Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 03:09 AM EST

PDB ID	:	1YJ9
Title	:	Crystal Structure Of The Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui Containing a three residue deletion in L22
Authors	:	Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2005-01-13
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

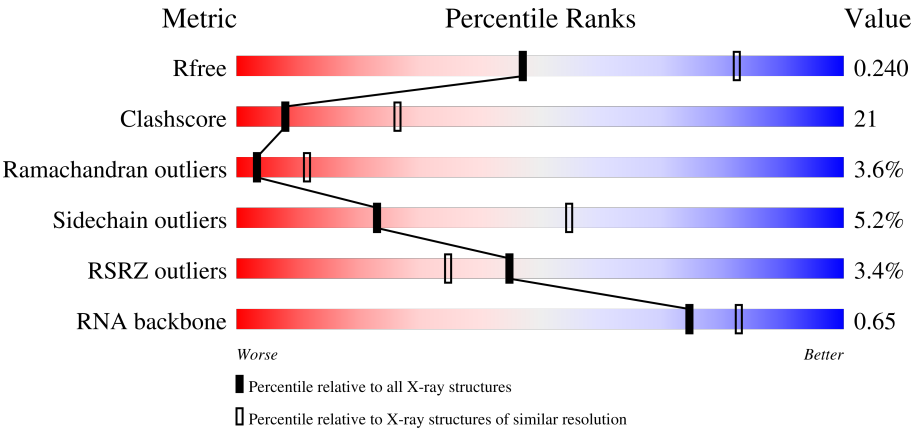
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	51% 38% 5% 6%
2	9	122	2% 38% 53% 8%
3	A	240	3% 50% 41% 7%
4	B	338	% 43% 49% 8%

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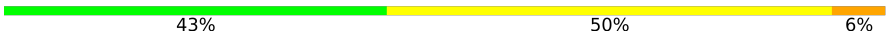
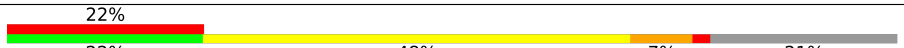
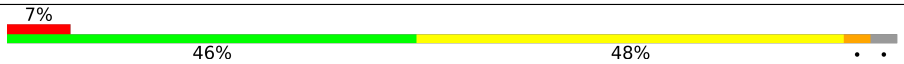
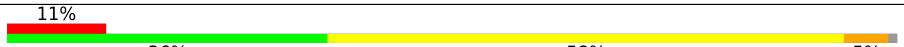
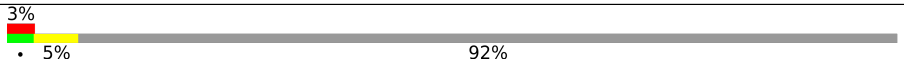
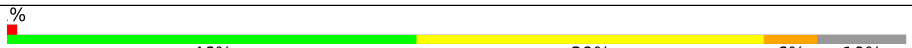
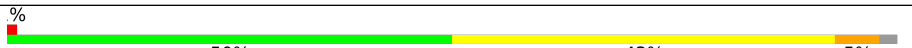
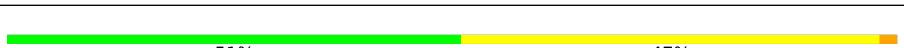
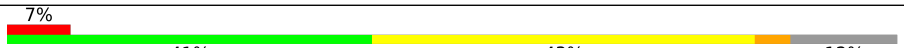
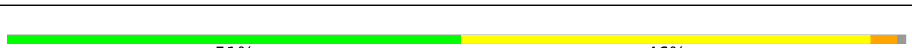
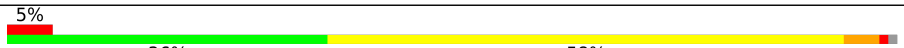
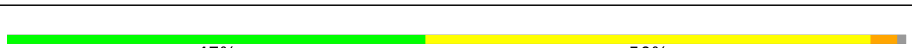
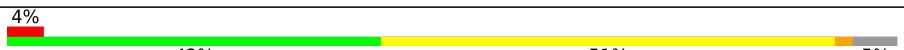
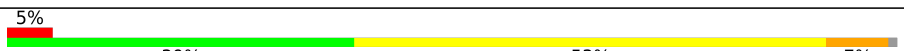
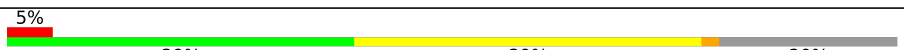
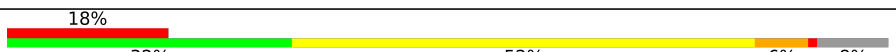
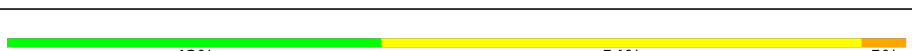
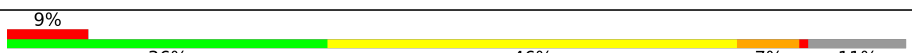
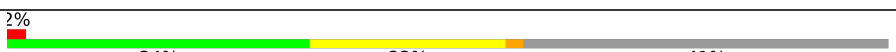
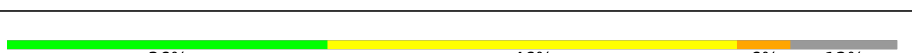
Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	152	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	6% 48% 46%
31	3	92	% 63% 34%

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
34	NA	0	8526	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	R	8586	-	-	-	X
35	CL	0	8815	-	-	-	X
35	CL	J	8801	-	-	X	-
35	CL	J	8802	-	-	X	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 99031 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	59041	26358	10875	19062	2746	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

- 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	2599	1160	471	847	121	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	147	Total	C	N	O	S	0	0	0
			1123	699	204	216	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLN	deletion	UNP P10970
R	?	-	GLN	deletion	UNP P10970
R	?	-	GLY	deletion	UNP P10970

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	49	Total	C	N	O	S	0	0	0
			421	254	93	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	107	Total	Mg	0	0
			107	107		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	74	Total	Na	0	0
			74	74		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	9	2	Total Na 2 2	0	0
34	A	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	Q	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	5866	Total O 5866 5866	0	0
37	9	143	Total O 143 143	0	0
37	A	119	Total O 119 119	0	0
37	B	148	Total O 148 148	0	0
37	C	180	Total O 180 180	0	0
37	D	46	Total O 46 46	0	0
37	E	45	Total O 45 45	0	0
37	F	27	Total O 27 27	0	0
37	G	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	69	Total O 69 69	0	0
37	I	9	Total O 9 9	0	0
37	J	57	Total O 57 57	0	0
37	K	54	Total O 54 54	0	0
37	L	84	Total O 84 84	0	0
37	M	130	Total O 130 130	0	0
37	N	64	Total O 64 64	0	0
37	O	45	Total O 45 45	0	0
37	P	64	Total O 64 64	0	0
37	Q	53	Total O 53 53	0	0
37	R	58	Total O 58 58	0	0
37	S	34	Total O 34 34	0	0
37	T	32	Total O 32 32	0	0
37	U	26	Total O 26 26	0	0
37	V	14	Total O 14 14	0	0
37	W	72	Total O 72 72	0	0
37	X	24	Total O 24 24	0	0
37	Y	104	Total O 104 104	0	0
37	Z	34	Total O 34 34	0	0
37	1	63	Total O 63 63	0	0
37	2	32	Total O 32 32	0	0

