
5:B:83:ALA:HB2	5:B:101:TRP:CD2	2.54	0.42
7:D:54:ALA:O	7:D:65:GLU:O	2.37	0.42
1:0:370:G:O2'	1:0:371:U:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:191:A:H2'	1:0:237:G:O6	2.19	0.42
1:0:821:U:H2'	1:0:822:C:C6	2.54	0.42
1:0:902:G:N7	14:K:18:HIS:CD2	2.85	0.42
14:K:124:ASP:OD1	14:K:149:ARG:NH2	2.53	0.42
1:0:1517:U:H2'	1:0:1518:A:C8	2.54	0.42
1:0:1714:C:H4'	1:0:2745:C:O2	2.19	0.42
15:L:137:ASP:O	15:L:142:LYS:HE3	2.19	0.42
1:0:317:A:H5'	22:S:52:ARG:HD2	2.01	0.42
1:0:2824:C:H5"	1:0:2825:C:H5'	2.01	0.42
1:0:2039:A:H2'	1:0:2040:C:C6	2.55	0.42
1:0:307:G:C2	1:0:309:C:C4	3.06	0.42
1:0:770:C:O2'	1:0:771:G:H5'	2.18	0.42
18:O:84:ALA:C	18:O:86:ALA:H	2.23	0.42
13:J:19:THR:HB	13:J:94:ALA:HB2	2.01	0.42
1:0:2651:C:H2'	1:0:2652:U:O4'	2.19	0.42
9:F:4:VAL:HA	9:F:76:PHE:CE1	2.54	0.42
12:I:130:VAL:HG12	12:I:131:THR:N	2.32	0.42
18:O:103:THR:O	18:O:107:GLU:HG3	2.20	0.42
1:0:1996:U:H6	1:0:2586:U:O2	2.03	0.42
16:M:69:TYR:HE2	16:M:183:ASP:OD2	2.03	0.42
8:E:15:GLN:NE2	8:E:40:VAL:O	2.52	0.42
10:G:20:VAL:O	10:G:24:VAL:HG23	2.20	0.42
29:Z:25:LYS:HD2	30:1:48:ASP:HA	2.02	0.42
5:B:132:HIS:CE1	5:B:171:VAL:CG2	3.03	0.42
7:D:95:THR:C	7:D:97:GLN:N	2.71	0.42
1:0:2413:A:N7	16:M:109:PRO:CB	2.81	0.42
1:0:1574:C:H2'	1:0:1575:C:C6	2.55	0.42
1:0:92:G:H4'	24:U:44:GLY:HA3	2.00	0.42
19:P:42:LYS:HD2	19:P:42:LYS:HA	1.93	0.42
1:0:1217:G:H2'	1:0:1218:U:H6	1.85	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.55	0.42
1:0:1320:U:H2'	1:0:1321:A:C8	2.55	0.42
1:0:709:G:O2'	17:N:25:VAL:CG1	2.67	0.42
38:0:4613:HOH:O	15:L:79:LYS:HD3	2.20	0.42
8:E:116:THR:HG22	8:E:151:LEU:HD22	2.00	0.42
1:0:2670:G:H4'	5:B:112:THR:HG22	2.02	0.42
1:0:846:A:O2'	1:0:847:C:H5'	2.19	0.42
1:0:1014:A:H5"	2:9:3101:G:O2'	2.20	0.42
1:0:1200:A:H2'	38:0:6645:HOH:O	2.20	0.42
1:0:585:C:H2'	1:0:586:C:C6	2.54	0.42
6:C:200:PRO:HB3	6:C:212:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:34:LEU:HA	16:M:47:LEU:CD2	2.50	0.42
16:M:67:ALA:O	16:M:69:TYR:N	2.53	0.42
14:K:73:VAL:HG11	14:K:118:LEU:HD21	2.02	0.42
1:0:255:A:H2'	1:0:256:C:H6	1.83	0.42
14:K:40:PHE:C	14:K:40:PHE:CD1	2.92	0.42
1:0:1511:U:O2'	1:0:1512:G:H5'	2.19	0.42
28:Y:42:CYS:SG	28:Y:43:GLY:N	2.93	0.42
1:0:169:A:O2'	31:2:48:ASN:ND2	2.53	0.42
1:0:2478:U:H2'	1:0:2479:A:H8	1.85	0.42
1:0:1992:U:H2'	1:0:1994:A:OP2	2.20	0.42
5:B:183:GLU:OE1	5:B:183:GLU:HA	2.20	0.42
1:0:1976:G:H1'	1:0:2005:G:N2	2.35	0.42
1:0:2004:U:H2'	1:0:2005:G:OP1	2.19	0.42
28:Y:13:ARG:NH1	28:Y:14:PHE:CZ	2.87	0.42
30:1:22:PRO:HG2	30:1:25:VAL:HG23	2.02	0.42
1:0:2327:A:H2'	1:0:2328:U:C6	2.55	0.42
1:0:750:A:O3'	6:C:101:ASP:HB2	2.20	0.42
4:A:16:PHE:HB3	38:A:8556:HOH:O	2.20	0.42
1:0:1236:A:H2'	1:0:1237:U:O4'	2.20	0.42
1:0:1597:A:O4'	18:O:95:GLU:HG2	2.20	0.42
22:S:80:GLU:OE2	22:S:84:GLY:HA2	2.20	0.42
1:0:1477:C:O2'	1:0:1478:U:H5'	2.19	0.42
1:0:424:C:H2'	1:0:425:U:C6	2.53	0.42
1:0:424:C:H2'	1:0:425:U:H6	1.85	0.42
1:0:1362:U:H5'	38:0:4214:HOH:O	2.19	0.42
1:0:35:U:O2'	1:0:36:C:H5'	2.20	0.42
11:H:47:GLU:CB	11:H:133:ILE:CD1	2.95	0.42
11:H:29:ALA:CB	11:H:65:ARG:HH12	2.18	0.42
7:D:41:LEU:O	7:D:44:ILE:HG22	2.20	0.42
5:B:27:ASN:HB3	38:B:8641:HOH:O	2.19	0.42
12:I:19:MET:CE	12:I:78:ILE:HG22	2.49	0.42
1:0:1666:C:H2'	1:0:1667:A:C8	2.54	0.42
16:M:154:LEU:HG	16:M:155:GLU:H	1.84	0.42
16:M:157:PRO:HG3	38:M:8526:HOH:O	2.19	0.42
25:V:65:VAL:HA	25:V:68:THR:HG22	2.01	0.42
9:F:21:GLU:O	9:F:24:ARG:CG	2.65	0.42
5:B:5:ARG:HD2	5:B:8:LYS:HZ1	1.82	0.42
1:0:39:G:N2	1:0:444:C:C2	2.88	0.42
23:T:37:GLU:O	23:T:40:ALA:HB3	2.20	0.42
9:F:23:ALA:HB1	38:F:5413:HOH:O	2.19	0.42
1:0:1276:U:H3'	17:N:19:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.42
8:E:3:VAL:HG22	8:E:49:ILE:HB	2.01	0.42
15:L:49:ALA:C	15:L:54:TYR:HB3	2.40	0.42
7:D:81:GLU:O	7:D:84:LEU:N	2.52	0.42
1:0:17:G:H2'	1:0:18:C:C6	2.54	0.42
14:K:12:THR:HG21	14:K:16:GLY:O	2.19	0.42
28:Y:57:CYS:C	28:Y:59:HIS:N	2.73	0.42
11:H:147:ARG:HA	11:H:150:LYS:HZ2	1.85	0.42
11:H:150:LYS:HA	11:H:153:VAL:HG22	2.01	0.42
1:0:1988:C:C2	1:0:2001:G:N2	2.88	0.42
1:0:2895:C:H4'	38:W:4132:HOH:O	2.19	0.42
1:0:462:A:C8	30:1:37:HIS:CE1	3.08	0.42
1:0:1268:C:O2'	1:0:1269:G:H5'	2.19	0.42
20:Q:19:ARG:HA	20:Q:142:ASP:OD1	2.20	0.42
1:0:2055:A:H4'	20:Q:132:ARG:NH2	2.35	0.42
1:0:1769:C:O2'	1:0:1770:U:H5'	2.20	0.42
1:0:2406:U:C2	1:0:2407:G:C8	3.08	0.42
1:0:1289:C:O2'	1:0:1290:G:H5'	2.20	0.42
1:0:2869:G:H2'	1:0:2870:C:C6	2.54	0.42
1:0:757:C:H2'	1:0:758:A:C8	2.55	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.20	0.42
1:0:630:A:H5"	38:0:5660:HOH:O	2.19	0.42
22:S:69:LYS:O	22:S:71:VAL:HG23	2.20	0.42
6:C:114:ALA:HB1	6:C:223:LEU:HB3	2.01	0.42
1:0:2381:C:H4'	31:2:80:ARG:NH1	2.34	0.42
8:E:15:GLN:HB2	8:E:20:ILE:HA	2.02	0.42
18:O:59:ARG:O	18:O:62:ALA:HB3	2.20	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.35	0.42
4:A:130:THR:HG22	4:A:131:HIS:N	2.33	0.42
1:0:2782:G:O6	1:0:2790:C:H5"	2.19	0.42
20:Q:29:LYS:CD	38:Q:8542:HOH:O	2.60	0.42
1:0:668:C:H2'	1:0:669:G:C8	2.55	0.42
1:0:1352:A:P	6:C:92:PRO:HG3	2.60	0.42
1:0:319:A:H2'	1:0:320:G:C8	2.55	0.42
4:A:65:ARG:NH1	4:A:65:ARG:HG2	2.35	0.42
6:C:21:VAL:C	6:C:23:GLU:N	2.72	0.42
1:0:660:A:N6	1:0:746:A:O4'	2.53	0.42
1:0:441:A:H1'	1:0:442:A:N7	2.35	0.42
1:0:73:C:O2'	1:0:74:A:H5'	2.19	0.42
1:0:2445:U:H2'	1:0:2446:G:C8	2.55	0.42
1:0:1905:U:H2'	1:0:1906:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:84:ALA:C	18:O:86:ALA:N	2.73	0.42
1:0:834:G:H5"	1:0:835:U:O5'	2.19	0.42
1:0:2604:A:H5'	38:0:6679:HOH:O	2.19	0.42
1:0:2866:U:H4'	1:0:2867:G:H5'	2.02	0.42
1:0:1520:G:H2'	1:0:1521:C:C6	2.54	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.01	0.42
15:L:87:MET:HE3	38:L:8596:HOH:O	2.18	0.41
6:C:236:THR:HG21	38:C:8382:HOH:O	2.20	0.41
1:0:1116:U:C2'	1:0:1118:A:C2	3.03	0.41