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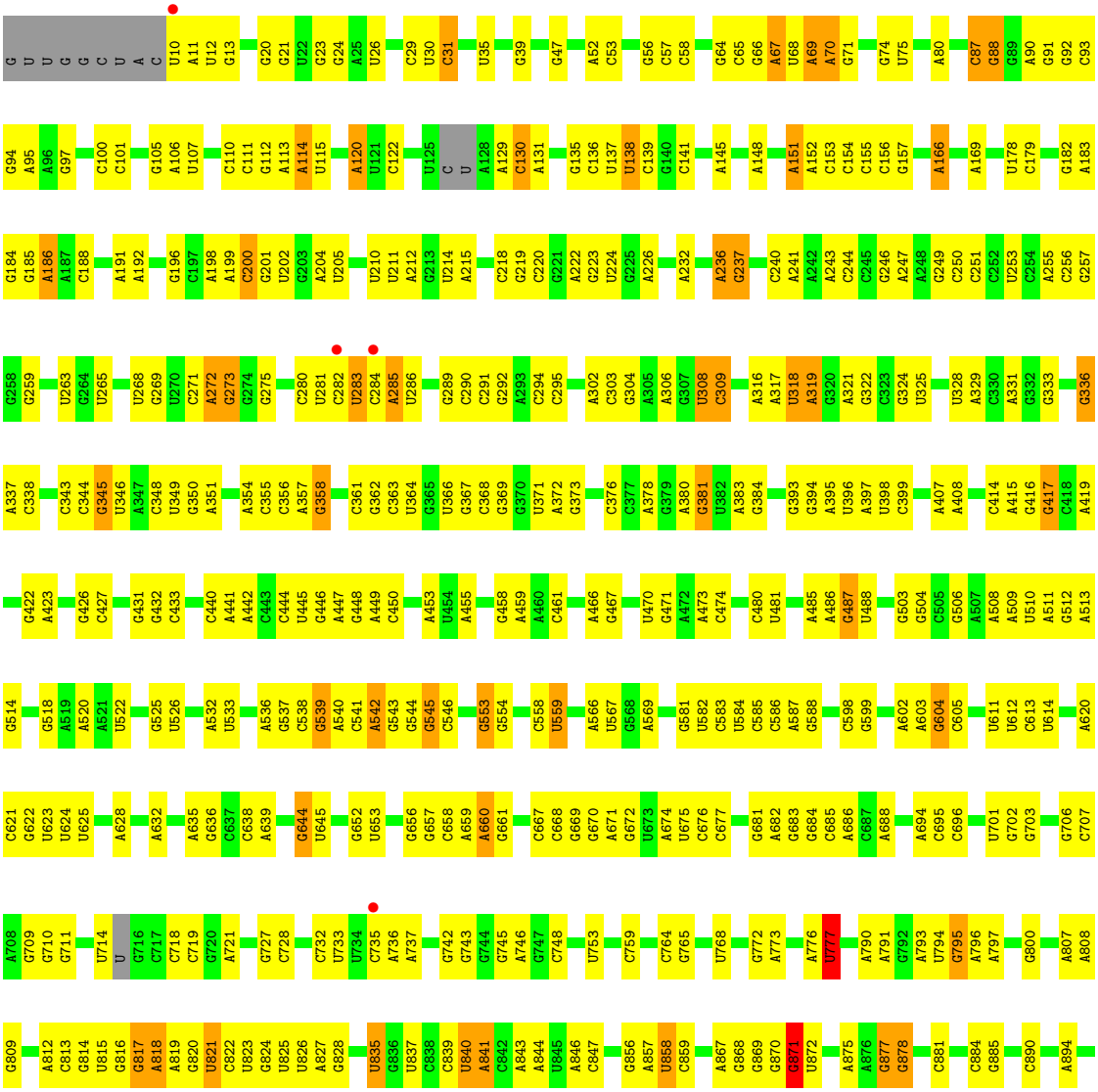
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	69	Total 69	O 69	0	0

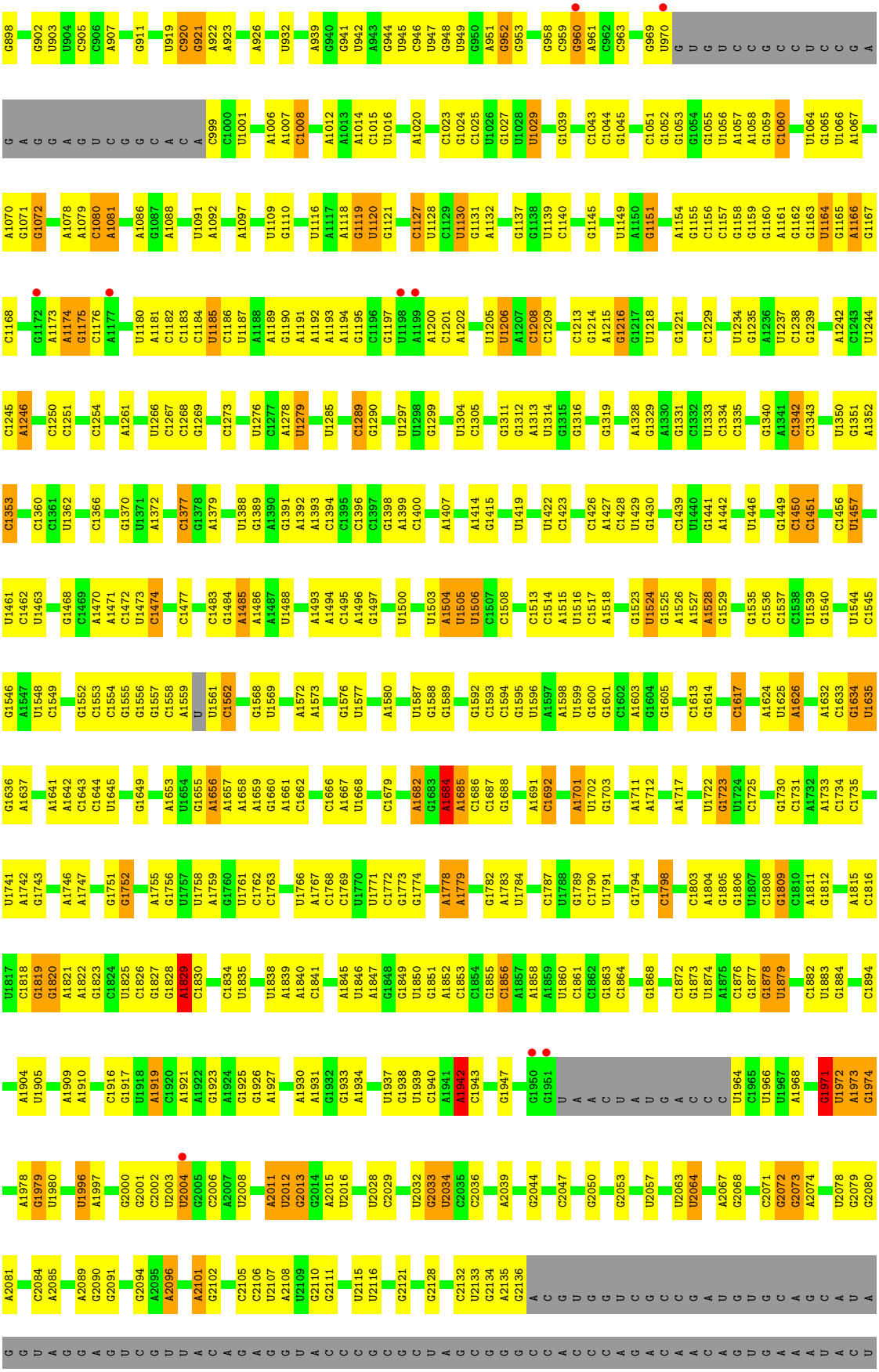
3 Residue-property plots (i)

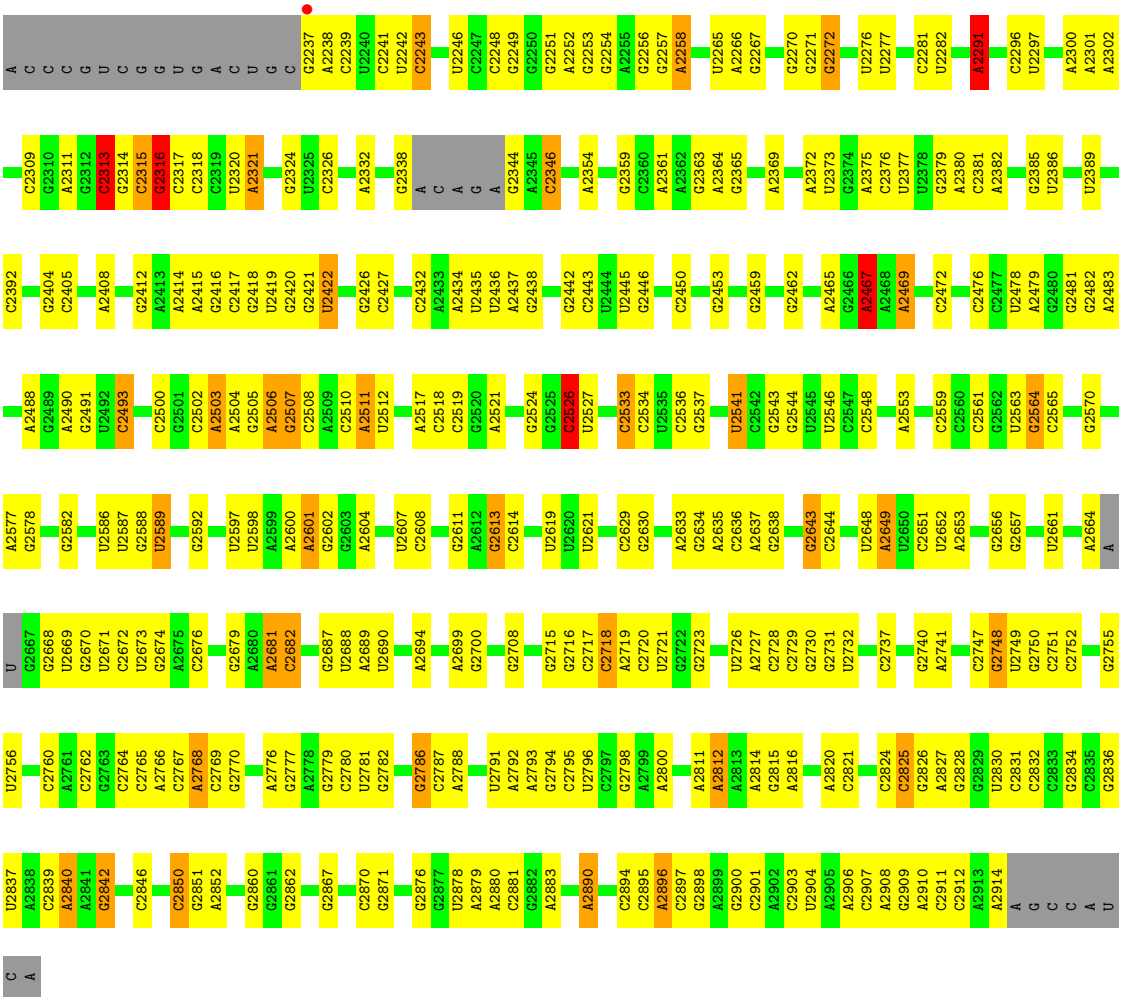
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 0:

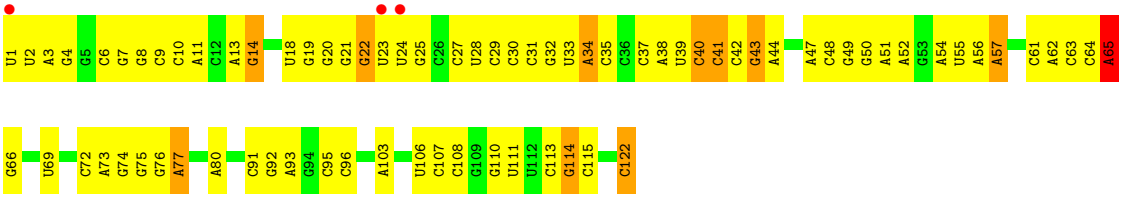






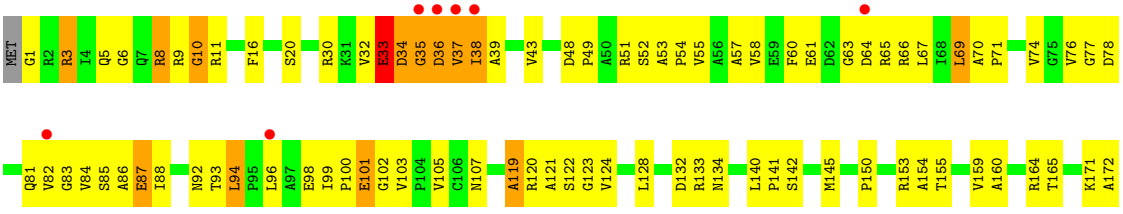
• Molecule 2: 5S Ribosomal RNA

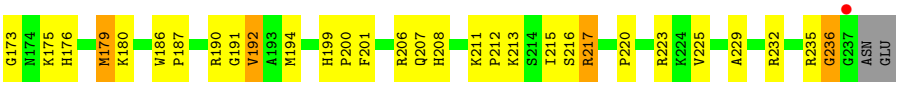
Chain 9:



• Molecule 3: 50S ribosomal protein L2P

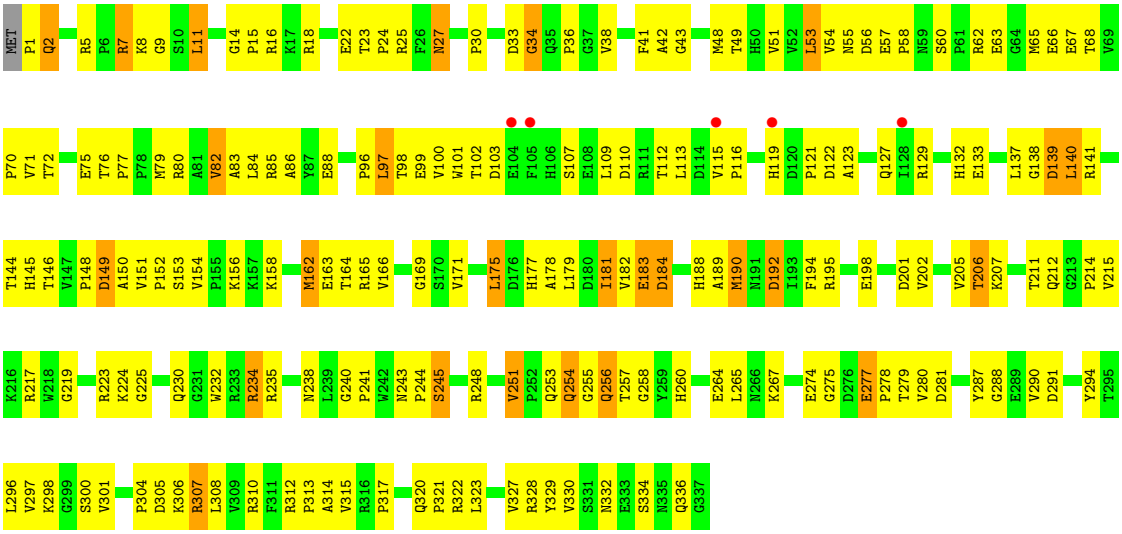
Chain A:





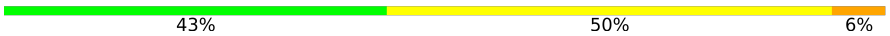
• Molecule 4: 50S ribosomal protein L3P

Chain B:



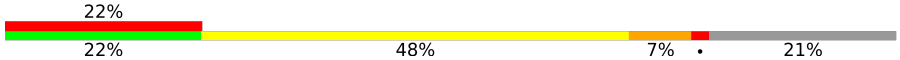
• Molecule 5: 50S ribosomal protein L4E

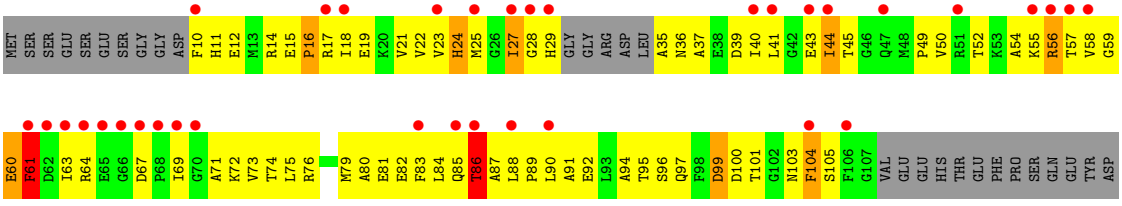
Chain C:

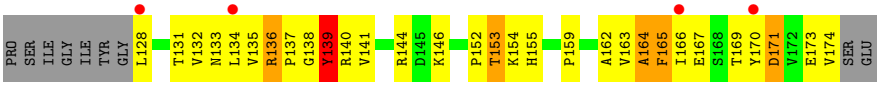


• Molecule 6: 50S ribosomal protein L5P

Chain D:

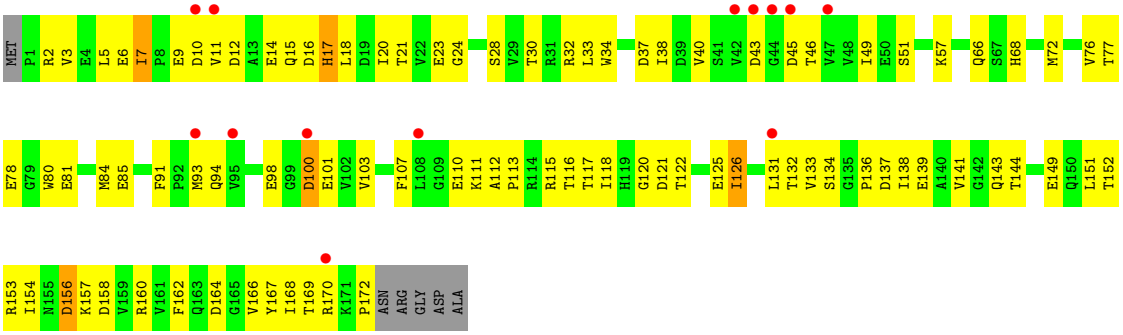






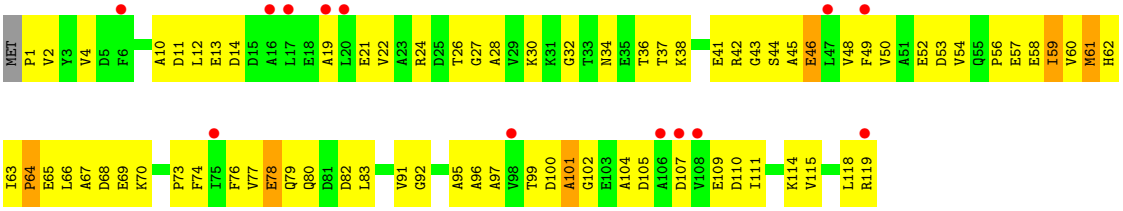
• Molecule 7: 50S ribosomal protein L6P

Chain E:



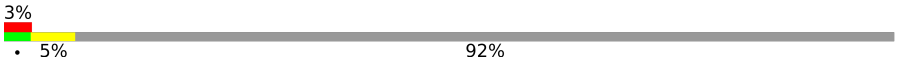
• Molecule 8: 50S ribosomal protein L7AE