5:B:304:PRO:HD2	5:B:307:ARG:HH11	1.83	0.41
20:Q:44:VAL:HG13	20:Q:89:LEU:HD22	2.01	0.41
11:H:75:SER:HB3	11:H:79:ALA:HB1	2.02	0.41
16:M:102:LEU:HG	16:M:104:ILE:CG2	2.50	0.41
14:K:124:ASP:CG	14:K:125:PHE:N	2.73	0.41
1:0:2301:A:H5"	1:0:2302:A:H5'	2.02	0.41
1:0:1514:C:H2'	1:0:1515:A:C8	2.55	0.41
15:L:133:LEU:O	15:L:134:ILE:HD13	2.20	0.41
30:1:36:ASN:HB3	30:1:39:ARG:HG3	2.01	0.41
7:D:140:ARG:HH11	7:D:140:ARG:HG3	1.84	0.41
1:0:2253:G:O2'	1:0:2254:G:H5'	2.21	0.41
1:0:145:A:H4'	15:L:137:ASP:OD2	2.20	0.41
1:0:2389:U:H4'	19:P:53:HIS:CD2	2.54	0.41
1:0:1524:U:O2'	1:0:1525:G:P	2.78	0.41
5:B:139:ASP:HB2	38:B:8532:HOH:O	2.19	0.41
20:Q:123:GLN:HA	20:Q:137:ASN:OD1	2.20	0.41
1:0:163:U:O3'	1:0:896:C:H4'	2.19	0.41
1:0:51:G:O2'	1:0:52:A:H5'	2.20	0.41
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.41
21:R:8:PRO:HD2	24:U:32:ALA:HA	2.02	0.41
26:W:74:ALA:HB2	26:W:85:VAL:HG13	2.01	0.41
1:0:2502:C:C4'	11:H:151:MET:CG	2.98	0.41
1:0:1044:C:H5"	38:0:3019:HOH:O	2.19	0.41
1:0:1334:C:H2'	1:0:1335:C:H6	1.85	0.41
14:K:90:ARG:HA	14:K:119:THR:HB	2.02	0.41
12:I:70:PHE:CD2	12:I:70:PHE:O	2.73	0.41
25:V:34:LEU:HD12	25:V:100:LEU:HD13	2.02	0.41
1:0:689:G:H2'	1:0:690:G:H8	1.84	0.41
1:0:883:U:C2'	1:0:883:U:O2	2.67	0.41
25:V:28:HIS:HD2	25:V:31:HIS:CE1	2.38	0.41
2:9:3011:A:O2'	2:9:3012:C:H3'	2.20	0.41
2:9:3036:C:C5	2:9:3037:C:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1409:G:H5'	38:0:4658:HOH:O	2.19	0.41
19:P:66:LYS:HB2	19:P:70:ALA:O	2.19	0.41
6:C:35:VAL:HG21	6:C:227:GLY:HA2	2.02	0.41
22:S:53:GLY:HA3	38:S:6384:HOH:O	2.20	0.41
2:9:3056:A:C3'	2:9:3057:A:H5"	2.50	0.41
26:W:76:ARG:NH1	26:W:76:ARG:CG	2.79	0.41
16:M:67:ALA:HA	16:M:71:TRP:HB3	2.02	0.41
1:0:251:C:H5'	15:L:140:ALA:HA	2.02	0.41
16:M:141:ARG:HB3	38:M:8569:HOH:O	2.20	0.41
4:A:130:THR:HG22	4:A:131:HIS:O	2.20	0.41
1:0:2781:U:H2'	1:0:2782:G:C5'	2.50	0.41
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.20	0.41
23:T:6:CYS:HA	23:T:13:ILE:HD11	2.02	0.41
4:A:186:TRP:CG	4:A:187:PRO:HA	2.55	0.41
1:0:1735:C:H5'	5:B:235:ARG:NH2	2.35	0.41
1:0:294:C:H2'	1:0:295:C:O4'	2.20	0.41
1:0:2737:C:H3'	1:0:2738:G:H5"	2.02	0.41
1:0:876:A:H2'	1:0:876:A:N3	2.35	0.41
27:X:197:ASP:OD1	27:X:199:ASP:HB2	2.20	0.41
19:P:88:ALA:O	19:P:90:HIS:N	2.53	0.41
22:S:43:ASN:C	22:S:45:GLY:H	2.24	0.41
16:M:71:TRP:CE2	16:M:73:ALA:HB3	2.55	0.41
2:9:3008:G:O6	16:M:11:ARG:NH1	2.54	0.41
1:0:1150:A:C2	10:G:20:VAL:HG21	2.55	0.41
1:0:1150:A:N7	10:G:69:ARG:NH2	2.69	0.41
16:M:24:LEU:O	16:M:28:LYS:HG2	2.21	0.41
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.41
31:2:38:ARG:O	31:2:42:ARG:HB2	2.20	0.41
1:0:1586:G:H2'	1:0:1587:U:H6	1.85	0.41
1:0:213:G:O2'	1:0:214:U:OP2	2.37	0.41
1:0:311:C:H2'	1:0:312:U:C6	2.56	0.41
1:0:474:C:O3'	6:C:73:LEU:HD21	2.20	0.41
15:L:78:ASN:O	15:L:79:LYS:HG2	2.20	0.41
11:H:82:LYS:HB2	11:H:82:LYS:NZ	2.36	0.41
16:M:50:LEU:HA	16:M:50:LEU:HD12	1.74	0.41
20:Q:34:GLU:HG2	20:Q:46:TYR:CZ	2.56	0.41
1:0:2703:A:H2'	1:0:2704:C:H6	1.85	0.41
15:L:46:LEU:HB2	38:L:8611:HOH:O	2.20	0.41
25:V:146:ILE:HG23	25:V:150:LEU:HD12	2.02	0.41
1:0:1711:A:O2'	1:0:1712:A:H5'	2.20	0.41
17:N:42:GLU:HB2	38:N:2176:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1365:C:H2'	1:0:1366:C:H6	1.85	0.41
1:0:541:C:H2'	1:0:542:A:H5'	2.01	0.41
6:C:2:GLN:HB3	38:C:8342:HOH:O	2.20	0.41
1:0:1666:C:C2'	1:0:1667:A:C5'	2.97	0.41
18:O:76:GLY:O	18:O:79:SER:HB2	2.21	0.41
1:0:1003:U:O2'	11:H:90:PHE:HE1	2.03	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.85	0.41
6:C:187:ARG:HD2	6:C:188:ARG:N	2.35	0.41
15:L:137:ASP:HA	15:L:142:LYS:HE3	2.02	0.41
15:L:71:SER:CB	15:L:92:THR:HG22	2.51	0.41
1:0:734:U:H2'	1:0:736:A:OP2	2.21	0.41
1:0:736:A:H2'	1:0:737:A:O4'	2.20	0.41
1:0:2135:A:O2'	1:0:2136:G:H5'	2.20	0.41
1:0:2501:G:H1'	38:0:5452:HOH:O	2.20	0.41
21:R:23:LYS:HE2	38:R:8333:HOH:O	2.20	0.41
38:0:4776:HOH:O	11:H:11:LYS:HE2	2.20	0.41
15:L:69:LYS:HD3	15:L:125:ARG:HA	2.02	0.41
11:H:47:GLU:CG	11:H:133:ILE:CD1	2.99	0.41
1:0:1192:A:H3'	1:0:1193:A:H5'	2.02	0.41
28:Y:57:CYS:C	28:Y:59:HIS:H	2.23	0.41
20:Q:99:ALA:HB1	20:Q:109:MET:HE3	1.99	0.41
25:V:6:GLN:CB	25:V:26:ILE:HD12	2.39	0.41
9:F:58:GLU:CA	9:F:61:MET:HG3	2.46	0.41
12:I:74:ARG:HD3	38:I:5061:HOH:O	2.21	0.41
31:2:70:ARG:HB3	38:2:8576:HOH:O	2.20	0.41
1:0:1473:U:O2'	1:0:1474:C:H5"	2.20	0.41
14:K:122:ALA:HB3	14:K:125:PHE:CZ	2.56	0.41
1:0:168:C:C2'	1:0:169:A:H5'	2.50	0.41
1:0:1626:A:C2'	1:0:1627:G:H5'	2.51	0.41
16:M:180:LEU:O	16:M:181:ASP:CB	2.69	0.41
1:0:1375:A:C2'	1:0:1376:G:H5'	2.50	0.41
1:0:2686:C:O2'	1:0:2687:G:H5'	2.21	0.41
17:N:25:VAL:HG23	17:N:26:TRP:N	2.36	0.41
1:0:128:A:H3'	1:0:128:A:C8	2.55	0.41
1:0:1780:G:O2'	1:0:1781:G:H5'	2.20	0.41
38:0:3197:HOH:O	4:A:11:ARG:HD3	2.20	0.41
1:0:2443:C:O3'	14:K:56:LYS:HE3	2.20	0.41
1:0:1323:G:C2	1:0:1324:G:C8	3.09	0.41
1:0:2082:G:O2'	1:0:2083:A:H5'	2.20	0.41
1:0:2656:G:C2'	1:0:2657:G:H5'	2.50	0.41
6:C:237:GLU:N	38:C:8461:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:63:VAL:HG21	15:L:109:PHE:CE1	2.56	0.41
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.96	0.41
4:A:169:PHE:O	4:A:170:VAL:HB	2.21	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.85	0.41
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.43	0.41
23:T:9:CYS:CA	23:T:52:THR:HG23	2.46	0.41
2:9:3007:G:OP1	16:M:23:ARG:NE	2.53	0.41
5:B:320:GLN:HG3	5:B:321:PRO:CD	2.51	0.41
1:0:2898:G:H2'	1:0:2899:A:H8	1.84	0.41
23:T:14:GLU:HA	23:T:15:PRO:HD2	1.92	0.41
1:0:778:C:C4	1:0:779:U:C4	3.09	0.41
1:0:2599:A:C6	1:0:2600:A:N1	2.89	0.41
24:U:42:ASN:O	24:U:44:GLY:N	2.53	0.41
15:L:173:LEU:HD23	15:L:183:VAL:HG12	2.02	0.41
4:A:105:VAL:HG13	4:A:155:THR:O	2.20	0.41
20:Q:17:MET:HE1	20:Q:19:ARG:NH2	2.36	0.41