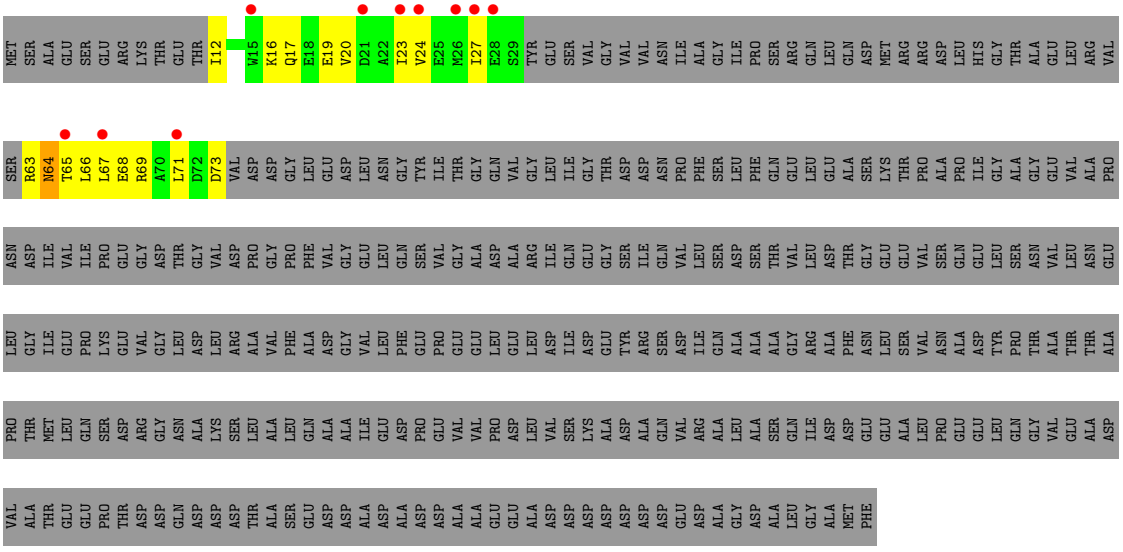
Chain F:



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

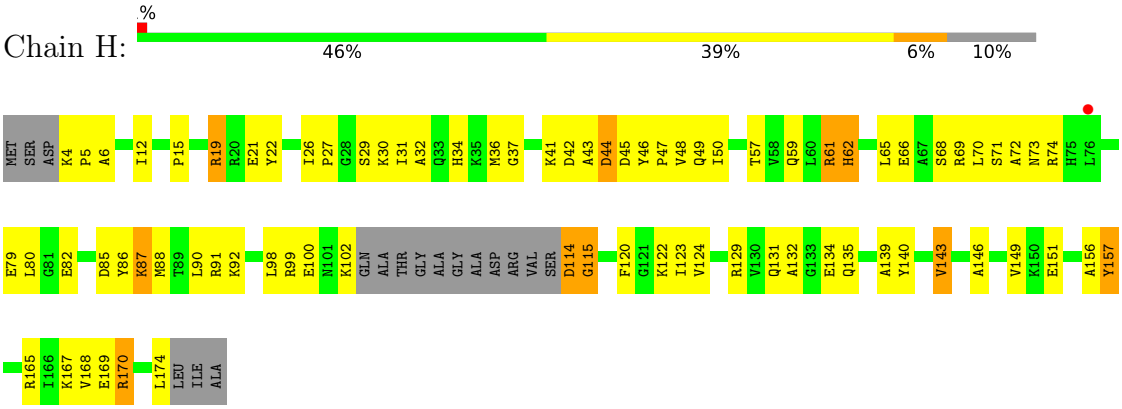
Chain G:





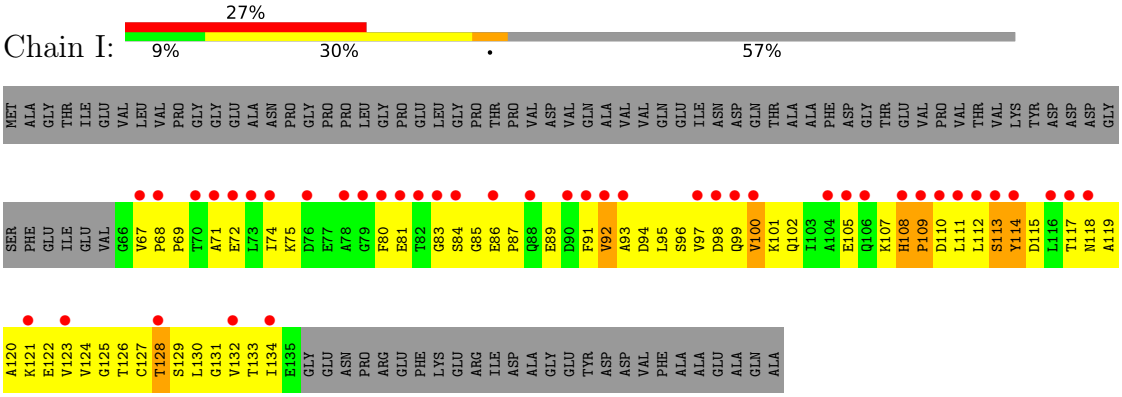
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain H:



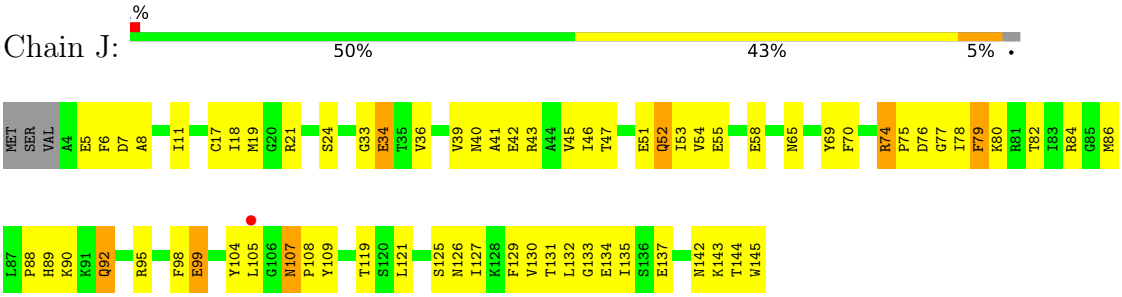
• Molecule 11: 50S RIBOSOMAL PROTEIN L11P

Chain I:



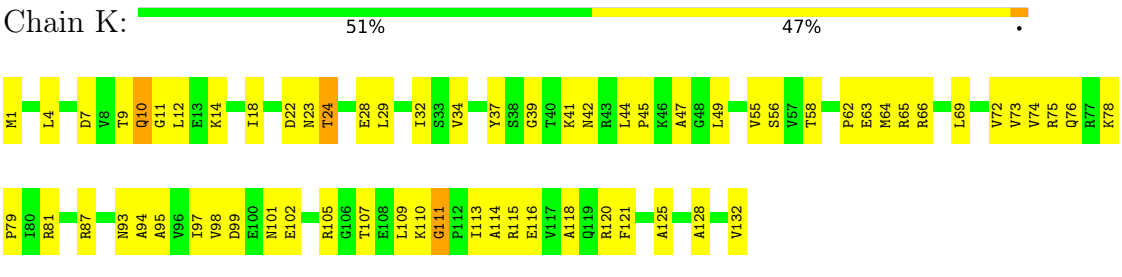
• Molecule 12: 50S ribosomal protein L13P

Chain J:



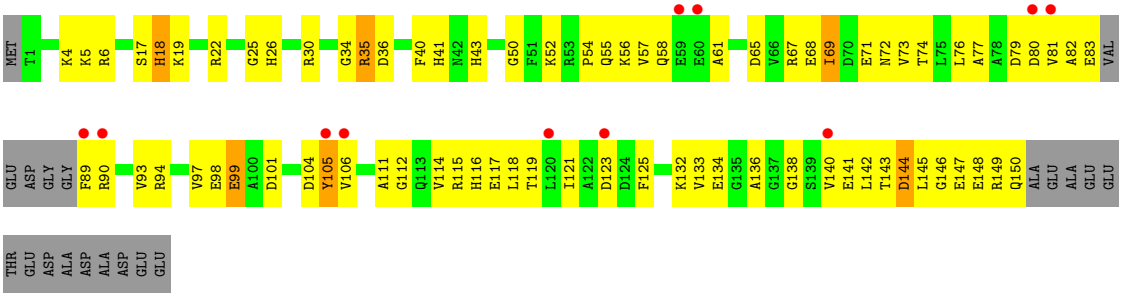
• Molecule 13: 50S ribosomal protein L14P