1:0:2478:U:O2'	1:0:2479:A:H5'	2.20	0.41
2:9:3034:A:H2'	2:9:3035:C:O4'	2.21	0.41
1:0:345:G:N2	1:0:346:U:H1'	2.35	0.41
1:0:711:G:N2	1:0:718:C:C2	2.88	0.41
1:0:2833:C:H2'	1:0:2834:G:H8	1.85	0.41
1:0:681:G:N3	1:0:681:G:H5'	2.36	0.41
1:0:166:A:N7	14:K:25:GLY:HA2	2.35	0.41
1:0:2551:C:O2'	1:0:2552:C:H5'	2.21	0.41
1:0:2831:C:H2'	1:0:2832:C:H5'	2.02	0.41
16:M:35:VAL:HG12	16:M:37:ARG:HG2	2.02	0.41
25:V:139:GLY:O	25:V:141:HIS:CD2	2.74	0.41
12:I:74:ARG:C	12:I:76:ASP:N	2.74	0.41
4:A:36:ASP:HB2	4:A:85:ASP:H	1.86	0.41
1:0:2381:C:H4'	31:2:80:ARG:CZ	2.51	0.41
31:2:55:VAL:O	31:2:56:PRO:C	2.58	0.41
1:0:380:A:H5"	15:L:48:ARG:NH2	2.35	0.41
4:A:75:GLY:HA2	28:Y:63:LYS:O	2.21	0.41
1:0:1003:U:O2	11:H:90:PHE:HZ	2.03	0.41
1:0:952:G:N3	1:0:2302:A:H2'	2.35	0.41
15:L:59:GLY:HA3	15:L:141:ILE:CD1	2.50	0.41
1:0:2688:U:H2'	1:0:2689:A:H8	1.85	0.41
1:0:138:U:OP2	1:0:139:C:H5	2.03	0.41
1:0:2737:C:H3'	1:0:2738:G:C5'	2.51	0.41
1:0:1525:G:H5'	1:0:1526:A:OP2	2.20	0.41
1:0:329:A:OP2	6:C:206:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:26:PHE:CE1	5:B:310:ARG:HB3	2.55	0.41
1:0:1616:A:H2'	1:0:1618:G:C8	2.55	0.41
4:A:123:GLY:HA3	4:A:162:GLY:HA2	2.03	0.41
1:0:716:G:O2'	1:0:717:C:H5'	2.21	0.41
12:I:24:SER:HA	12:I:86:MET:SD	2.61	0.41
24:U:5:VAL:HG23	38:U:2271:HOH:O	2.20	0.41
1:0:1165:G:OP1	1:0:1165:G:H3'	2.21	0.41
1:0:1196:C:C2'	1:0:1197:G:H5'	2.51	0.41
1:0:358:G:O2'	1:0:359:U:OP2	2.39	0.41
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.41
11:H:55:GLN:NE2	11:H:124:ARG:NE	2.59	0.41
7:D:23:VAL:CG2	7:D:23:VAL:O	2.69	0.41
11:H:140:PRO:HA	11:H:142:VAL:CG1	2.50	0.41
15:L:35:PRO:HD2	15:L:38:VAL:HG21	2.01	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.79	0.41
25:V:139:GLY:O	25:V:141:HIS:HD2	2.03	0.41
11:H:127:GLY:O	11:H:128:ALA:CB	2.66	0.41
7:D:57:THR:CG2	7:D:63:ILE:HG22	2.48	0.41
5:B:168:GLY:O	5:B:169:GLY:O	2.39	0.41
14:K:73:VAL:HG21	14:K:116:HIS:CD2	2.56	0.41
5:B:254:GLN:HG2	5:B:255:GLY:H	1.85	0.41
12:I:107:ASN:HD22	12:I:108:PRO:N	2.19	0.41
1:0:2134:G:C6	1:0:2258:A:C8	3.09	0.41
1:0:926:A:H5'	14:K:39:GLU:OE2	2.20	0.41
14:K:98:GLU:O	14:K:99:GLU:HB2	2.21	0.41
27:X:130:ARG:HB2	27:X:142:SER:O	2.20	0.41
1:0:1224:G:H2'	1:0:1225:C:C6	2.55	0.41
1:0:61:G:OP1	30:1:17:GLN:HG2	2.21	0.41
1:0:331:A:C6	1:0:332:G:C4	3.08	0.41
1:0:1269:G:H2'	1:0:1270:U:H6	1.86	0.41
23:T:31:PHE:CG	23:T:37:GLU:HG2	2.56	0.41
18:O:98:ILE:O	18:O:98:ILE:HD13	2.20	0.41
27:X:126:PRO:HG2	27:X:128:PHE:CZ	2.56	0.41
24:U:59:ILE:O	24:U:63:GLU:HG2	2.21	0.41
1:0:818:A:H2	28:Y:13:ARG:HA	1.86	0.41
6:C:7:ASP:O	6:C:9:ASP:N	2.54	0.41
5:B:310:ARG:HD2	38:B:8663:HOH:O	2.21	0.41
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.95	0.41
1:0:2042:U:H2'	1:0:2043:U:C6	2.56	0.41
1:0:1748:U:H4'	38:0:8399:HOH:O	2.21	0.41
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:701:U:C2	1:0:744:G:C2	3.08	0.41
1:0:2281:C:C2'	1:0:2282:U:H5'	2.49	0.41
1:0:1562:C:H2'	1:0:1562:C:O2	2.21	0.41
1:0:2664:A:H8	1:0:2664:A:OP1	2.04	0.41
27:X:163:THR:HG23	38:X:8529:HOH:O	2.20	0.41
1:0:1697:G:O2'	1:0:1698:U:H5'	2.20	0.41
26:W:7:GLU:HA	26:W:75:ALA:HA	2.03	0.41
29:Z:10:LYS:HG3	38:Z:2979:HOH:O	2.20	0.41
25:V:133:LYS:HG3	38:V:5904:HOH:O	2.20	0.41
1:0:899:C:H5'	38:0:4153:HOH:O	2.21	0.41
25:V:35:VAL:HA	25:V:36:PRO:HD3	1.85	0.41
1:0:2385:G:H2'	1:0:2386:U:C6	2.55	0.41
12:I:131:THR:CG2	12:I:134:GLU:HG3	2.51	0.41
18:O:115:SER:C	18:O:117:SER:N	2.74	0.41
9:F:60:VAL:O	9:F:61:MET:C	2.59	0.41
16:M:71:TRP:CZ2	16:M:73:ALA:HB3	2.56	0.41
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.84	0.41
16:M:25:ARG:O	16:M:28:LYS:HB2	2.21	0.41
1:0:2539:U:C5	32:0:9500:SLD:H7	2.56	0.41
1:0:255:A:H2'	1:0:256:C:O4'	2.21	0.41
1:0:1552:G:H2'	1:0:1553:C:H6	1.84	0.41
1:0:10:U:O2'	1:0:11:A:H8	2.03	0.41
4:A:93:THR:HG23	4:A:154:ALA:O	2.21	0.41
25:V:108:ARG:HE	25:V:114:PRO:CG	2.33	0.41
1:0:1269:G:O2'	1:0:1270:U:H5'	2.21	0.41
1:0:2531:U:H2'	1:0:2532:A:O4'	2.20	0.41
2:9:3103:A:O2'	2:9:3104:A:H5'	2.21	0.41
1:0:1616:A:H5"	1:0:1617:C:OP1	2.21	0.41
26:W:75:ALA:O	26:W:83:ALA:HA	2.21	0.41
15:L:115:LEU:HD13	15:L:115:LEU:C	2.41	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.21	0.41
1:0:1679:C:H5'	38:0:3303:HOH:O	2.20	0.41
25:V:105:THR:HA	25:V:109:GLU:OE1	2.20	0.41
1:0:968:G:O2'	1:0:969:G:H5'	2.20	0.41
18:O:132:ASP:O	18:O:133:SER:HB3	2.20	0.41
1:0:1427:A:H61	1:0:1440:U:H1'	1.85	0.41
25:V:132:VAL:HG23	25:V:138:LEU:O	2.21	0.41
1:0:1896:G:C6	1:0:1897:U:C4	3.08	0.41
6:C:37:ALA:O	6:C:41:ASN:ND2	2.54	0.41
1:0:2284:G:H5'	38:0:3431:HOH:O	2.20	0.41
6:C:127:ARG:HD2	6:C:229:PRO:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1242:A:H5'	12:I:82:THR:CG2	2.37	0.40
15:L:67:ILE:HG21	15:L:97:ILE:HG23	2.03	0.40
1:0:56:G:C5'	24:U:50:ARG:HH12	2.25	0.40
1:0:1853:C:H4'	4:A:217:ARG:HH22	1.87	0.40
1:0:2120:U:H2'	1:0:2121:G:O4'	2.22	0.40
12:I:40:ASN:OD1	12:I:106:GLY:HA2	2.21	0.40
22:S:48:VAL:CG1	22:S:96:VAL:HG13	2.51	0.40
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.54	0.40
19:P:11:ARG:HD3	38:P:5620:HOH:O	2.20	0.40
13:J:82:ARG:HH21	13:J:115:ARG:HG2	1.86	0.40
14:K:125:PHE:CE2	14:K:140:VAL:HG22	2.56	0.40
1:0:860:U:H2'	1:0:861:A:C8	2.56	0.40
24:U:42:ASN:N	24:U:43:PRO:HD3	2.36	0.40
1:0:1472:C:H6	1:0:1472:C:O5'	2.04	0.40
1:0:1624:A:H4'	1:0:1626:A:H5"	2.03	0.40
22:S:89:ARG:HG3	22:S:89:ARG:O	2.21	0.40
1:0:244:C:H6	1:0:244:C:O5'	2.04	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.56	0.40
20:Q:57:VAL:HG21	20:Q:81:PRO:HD2	2.03	0.40
1:0:2472:C:O2'	1:0:2634:G:H4'	2.21	0.40
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.35	0.40
15:L:74:ARG:HD3	15:L:91:ILE:HD12	2.04	0.40
15:L:97:ILE:CD1	15:L:127:LYS:HD2	2.51	0.40
1:0:2890:A:H1'	23:T:56:ARG:HH21	1.80	0.40
1:0:558:C:C2'	1:0:559:U:C5'	2.99	0.40
1:0:1159:G:H1	1:0:1208:C:H42	1.69	0.40
16:M:154:LEU:CG	16:M:155:GLU:H	2.34	0.40
1:0:816:G:C6	1:0:817:G:N1	2.89	0.40
4:A:55:VAL:HG11	4:A:67:LEU:HD13	2.02	0.40
1:0:2001:G:C2'	1:0:2002:C:H5'	2.52	0.40
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.56	0.40
13:J:72:VAL:O	13:J:95:ALA:HA	2.21	0.40
1:0:485:A:O2'	1:0:487:G:H5'	2.22	0.40
1:0:1767:A:O2'	1:0:1768:C:H5'	2.21	0.40
27:X:117:LEU:HA	27:X:174:VAL:HG11	2.03	0.40
1:0:834:G:H3'	1:0:835:U:H4'	2.04	0.40
11:H:82:LYS:CB	11:H:82:LYS:NZ	2.85	0.40
17:N:105:ASN:HD21	17:N:109:SER:H	1.68	0.40
5:B:84:LEU:HD13	5:B:84:LEU:C	2.41	0.40
11:H:118:PRO:HD2	38:H:8341:HOH:O	2.20	0.40
1:0:1314:U:H2'	38:0:6761:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:74:ASN:ND2	11:H:141:ASN:OD1	2.55	0.40
12:I:14:ALA:HB1	12:I:44:ALA:HB2	2.02	0.40
2:9:3072:C:O2'	2:9:3073:G:H5'	2.21	0.40
1:0:1001:U:O2'	1:0:1002:G:H5'	2.21	0.40
22:S:113:GLU:O	22:S:114:SER:C	2.58	0.40
30:1:41:HIS:CD2	30:1:44:ARG:H	2.34	0.40
4:A:211:LYS:HD3	38:A:8623:HOH:O	2.20	0.40
1:0:2852:A:H5"	38:0:6132:HOH:O	2.21	0.40
6:C:219:ASN:N	6:C:222:ASP:OD1	2.52	0.40
2:9:3013:A:H3'	2:9:3014:G:H5'	2.02	0.40
7:D:94:ALA:O	7:D:95:THR:O	2.39	0.40
31:2:84:ARG:HG3	31:2:84:ARG:HH11	1.86	0.40
28:Y:50:ALA:HB3	28:Y:54:ILE:CG2	2.49	0.40
1:0:2050:G:OP1	20:Q:79:ARG:HB3	2.21	0.40
7:D:58:VAL:CG1	7:D:59:GLY:N	2.83	0.40
1:0:514:G:H8	1:0:514:G:O5'	2.04	0.40
4:A:107:ASN:OD1	4:A:116:GLY:HA3	2.21	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
1:0:1897:U:O2'	1:0:1898:G:H5'	2.21	0.40
5:B:209:LYS:HE2	38:B:8579:HOH:O	2.21	0.40
8:E:21:THR:HG23	8:E:30:THR:OG1	2.21	0.40
1:0:873:G:H2'	1:0:875:A:N7	2.37	0.40
2:9:3067:C:H2'	2:9:3068:G:H8	1.86	0.40
14:K:146:GLY:C	14:K:148:GLU:H	2.25	0.40
31:2:11:CYS:SG	31:2:14:CYS:HB2	2.61	0.40
22:S:32:ARG:HH12	22:S:38:ARG:HH12	1.67	0.40
22:S:48:VAL:HG13	22:S:96:VAL:HG13	2.03	0.40
1:0:775:G:OP1	29:Z:16:HIS:HE1	2.03	0.40
1:0:2134:G:N2	1:0:2242:U:C2	2.90	0.40
1:0:2546:U:H2'	1:0:2547:C:C6	2.57	0.40
1:0:1572:A:H2'	1:0:1573:A:C8	2.55	0.40
1:0:1331:A:O2'	1:0:1332:C:H5'	2.21	0.40
15:L:183:VAL:HG12	15:L:184:ARG:N	2.37	0.40
1:0:1497:G:O2'	1:0:1498:G:H5'	2.22	0.40
2:9:3045:A:H2'	2:9:3046:C:C6	2.55	0.40
1:0:230:C:H2'	1:0:231:G:C8	2.57	0.40
17:N:26:TRP:CE3	17:N:26:TRP:HA	2.57	0.40
1:0:2653:A:H2'	1:0:2654:C:C6	2.57	0.40
1:0:929:A:H8	1:0:929:A:O5'	2.04	0.40
1:0:2124:G:H2'	1:0:2125:G:C8	2.57	0.40
5:B:108:GLU:HB3	5:B:111:ARG:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:34:LYS:HB2	31:2:37:ASP:OD2	2.20	0.40
1:0:1743:G:H1'	38:0:5797:HOH:O	2.22	0.40
1:0:1682:A:H5"	38:0:3430:HOH:O	2.21	0.40
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.22	0.40
1:0:422:G:H2'	1:0:423:A:H8	1.85	0.40
15:L:66:ALA:HB2	15:L:128:TRP:NE1	2.37	0.40
1:0:2658:G:H4'	1:0:2842:G:C8	2.56	0.40
1:0:870:G:C3'	1:0:871:G:H5"	2.52	0.40
16:M:119:GLN:HE21	16:M:129:ILE:CG2	2.34	0.40
7:D:18:ILE:HG12	7:D:134:LEU:HD21	2.04	0.40
16:M:37:ARG:HD3	36:M:8507:CL:CL	2.58	0.40
28:Y:20:LEU:O	28:Y:21:LYS:C	2.59	0.40
1:0:588:G:O6	25:V:154:ARG:NH1	2.55	0.40
11:H:58:HIS:CE1	11:H:59:ASN:HD21	2.40	0.40
9:F:22:VAL:CG2	9:F:104:ALA:HB2	2.52	0.40
1:0:2255:A:N1	1:0:2256:G:C4	2.90	0.40
23:T:49:LEU:HD13	23:T:51:TRP:CZ2	2.57	0.40
1:0:2011:A:O4'	1:0:2013:G:C8	2.75	0.40
4:A:94:LEU:N	4:A:94:LEU:CD2	2.83	0.40
1:0:1211:G:O2'	1:0:1212:C:H5'	2.21	0.40
31:2:55:VAL:HG22	38:2:8509:HOH:O	2.22	0.40
12:I:75:PRO:HG2	12:I:105:LEU:CD2	2.49	0.40
5:B:5:ARG:HA	5:B:6:PRO:HD3	2.00	0.40
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.52	0.40
11:H:57:ARG:HG3	11:H:57:ARG:HH11	1.86	0.40
1:0:1345:A:H2'	1:0:1346:U:H6	1.85	0.40
15:L:169:ARG:HD2	38:L:8593:HOH:O	2.21	0.40
1:0:1792:C:H2'	1:0:1793:C:C6	2.56	0.40
1:0:473:A:OP1	29:Z:51:GLN:NE2	2.55	0.40
1:0:675:U:H2'	1:0:676:C:H5'	2.03	0.40
4:A:165:THR:O	4:A:165:THR:HG22	2.20	0.40
1:0:1675:C:H5"	30:1:5:LYS:HD2	2.04	0.40
1:0:1235:G:C1'	12:I:63:ILE:HG23	2.51	0.40
1:0:1609:C:H2'	1:0:1610:G:H8	1.87	0.40
18:O:11:ALA:HB2	18:O:18:LYS:HA	2.03	0.40
1:0:2659:U:H4'	20:Q:76:ASP:HB3	2.04	0.40
5:B:185:GLY:HA2	38:B:8647:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	11 46
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	9 40
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	16 56
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1 4
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	30 72
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	7 33
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	4 21
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	7 33
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	9 40
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	13 50
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	14 51
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	7 33
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	4 22
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	21 64
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	26 70
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	8 38
20	Q	148/154 (96%)	134 (90%)	14 (10%)	0	100 100
21	R	79/84 (94%)	76 (96%)	3 (4%)	0	100 100
22	S	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11 46
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	9 41
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5 27
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	26 70
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	7 34
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100 100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	3 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	8	38
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	9	41