Chain K:



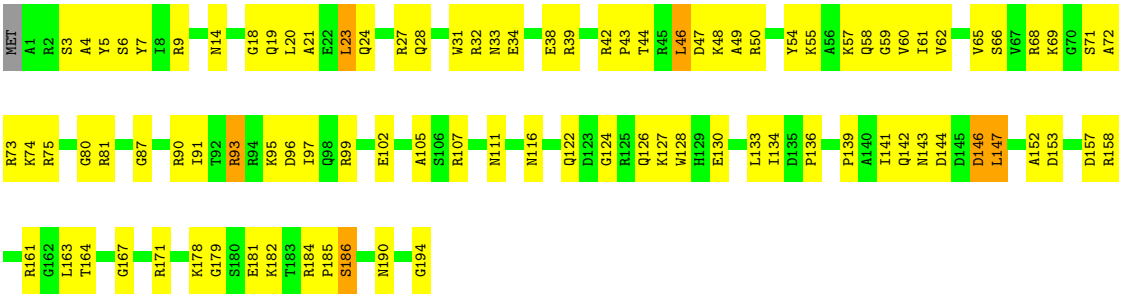
• Molecule 14: 50S ribosomal protein L15P

Chain L:



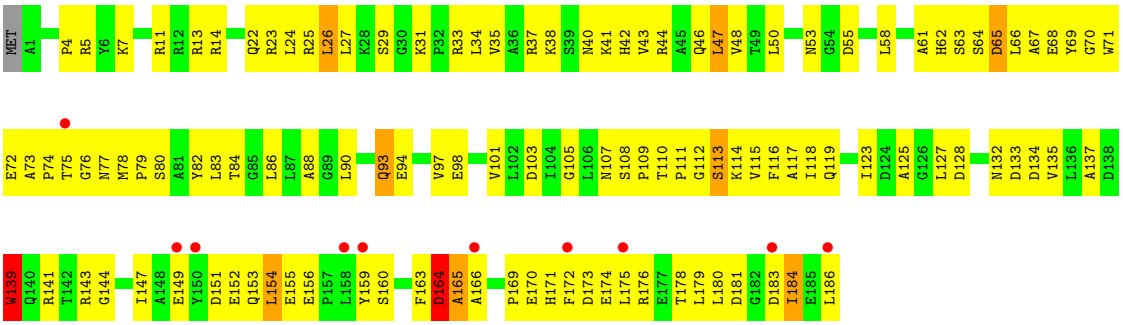
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



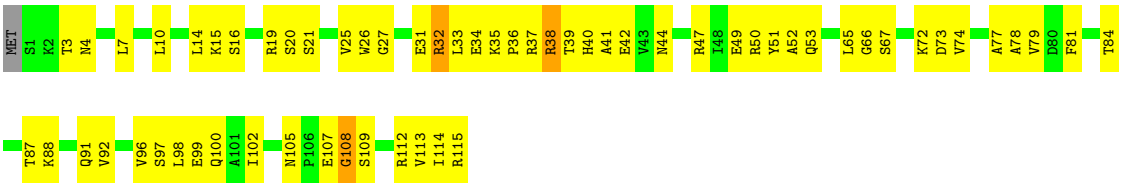
• Molecule 16: 50S ribosomal protein L18P

Chain N:



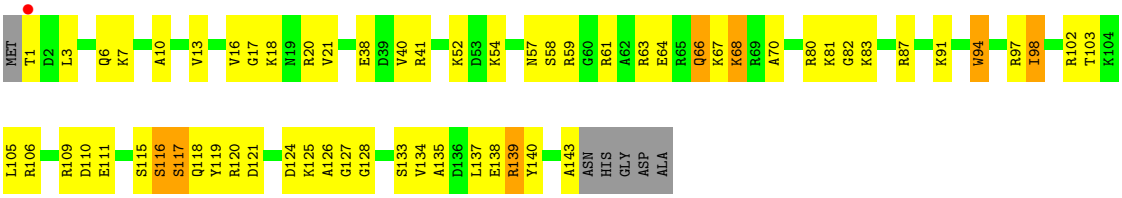
• Molecule 17: 50S ribosomal protein L18e

Chain O:



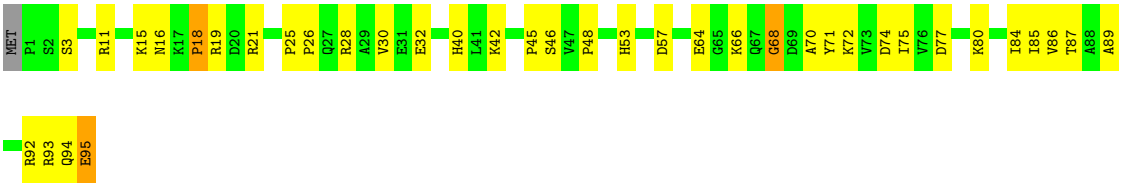
• Molecule 18: 50S ribosomal protein L19E

Chain P:



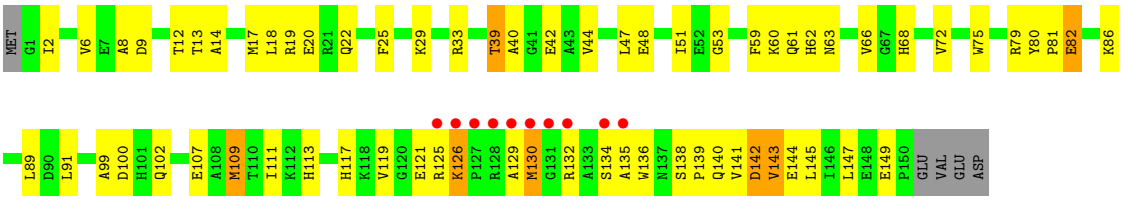
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



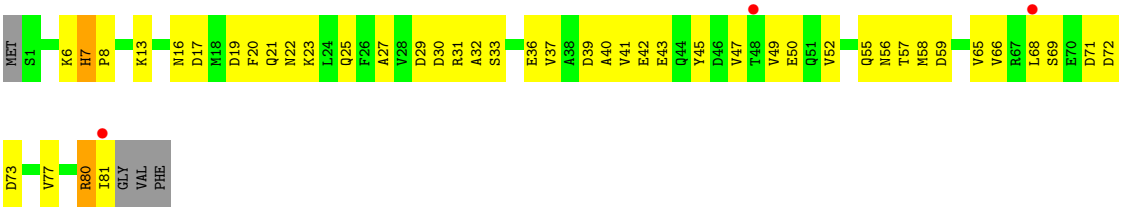
• Molecule 20: 50S ribosomal protein L22P