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	138	PRO
11	H	162	SER
12	I	5	GLU
16	M	139	TRP
16	M	154	LEU
16	M	162	ASP
16	M	164	ASP
16	M	183	ASP
28	Y	20	LEU
28	Y	81	LYS
31	2	56	PRO
5	B	34	GLY
5	B	107	SER
5	B	169	GLY
6	C	8	LEU
7	D	11	HIS
7	D	16	PRO
7	D	20	LYS
7	D	61	PHE
7	D	147	ALA
10	G	72	ASP
11	H	164	ALA
12	I	89	HIS
12	I	143	LYS
14	K	80	ASP
15	L	148	SER
16	M	181	ASP

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Mol	Chain	Res	Type
18	O	116	SER
22	S	53	GLY
24	U	43	PRO
28	Y	28	ASP
31	2	57	GLY
4	A	34	ASP
4	A	132	ASP
5	B	184	ASP
7	D	171	ASP
11	H	40	PRO
13	J	119	GLN
14	K	105	TYR
15	L	18	GLY
15	L	140	ALA
26	W	77	PHE
4	A	62	ASP
5	B	185	GLY
17	N	20	SER
23	T	7	ASP
26	W	70	ILE
5	B	2	GLN
6	C	145	GLU
7	D	36	ASN
7	D	60	GLU
9	F	61	MET
9	F	64	PRO
13	J	126	SER
15	L	15	PRO
16	M	68	GLU
25	V	77	ALA
4	A	37	VAL
15	L	71	SER
22	S	44	ALA
8	E	44	GLY
24	U	40	PRO
19	P	18	PRO
6	C	19	PRO
19	P	54	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/181 (99%)	168 (94%)	11 (6%)	23	61
5	B	282/282 (100%)	264 (94%)	18 (6%)	22	59
6	C	193/193 (100%)	178 (92%)	15 (8%)	16	49
7	D	117/147 (80%)	108 (92%)	9 (8%)	16	50
8	E	152/155 (98%)	146 (96%)	6 (4%)	39	77
9	F	92/92 (100%)	91 (99%)	1 (1%)	80	94
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	12	41
12	I	118/121 (98%)	110 (93%)	8 (7%)	20	56
13	J	106/106 (100%)	102 (96%)	4 (4%)	40	78
14	K	113/126 (90%)	108 (96%)	5 (4%)	35	74
15	L	166/166 (100%)	157 (95%)	9 (5%)	27	66
16	M	149/149 (100%)	141 (95%)	8 (5%)	27	66
17	N	93/93 (100%)	90 (97%)	3 (3%)	46	82
18	O	113/116 (97%)	109 (96%)	4 (4%)	43	80
19	P	79/79 (100%)	75 (95%)	4 (5%)	29	69
20	Q	117/121 (97%)	114 (97%)	3 (3%)	54	85
21	R	71/73 (97%)	69 (97%)	2 (3%)	51	84
22	S	105/105 (100%)	100 (95%)	5 (5%)	31	71
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	39	77
25	V	130/130 (100%)	122 (94%)	8 (6%)	23	60
26	W	66/73 (90%)	62 (94%)	4 (6%)	23	61
27	X	120/195 (62%)	113 (94%)	7 (6%)	25	63
28	Y	56/56 (100%)	52 (93%)	4 (7%)	18	54
29	Z	46/46 (100%)	45 (98%)	1 (2%)	60	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	1	42/44 (96%)	41 (98%)	1 (2%)	57 87
31	2	79/79 (100%)	75 (95%)	4 (5%)	29 69
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	29 68

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	55	VAL
4	A	68	ILE
4	A	69	LEU
4	A	94	LEU
4	A	131	HIS
4	A	153	ARG
4	A	179	MET
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	33	ASP
5	B	63	GLU
5	B	97	LEU
5	B	98	THR
5	B	103	ASP
5	B	162	MET
5	B	234	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	264	GLU
5	B	304	PRO
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	78	ARG

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Mol	Chain	Res	Type
6	C	115	LEU
6	C	136	VAL
6	C	180	SER
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	131	THR
7	D	133	ASN
7	D	136	ARG
7	D	137	PRO
7	D	149	ARG
8	E	7	ILE
8	E	12	ASP
8	E	15	GLN
8	E	54	ASP
8	E	102	VAL
8	E	164	ASP
9	F	64	PRO
11	H	18	GLU
11	H	59	ASN
11	H	61	LEU
11	H	72	VAL
11	H	73	GLN
11	H	82	LYS
11	H	86	ARG
11	H	94	ARG
11	H	109	ASP
11	H	142	VAL
11	H	150	LYS
12	I	46	ILE
12	I	47	THR
12	I	52	GLN
12	I	74	ARG
12	I	79	PHE

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Mol	Chain	Res	Type
12	I	107	ASN
12	I	127	ILE
12	I	131	THR
13	J	10	GLN
13	J	49	LEU
13	J	56	SER
13	J	98	VAL
14	K	30	ARG
14	K	35	ARG
14	K	80	ASP
14	K	83	GLU
14	K	117	GLU
15	L	38	VAL
15	L	46	LEU
15	L	68	ARG
15	L	87	MET
15	L	93	ARG
15	L	99	ARG
15	L	159	THR
15	L	164	THR
15	L	170	CYS
16	M	26	LEU
16	M	47	LEU
16	M	49	THR
16	M	80	SER
16	M	127	LEU
16	M	128	ASP
16	M	152	GLU
16	M	163	PHE
17	N	3	THR
17	N	98	LEU
17	N	111	VAL
18	O	52	LYS
18	O	81	LYS
18	O	91	LYS
18	O	98	ILE
19	P	11	ARG
19	P	16	ASN
19	P	57	ASP
19	P	95	GLU
20	Q	13	THR
20	Q	39	THR

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Mol	Chain	Res	Type
20	Q	82	GLU
21	R	10	VAL
21	R	80	ARG
22	S	23	VAL
22	S	26	THR
22	S	39	ASN
22	S	48	VAL
22	S	73	HIS
24	U	22	ASP
24	U	65	ASP
25	V	35	VAL
25	V	52	VAL
25	V	73	LEU
25	V	122	ARG
25	V	128	VAL
25	V	142	ASP
25	V	146	ILE
25	V	154	ARG
26	W	15	ARG
26	W	27	ASP
26	W	49	ARG
26	W	72	VAL
27	X	115	ARG
27	X	154	ARG
27	X	163	THR
27	X	189	ASN
27	X	203	VAL
27	X	204	ARG
27	X	235	GLU
28	Y	11	THR
28	Y	42	CYS
28	Y	64	ILE
28	Y	68	CYS
29	Z	36	SER
30	1	18	ASN
31	2	42	ARG
31	2	56	PRO
31	2	65	THR
31	2	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	47	HIS
4	A	92	ASN
4	A	125	ASN
4	A	127	GLN
4	A	176	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	85	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	17	GLN
10	G	64	ASN
11	H	35	ASN
11	H	45	GLN
11	H	55	GLN
11	H	58	HIS
11	H	59	ASN
11	H	69	ASN
11	H	74	ASN
11	H	80	ASN
11	H	91	HIS
11	H	129	ASN
11	H	130	HIS
11	H	137	ASN
11	H	166	ASN
12	I	52	GLN
12	I	107	ASN
13	J	10	GLN
14	K	18	HIS
14	K	41	HIS
15	L	26	HIS

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Mol	Chain	Res	Type
15	L	58	GLN
15	L	176	GLN
16	M	40	ASN
16	M	107	ASN
16	M	119	GLN
16	M	132	ASN
16	M	153	GLN
17	N	53	GLN
18	O	50	GLN
18	O	66	GLN
18	O	73	HIS
18	O	118	GLN
19	P	16	ASN
19	P	40	HIS
20	Q	61	GLN
20	Q	94	ASN
20	Q	98	ASN
20	Q	113	HIS
20	Q	117	HIS
21	R	53	ASN
22	S	39	ASN
22	S	73	HIS
23	T	39	ASN
24	U	60	GLN
25	V	27	HIS
25	V	28	HIS
25	V	59	GLN
25	V	87	HIS
25	V	110	GLN
25	V	119	HIS
25	V	125	HIS
25	V	141	HIS
26	W	23	HIS
26	W	36	HIS
27	X	134	HIS
27	X	149	GLN
27	X	189	ASN
28	Y	70	GLN
29	Z	8	GLN
29	Z	16	HIS
29	Z	28	HIS
30	1	16	ASN