Chain R:



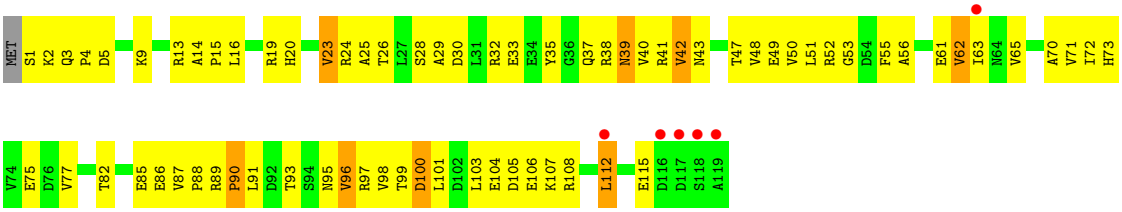
• Molecule 21: 50S ribosomal protein L23P

Chain S:

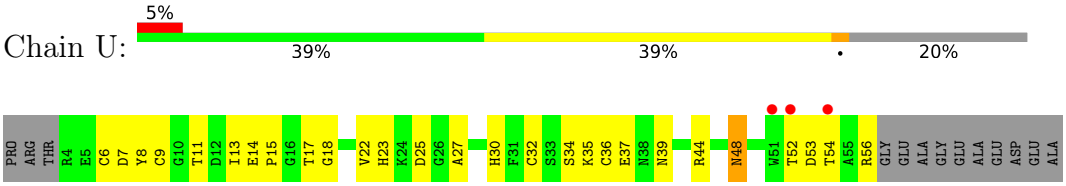


• Molecule 22: 50S ribosomal protein L24P

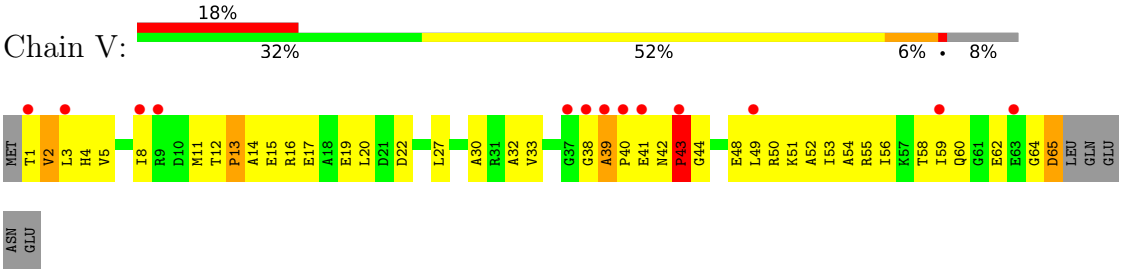
Chain T:



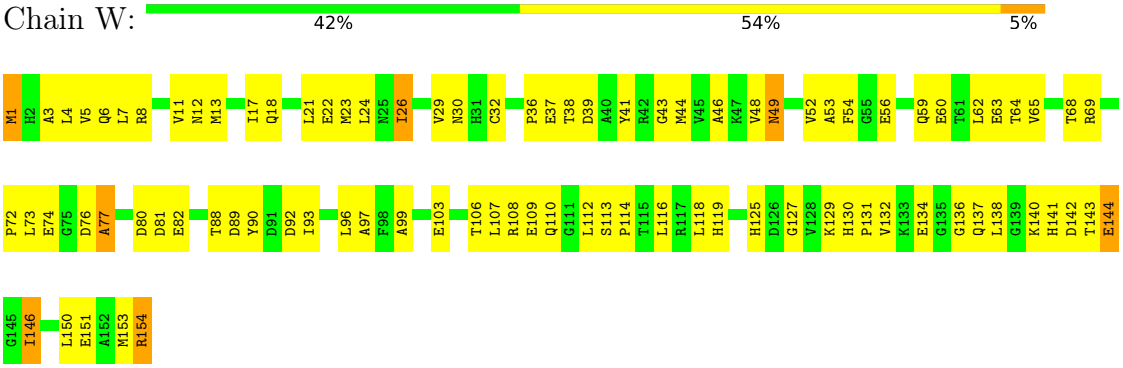
• Molecule 23: 50S ribosomal protein L24E



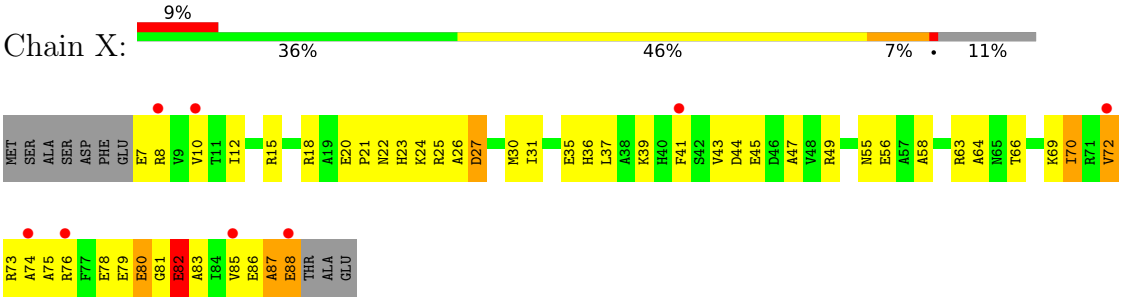
• Molecule 24: 50S ribosomal protein L29P



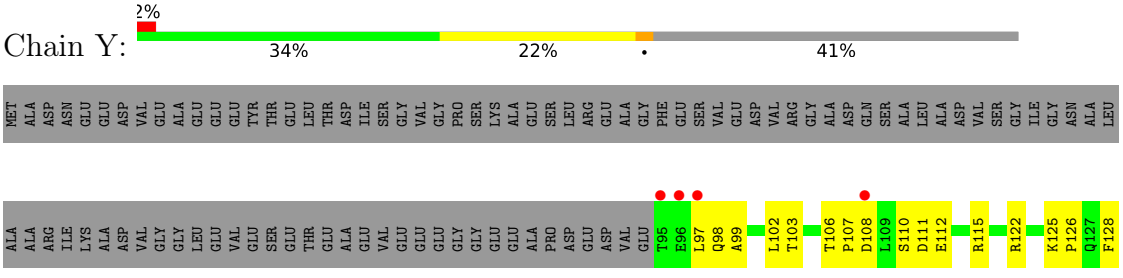
• Molecule 25: 50S ribosomal protein L30P