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Mol	Chain	Res	Type
30	1	18	ASN
30	1	41	HIS
30	1	45	ASN
31	2	13	HIS
31	2	30	GLN
31	2	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	241 (8%)	25 (0%)
2	9	121/122 (99%)	18 (14%)	3 (2%)
3	4	2/3 (66%)	1 (50%)	0
All	All	2868/3047 (94%)	260 (9%)	28 (0%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C

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Mol	Chain	Res	Type
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	317	A
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	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G

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Mol	Chain	Res	Type
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	938	G
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G

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Mol	Chain	Res	Type
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	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	1460	G
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	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
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

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Mol	Chain	Res	Type
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	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	1904	A
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G

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Mol	Chain	Res	Type
1	0	2272	G
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2540	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	2637	A
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A

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Mol	Chain	Res	Type
1	0	2812	A
1	0	2825	C
1	0	2850	C
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	3026	C
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
3	4	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	604	G
1	0	834	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1164	U
1	0	1237	U

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Mol	Chain	Res	Type
1	0	1352	A
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2320	U
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2791	U
2	9	3024	U
2	9	3065	A
2	9	3103	A

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	SLD	0	9500	-	38,39,39	5.63	18 (47%)	46,53,53	2.67	19 (41%)

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	SLD	0	9500	-	-	0/23/51/51	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C9S-C8S	-9.70	1.35	1.50
32	0	9500	SLD	C9S-C0S	-5.75	1.43	1.51
32	0	9500	SLD	O1-C7	-3.43	1.41	1.46
32	0	9500	SLD	C4-C2	2.07	1.43	1.39
32	0	9500	SLD	C3-C12	2.74	1.46	1.41
32	0	9500	SLD	F1-C11	3.56	1.44	1.35
32	0	9500	SLD	O1-C6	3.62	1.40	1.35
32	0	9500	SLD	C1S-N2S	3.72	1.45	1.38
32	0	9500	SLD	C7S-C5S	4.15	1.57	1.50
32	0	9500	SLD	C12-C2B	4.58	1.54	1.47
32	0	9500	SLD	C4-C11	5.02	1.46	1.37
32	0	9500	SLD	C3-C1	5.04	1.47	1.38
32	0	9500	SLD	C1-C2	5.65	1.50	1.39
32	0	9500	SLD	C6S-C1S	7.28	1.58	1.44
32	0	9500	SLD	C6-N1	8.58	1.45	1.36
32	0	9500	SLD	C5S-N4S	10.86	1.45	1.33
32	0	9500	SLD	C12-C11	12.70	1.53	1.39
32	0	9500	SLD	C8S-C6S	21.71	1.58	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	9500	SLD	O3-C6-N1	-8.51	122.04	128.87
32	0	9500	SLD	C5-N1-C6	-5.40	108.17	111.24
32	0	9500	SLD	C9S-C0S-N5S	-3.36	109.95	117.07
32	0	9500	SLD	C7-O1-C6	-2.88	107.83	110.20
32	0	9500	SLD	O1-C6-N1	-2.77	108.18	109.97
32	0	9500	SLD	C7-C8-N2	-2.46	106.40	112.11
32	0	9500	SLD	CAS-N5S-C0S	-2.29	118.28	122.79
32	0	9500	SLD	C1-C2-N1	-2.21	116.91	120.17
32	0	9500	SLD	C4-C11-C12	-2.04	123.18	124.34
32	0	9500	SLD	C8-N2-C9	2.14	126.33	122.77
32	0	9500	SLD	C3-C12-C11	2.20	117.72	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	9500	SLD	F1-C11-C12	2.61	121.61	117.99
32	0	9500	SLD	CAS-C5B-C4B	2.76	122.35	113.27
32	0	9500	SLD	O2S-C0S-C9S	2.91	126.61	121.00
32	0	9500	SLD	C5B-CAS-N5S	3.14	121.40	112.19
32	0	9500	SLD	O1-C7-C5	3.25	107.91	104.59
32	0	9500	SLD	C2-N1-C6	4.65	131.36	125.80
32	0	9500	SLD	C3S-N4S-C5S	5.04	123.64	118.82
32	0	9500	SLD	O1-C6-O3	6.36	129.77	122.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9500	SLD	4	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	2754/2922 (94%)	-0.43	34 (1%) 81 55	35, 63, 107, 150	0
2	9	122/122 (100%)	0.01	5 (4%) 41 16	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.41	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.46	3 (1%) 79 53	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.36	2 (0%) 90 73	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.53	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.35	12 (8%) 13 4	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.26	3 (1%) 73 45	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.05	4 (3%) 49 21	70, 88, 112, 118	0
10	G	29/348 (8%)	0.11	1 (3%) 49 21	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.28	2 (1%) 79 53	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.50	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.37	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.27	2 (1%) 78 51	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.62	0 100 100	47, 62, 79, 90	0
16	M	186/186 (100%)	-0.02	7 (3%) 44 18	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.33	1 (0%) 85 64	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.47	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.46	1 (1%) 82 58	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.52	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.33	1 (1%) 81 55	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.32	3 (2%) 61 30	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.29	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	0.13	5 (7%) 16 6	68, 91, 123, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	V	154/154 (100%)	-0.53	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.23	2 (2%) 62 32	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.59	2 (1%) 78 51	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.25	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.70	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.12	2 (4%) 39 16	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.17	2 (2%) 65 35	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.37	94 (1%) 78 51	35, 69, 108, 150	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	6.3
1	0	2250	G	6.0
2	9	3025	G	4.9
22	S	116	ASP	4.9
24	U	1	THR	4.6
2	9	3023	U	4.6
1	0	2237	G	4.4
2	9	3002	U	4.3
1	0	735	C	4.3
7	D	66	GLY	3.8
31	2	56	PRO	3.8
7	D	10	PHE	3.8
14	K	80	ASP	3.8
24	U	40	PRO	3.7
24	U	38	GLY	3.7
1	0	2249	G	3.5
19	P	95	GLU	3.4
24	U	39	ALA	3.4
17	N	1	SER	3.3
30	1	35	ARG	3.2
1	0	960	G	3.2
1	0	1951	G	3.2
1	0	2251	G	3.2
7	D	43	GLU	3.0
7	D	12	GLU	3.0
1	0	970	U	2.9
1	0	362	G	2.9
1	0	1181	A	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	1199	A	2.9
8	E	10	ASP	2.9
4	A	133	ARG	2.8
1	0	2664	A	2.8
1	0	365	G	2.8
1	0	1527	A	2.8
7	D	57	THR	2.7
16	M	185	GLU	2.7
1	0	128	A	2.7
7	D	128	LEU	2.7
7	D	47	GLN	2.7
16	M	152	GLU	2.6
16	M	162	ASP	2.6
1	0	736	A	2.6
1	0	2253	G	2.6
26	W	80	GLU	2.6
7	D	63	ILE	2.6
1	0	1279	U	2.5
16	M	160	SER	2.5
27	X	108	ASP	2.5
11	H	35	ASN	2.5
16	M	56	ASP	2.5
24	U	37	GLY	2.5
1	0	1172	G	2.4
1	0	2344	G	2.4
31	2	55	VAL	2.4
7	D	170	TYR	2.4
1	0	1130	U	2.4
1	0	2254	G	2.4
22	S	115	GLU	2.4
30	1	36	ASN	2.4
10	G	72	ASP	2.4
4	A	237	GLY	2.4
5	B	118	ASP	2.4
8	E	45	ASP	2.4
9	F	119	ARG	2.4
1	0	1171	A	2.4
1	0	1950	G	2.4
1	0	1198	U	2.4
1	0	1525	G	2.3
5	B	83	ALA	2.3
21	R	1	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	0	2239	C	2.3
9	F	100	ASP	2.2
22	S	117	ASP	2.2
2	9	3024	U	2.2
1	0	1175	G	2.2
1	0	2508	C	2.2
4	A	31	LYS	2.2
8	E	16	ASP	2.2
14	K	150	GLN	2.1
11	H	167	ALA	2.1
1	0	1173	A	2.1
1	0	2252	A	2.1
26	W	88	GLU	2.1
1	0	2509	A	2.1
1	0	2238	A	2.1
7	D	64	ARG	2.1
16	M	138	ASP	2.1
27	X	235	GLU	2.1
7	D	85	GLN	2.0
9	F	44	SER	2.0
16	M	184	ILE	2.0
1	0	808	A	2.0
7	D	107	GLY	2.0
9	F	90	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	8356	1/1	0.94	0.96	55.52	73,73,73,73	0
35	NA	0	8371	1/1	0.66	0.72	38.24	69,69,69,69	0
35	NA	0	8377	1/1	0.93	0.58	31.35	75,75,75,75	0
35	NA	0	8323	1/1	0.81	0.44	30.91	66,66,66,66	0
34	K	0	8202	1/1	0.81	0.77	26.95	92,92,92,92	0
35	NA	0	8378	1/1	0.84	0.77	26.66	65,65,65,65	0
35	NA	0	8376	1/1	0.95	0.46	23.49	79,79,79,79	0
35	NA	0	8372	1/1	0.93	0.74	23.45	72,72,72,72	0
36	CL	0	8505	1/1	0.83	0.43	20.77	99,99,99,99	0
35	NA	0	8303	1/1	0.94	0.50	18.70	55,55,55,55	0
33	MG	0	8064	1/1	0.94	0.36	17.82	39,39,39,39	0
35	NA	0	8321	1/1	0.94	0.41	15.67	67,67,67,67	0
35	NA	0	8368	1/1	0.77	0.36	14.46	69,69,69,69	0
35	NA	0	8361	1/1	0.72	0.37	13.98	77,77,77,77	0
36	CL	B	8519	1/1	0.88	0.38	13.66	95,95,95,95	0
35	NA	Q	8386	1/1	0.42	0.64	11.18	107,107,107,107	0
35	NA	0	8379	1/1	0.97	0.24	10.88	48,48,48,48	0
35	NA	0	8350	1/1	0.85	0.28	10.75	57,57,57,57	0
36	CL	2	8504	1/1	0.90	0.49	10.69	100,100,100,100	0
33	MG	0	8044	1/1	0.96	0.27	10.09	59,59,59,59	0
35	NA	0	8366	1/1	0.82	0.36	9.71	82,82,82,82	0
33	MG	0	8108	1/1	0.93	0.27	9.57	102,102,102,102	0
35	NA	0	8332	1/1	0.81	0.37	9.01	50,50,50,50	0
35	NA	0	8325	1/1	0.86	0.28	8.96	64,64,64,64	0
35	NA	0	8362	1/1	0.81	0.24	8.55	79,79,79,79	0
35	NA	K	8380	1/1	0.97	0.36	8.20	85,85,85,85	0
33	MG	0	8053	1/1	0.95	0.30	7.74	63,63,63,63	0
35	NA	0	8364	1/1	0.89	0.24	7.43	66,66,66,66	0
35	NA	0	8333	1/1	0.89	0.26	5.99	40,40,40,40	0
33	MG	0	8006	1/1	0.98	0.28	5.96	60,60,60,60	0
35	NA	0	8308	1/1	0.93	0.25	5.75	77,77,77,77	0
35	NA	0	8324	1/1	0.71	0.39	5.62	58,58,58,58	0
35	NA	9	8383	1/1	0.78	0.40	4.75	67,67,67,67	0
35	NA	0	8373	1/1	0.94	0.24	4.74	57,57,57,57	0
35	NA	0	8326	1/1	0.81	0.30	4.56	73,73,73,73	0
35	NA	0	8367	1/1	0.96	0.25	4.36	85,85,85,85	0
33	MG	0	8020	1/1	0.94	0.19	4.07	53,53,53,53	0
35	NA	0	8365	1/1	0.83	0.42	3.68	47,47,47,47	0
36	CL	I	8521	1/1	0.95	0.25	3.38	69,69,69,69	0
33	MG	0	8038	1/1	0.99	0.19	2.85	56,56,56,56	0
35	NA	0	8320	1/1	0.98	0.21	2.81	40,40,40,40	0
35	NA	0	8335	1/1	0.95	0.17	2.60	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8049	1/1	0.66	0.32	2.52	90,90,90,90	0
33	MG	0	8054	1/1	0.93	0.19	2.50	45,45,45,45	0
35	NA	0	8310	1/1	0.92	0.20	2.39	46,46,46,46	0
36	CL	J	8512	1/1	0.96	0.21	2.01	67,67,67,67	0
35	NA	H	8309	1/1	0.98	0.26	1.91	49,49,49,49	0
32	SLD	0	9500	37/37	0.92	0.21	1.91	46,50,53,59	0
36	CL	N	8508	1/1	0.89	0.22	1.89	116,116,116,116	0
35	NA	Q	8337	1/1	0.91	0.26	1.52	64,64,64,64	0
33	MG	0	8060	1/1	0.96	0.15	1.41	63,63,63,63	0
35	NA	0	8359	1/1	0.94	0.15	1.32	81,81,81,81	0
33	MG	0	8014	1/1	0.98	0.18	1.22	46,46,46,46	0
33	MG	0	8001	1/1	0.96	0.17	1.13	46,46,46,46	0
33	MG	0	8004	1/1	0.97	0.19	1.09	50,50,50,50	0
33	MG	0	8008	1/1	0.96	0.16	1.03	52,52,52,52	0
33	MG	0	8013	1/1	0.85	0.17	0.85	60,60,60,60	0
33	MG	X	8109	1/1	0.96	0.18	0.77	66,66,66,66	0
35	NA	0	8374	1/1	0.88	0.14	0.46	77,77,77,77	0
33	MG	0	8017	1/1	0.99	0.15	0.35	43,43,43,43	0
35	NA	0	8353	1/1	0.93	0.14	0.34	43,43,43,43	0
33	MG	0	8112	1/1	0.93	0.15	0.27	64,64,64,64	0
35	NA	0	8339	1/1	0.94	0.14	0.05	33,33,33,33	0
33	MG	A	8065	1/1	0.99	0.15	0.05	55,55,55,55	0
33	MG	0	8003	1/1	0.89	0.15	-0.04	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.13	-0.19	54,54,54,54	0
33	MG	0	8019	1/1	0.97	0.15	-0.43	43,43,43,43	0
35	NA	0	8343	1/1	0.96	0.14	-0.51	48,48,48,48	0
34	K	0	8201	1/1	0.75	0.13	-0.62	141,141,141,141	0
35	NA	0	8344	1/1	0.97	0.11	-0.64	48,48,48,48	0
35	NA	0	8331	1/1	0.98	0.12	-0.65	60,60,60,60	0
33	MG	0	8058	1/1	0.98	0.11	-0.71	61,61,61,61	0
33	MG	0	8007	1/1	0.98	0.12	-0.73	47,47,47,47	0
33	MG	0	8067	1/1	0.94	0.12	-0.73	81,81,81,81	0
35	NA	L	8347	1/1	0.96	0.13	-0.86	55,55,55,55	0
33	MG	S	8073	1/1	0.89	0.14	-0.94	71,71,71,71	0
33	MG	0	8015	1/1	0.99	0.11	-0.99	60,60,60,60	0
37	CD	Y	8403	1/1	0.98	0.07	-1.30	84,84,84,84	0
33	MG	0	8057	1/1	0.96	0.09	-1.32	53,53,53,53	0
35	NA	0	8338	1/1	0.95	0.09	-1.35	66,66,66,66	0
35	NA	0	8317	1/1	0.94	0.11	-1.38	57,57,57,57	0
33	MG	0	8086	1/1	0.97	0.06	-1.41	62,62,62,62	0
37	CD	2	8404	1/1	0.99	0.09	-1.43	90,90,90,90	0
37	CD	Z	8402	1/1	0.99	0.07	-1.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	I	8346	1/1	0.99	0.08	-1.52	45,45,45,45	0
33	MG	9	8052	1/1	0.96	0.10	-1.64	60,60,60,60	0
33	MG	0	8039	1/1	0.98	0.10	-1.70	53,53,53,53	0
33	MG	4	8063	1/1	0.97	0.11	-1.73	62,62,62,62	0
33	MG	0	8062	1/1	0.94	0.09	-1.77	90,90,90,90	0
33	MG	0	8074	1/1	0.98	0.07	-1.81	51,51,51,51	0
33	MG	0	8107	1/1	0.93	0.09	-1.91	55,55,55,55	0
35	NA	0	8327	1/1	0.98	0.10	-1.96	46,46,46,46	0
33	MG	0	8027	1/1	0.98	0.07	-2.00	65,65,65,65	0
33	MG	0	8010	1/1	0.99	0.10	-2.00	47,47,47,47	0
35	NA	A	8345	1/1	0.96	0.10	-2.02	48,48,48,48	0
36	CL	L	8518	1/1	0.96	0.10	-2.09	69,69,69,69	0
35	NA	P	8348	1/1	0.89	0.09	-2.14	68,68,68,68	0
33	MG	0	8002	1/1	0.97	0.09	-2.15	51,51,51,51	0
37	CD	T	8401	1/1	0.99	0.07	-2.21	83,83,83,83	0
33	MG	0	8056	1/1	0.99	0.09	-2.47	60,60,60,60	0
33	MG	0	8080	1/1	0.99	0.08	-2.66	52,52,52,52	0
33	MG	B	8055	1/1	0.95	0.06	-2.68	71,71,71,71	0
33	MG	0	8018	1/1	0.95	0.09	-2.77	57,57,57,57	0
33	MG	2	8078	1/1	0.98	0.04	-2.99	65,65,65,65	0
33	MG	0	8096	1/1	0.96	0.09	-3.15	70,70,70,70	0
33	MG	0	8016	1/1	0.96	0.07	-3.25	71,71,71,71	0
33	MG	0	8091	1/1	0.99	0.06	-3.47	65,65,65,65	0
33	MG	0	8012	1/1	0.99	0.06	-3.51	42,42,42,42	0
33	MG	0	8032	1/1	0.98	0.08	-3.70	52,52,52,52	0
35	NA	0	8305	1/1	0.97	0.08	-3.81	42,42,42,42	0
33	MG	J	8069	1/1	0.94	0.05	-3.89	87,87,87,87	0
33	MG	0	8033	1/1	0.98	0.11	-4.56	48,48,48,48	0
33	MG	0	8059	1/1	0.98	0.06	-5.88	60,60,60,60	0
33	MG	0	8084	1/1	0.99	0.05	-6.30	70,70,70,70	0
33	MG	0	8035	1/1	0.94	0.06	-6.42	69,69,69,69	0
35	NA	R	8312	1/1	0.53	0.93	-	84,84,84,84	0
33	MG	0	8099	1/1	0.93	0.23	-	80,80,80,80	0
33	MG	0	8005	1/1	0.99	0.10	-	58,58,58,58	0
33	MG	0	8093	1/1	0.98	0.10	-	63,63,63,63	0
35	NA	0	8330	1/1	0.93	0.11	-	61,61,61,61	0
33	MG	0	8104	1/1	0.92	0.13	-	66,66,66,66	0
33	MG	0	8076	1/1	0.89	0.16	-	102,102,102,102	0
35	NA	0	8316	1/1	0.84	0.21	-	52,52,52,52	0
33	MG	0	8111	1/1	0.92	0.12	-	75,75,75,75	0
35	NA	0	8340	1/1	0.78	0.36	-	69,69,69,69	0
36	CL	I	8501	1/1	0.91	0.18	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8363	1/1	0.50	0.60	-	83,83,83,83	0
33	MG	0	8045	1/1	0.89	0.25	-	91,91,91,91	0
35	NA	0	8336	1/1	0.93	0.13	-	63,63,63,63	0
33	MG	0	8022	1/1	0.88	0.57	-	83,83,83,83	0
36	CL	0	8514	1/1	0.94	0.14	-	75,75,75,75	0
33	MG	0	8041	1/1	0.98	0.24	-	68,68,68,68	0
36	CL	I	8502	1/1	0.90	0.11	-	93,93,93,93	0
33	MG	0	8026	1/1	0.96	0.08	-	39,39,39,39	0
35	NA	0	8313	1/1	0.85	0.22	-	89,89,89,89	0
36	CL	K	8510	1/1	0.83	0.26	-	104,104,104,104	0
33	MG	0	8030	1/1	0.99	0.16	-	48,48,48,48	0
35	NA	C	8304	1/1	0.93	0.38	-	51,51,51,51	0
33	MG	0	8066	1/1	0.86	0.18	-	105,105,105,105	0
33	MG	0	8029	1/1	0.95	0.07	-	60,60,60,60	0
33	MG	0	8075	1/1	0.96	0.09	-	77,77,77,77	0
36	CL	0	8515	1/1	0.86	0.29	-	100,100,100,100	0
36	CL	P	8511	1/1	0.87	0.37	-	84,84,84,84	0
33	MG	0	8114	1/1	0.78	0.70	-	95,95,95,95	0
33	MG	0	8089	1/1	0.97	0.07	-	82,82,82,82	0
33	MG	0	8115	1/1	0.93	0.12	-	73,73,73,73	0
33	MG	0	8050	1/1	0.97	0.14	-	68,68,68,68	0
36	CL	X	8520	1/1	0.97	0.28	-	57,57,57,57	0
33	MG	0	8101	1/1	0.95	0.14	-	94,94,94,94	0
33	MG	0	8098	1/1	0.98	0.06	-	50,50,50,50	0
36	CL	0	8517	1/1	0.95	0.33	-	82,82,82,82	0
35	NA	0	8375	1/1	0.91	0.69	-	81,81,81,81	0
35	NA	0	8385	1/1	0.78	0.36	-	73,73,73,73	0
33	MG	0	8048	1/1	0.98	0.06	-	66,66,66,66	0
36	CL	A	8509	1/1	0.90	0.74	-	89,89,89,89	0
33	MG	0	8094	1/1	0.99	0.07	-	97,97,97,97	0
33	MG	0	8025	1/1	0.97	0.06	-	59,59,59,59	0
33	MG	0	8116	1/1	0.94	0.16	-	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	-	54,54,54,54	0
35	NA	0	8329	1/1	0.56	1.25	-	98,98,98,98	0
35	NA	0	8311	1/1	0.90	0.26	-	73,73,73,73	0
35	NA	9	8351	1/1	0.33	0.26	-	94,94,94,94	0
33	MG	0	8082	1/1	0.92	0.16	-	79,79,79,79	0
33	MG	0	8042	1/1	0.96	0.14	-	61,61,61,61	0
35	NA	0	8319	1/1	0.98	0.18	-	41,41,41,41	0
36	CL	0	8522	1/1	0.97	0.64	-	92,92,92,92	0
35	NA	0	8384	1/1	0.47	0.63	-	85,85,85,85	0
33	MG	A	8105	1/1	0.82	0.30	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8031	1/1	0.96	0.12	-	54,54,54,54	0
35	NA	0	8352	1/1	0.81	0.32	-	61,61,61,61	0
33	MG	0	8061	1/1	0.99	0.05	-	45,45,45,45	0
33	MG	0	8011	1/1	0.88	0.19	-	50,50,50,50	0
35	NA	0	8370	1/1	0.90	0.40	-	76,76,76,76	0
33	MG	0	8036	1/1	0.97	0.05	-	52,52,52,52	0
35	NA	0	8328	1/1	0.88	0.23	-	55,55,55,55	0
33	MG	0	8110	1/1	0.96	0.12	-	56,56,56,56	0
36	CL	Q	8506	1/1	0.92	0.23	-	80,80,80,80	0
35	NA	0	8382	1/1	0.79	0.18	-	89,89,89,89	0
33	MG	0	8043	1/1	0.97	0.07	-	64,64,64,64	0
36	CL	0	8513	1/1	0.92	0.24	-	74,74,74,74	0
37	CD	N	8405	1/1	0.81	0.23	-	150,150,150,150	0
33	MG	0	8040	1/1	0.96	0.08	-	88,88,88,88	0
35	NA	0	8369	1/1	0.84	0.35	-	96,96,96,96	0
33	MG	0	8023	1/1	0.99	0.06	-	46,46,46,46	0
33	MG	0	8088	1/1	0.96	0.22	-	40,40,40,40	0
35	NA	0	8355	1/1	0.96	0.40	-	77,77,77,77	0
33	MG	0	8117	1/1	0.98	0.07	-	45,45,45,45	0
35	NA	0	8318	1/1	0.97	0.23	-	48,48,48,48	0
33	MG	0	8009	1/1	0.96	0.18	-	44,44,44,44	0
33	MG	0	8070	1/1	0.97	0.06	-	63,63,63,63	0
33	MG	0	8079	1/1	0.96	0.12	-	53,53,53,53	0
35	NA	0	8307	1/1	0.83	0.32	-	71,71,71,71	0
33	MG	0	8087	1/1	0.95	0.07	-	82,82,82,82	0
36	CL	0	8503	1/1	0.94	0.29	-	82,82,82,82	0
33	MG	0	8047	1/1	0.98	0.10	-	90,90,90,90	0
35	NA	0	8349	1/1	0.98	0.44	-	69,69,69,69	0
33	MG	0	8034	1/1	0.95	0.10	-	46,46,46,46	0
33	MG	0	8085	1/1	0.88	0.22	-	92,92,92,92	0
33	MG	0	8092	1/1	0.87	0.36	-	111,111,111,111	0
33	MG	0	8100	1/1	0.92	0.19	-	97,97,97,97	0
35	NA	0	8360	1/1	0.84	0.41	-	69,69,69,69	0
33	MG	0	8046	1/1	0.86	0.15	-	86,86,86,86	0
33	MG	0	8068	1/1	0.99	0.07	-	64,64,64,64	0
35	NA	0	8334	1/1	0.96	0.20	-	48,48,48,48	0
35	NA	0	8357	1/1	0.92	0.26	-	61,61,61,61	0
33	MG	0	8102	1/1	0.84	0.40	-	91,91,91,91	0
33	MG	0	8113	1/1	0.84	0.10	-	60,60,60,60	0
33	MG	0	8097	1/1	0.91	0.30	-	53,53,53,53	0
33	MG	9	8095	1/1	0.93	0.36	-	106,106,106,106	0
35	NA	0	8341	1/1	0.79	0.33	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8083	1/1	0.98	0.07	-	65,65,65,65	0
33	MG	0	8021	1/1	0.99	0.18	-	54,54,54,54	0
35	NA	0	8306	1/1	0.96	0.38	-	59,59,59,59	0
33	MG	0	8071	1/1	0.84	0.07	-	104,104,104,104	0
36	CL	M	8507	1/1	0.94	0.24	-	86,86,86,86	0
33	MG	0	8051	1/1	0.95	0.19	-	97,97,97,97	0
33	MG	0	8103	1/1	0.92	0.42	-	97,97,97,97	0
35	NA	0	8301	1/1	0.96	0.12	-	59,59,59,59	0
36	CL	0	8516	1/1	0.96	0.26	-	64,64,64,64	0
33	MG	0	8081	1/1	0.92	0.08	-	67,67,67,67	0
33	MG	0	8024	1/1	0.75	0.62	-	98,98,98,98	0
35	NA	0	8314	1/1	0.97	0.23	-	53,53,53,53	0
35	NA	0	8315	1/1	0.98	0.20	-	70,70,70,70	0
35	NA	0	8302	1/1	0.96	0.16	-	55,55,55,55	0
35	NA	0	8354	1/1	0.92	0.41	-	58,58,58,58	0
35	NA	0	8358	1/1	0.96	0.28	-	109,109,109,109	0
33	MG	0	8028	1/1	0.90	0.17	-	57,57,57,57	0
33	MG	0	8106	1/1	0.97	0.26	-	78,78,78,78	0
35	NA	0	8381	1/1	0.87	0.30	-	69,69,69,69	0
35	NA	H	8322	1/1	0.70	0.42	-	78,78,78,78	0
33	MG	0	8090	1/1	0.95	0.33	-	81,81,81,81	0
33	MG	0	8072	1/1	0.95	0.34	-	78,78,78,78	0
35	NA	0	8342	1/1	0.98	0.14	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.