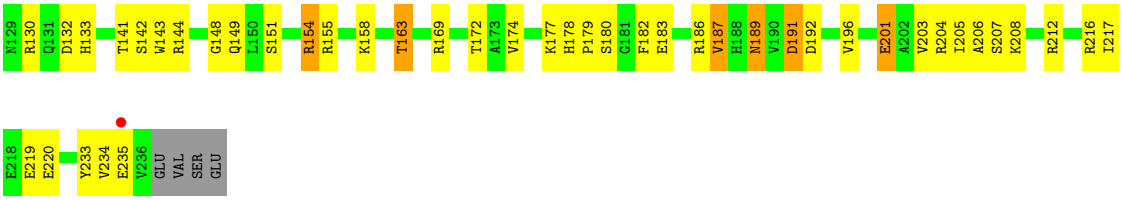


• Molecule 26: 50S ribosomal protein L31e

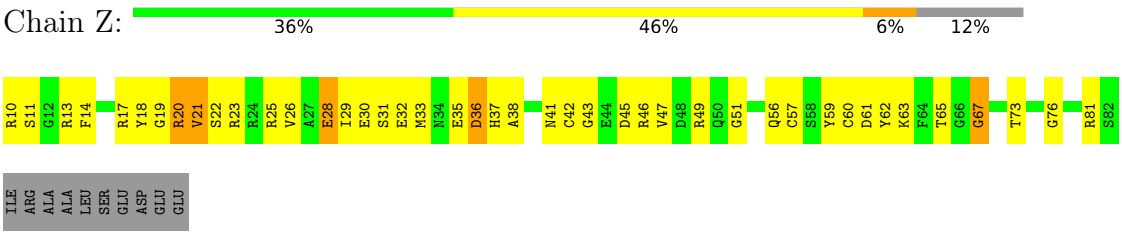


• Molecule 27: 50S ribosomal protein L32E

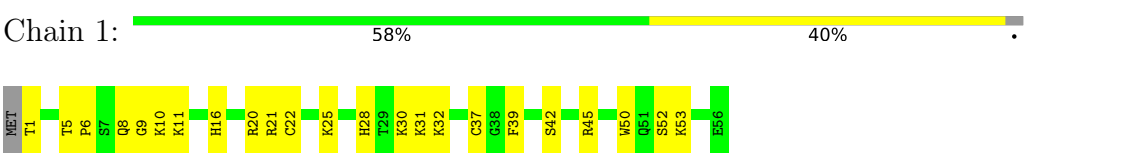




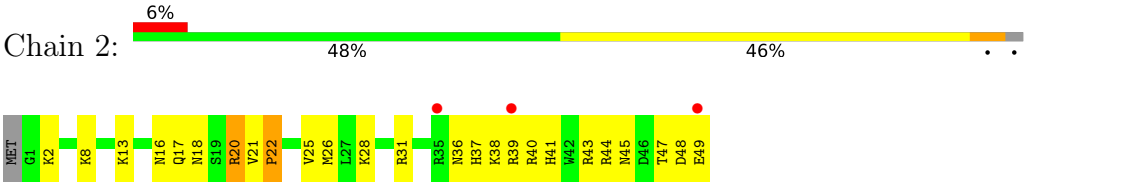
• Molecule 28: 50S ribosomal protein L37Ae



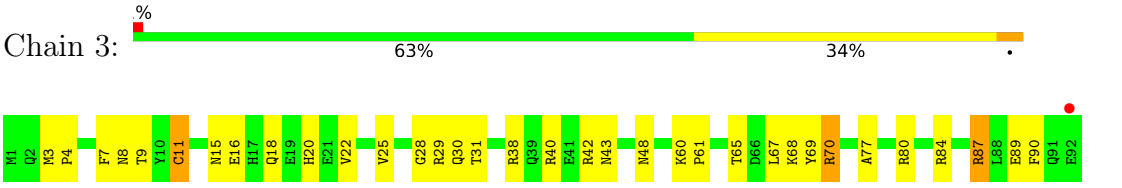
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.08Å 300.75Å 575.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 49.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.94-2.80) 89.2 (49.56-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.242 0.185 , 0.240	Depositor DCC
R_{free} test set	3987 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99031	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.42	0/65980	0.69	13/102903 (0.0%)
2	9	0.38	0/2904	0.70	1/4526 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.35	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.57	0/1498
7	E	0.35	0/1382	0.59	0/1880
8	F	0.34	0/901	0.59	0/1224
9	G	0.31	0/241	0.53	0/324
10	H	0.38	0/1302	0.70	1/1743 (0.1%)
11	I	0.31	0/526	0.59	0/716
12	J	0.40	0/1136	0.61	0/1530
13	K	0.37	0/1001	0.69	0/1347
14	L	0.36	0/1130	0.65	0/1509
15	M	0.36	0/1582	0.62	1/2117 (0.0%)
16	N	0.32	0/1474	0.64	0/1999
17	O	0.35	0/874	0.58	0/1181
18	P	0.37	0/1147	0.55	0/1528
19	Q	0.40	0/749	0.74	1/1005 (0.1%)
20	R	0.42	0/1146	0.63	0/1544
21	S	0.36	0/648	0.59	0/875
22	T	0.34	0/958	0.64	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.65	0/1655
26	X	0.36	0/664	0.62	0/895
27	Y	0.38	0/1146	0.65	0/1536
28	Z	0.38	0/589	0.63	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.41	0/427	0.61	0/566
31	3	0.40	0/771	0.58	0/1024
All	All	0.40	0/98725	0.68	17/147627 (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	46
2	9	0	1
All	All	0	47

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1942	A	C5'-C4'-C3'	7.17	127.47	116.00
1	0	1504	A	C1'-O4'-C4'	-6.38	104.80	109.90
1	0	2291	A	N9-C1'-C2'	6.19	122.05	114.00
19	Q	68	GLY	N-CA-C	-5.89	98.36	113.10
1	0	1504	A	N9-C1'-C2'	5.75	121.48	114.00
1	0	2467	A	C1'-O4'-C4'	-5.72	105.32	109.90
2	9	65	A	N9-C1'-C2'	5.66	121.35	114.00
1	0	1971	G	N9-C1'-C2'	5.52	121.18	114.00
1	0	2313	C	C5'-C4'-O4'	5.45	115.64	109.10
1	0	871	G	C5'-C4'-O4'	-5.39	102.63	109.10
1	0	2316	G	C5'-C4'-C3'	-5.30	107.52	116.00
10	H	115	GLY	N-CA-C	-5.23	100.01	113.10
1	0	840[A]	U	C5'-C4'-O4'	5.15	115.28	109.10
1	0	840[B]	U	C5'-C4'-O4'	5.15	115.28	109.10
15	M	194	GLY	N-CA-C	5.11	125.88	113.10
1	0	777	U	O4'-C1'-N1	5.02	112.22	108.20
1	0	1261	A	N9-C1'-C2'	5.01	120.51	114.00

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1131	G	Sidechain
1	0	1340	G	Sidechain
1	0	1351	G	Sidechain
1	0	1430	G	Sidechain
1	0	148	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1599	U	Sidechain
1	0	1635	U	Sidechain
1	0	1653	A	Sidechain
1	0	1684	A	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	2034	U	Sidechain
1	0	2101	A	Sidechain
1	0	2313	C	Sidechain
1	0	2315	C	Sidechain
1	0	2316	G	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	26	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	398	U	Sidechain
1	0	458	G	Sidechain
1	0	471	G	Sidechain
1	0	481	U	Sidechain
1	0	518	G	Sidechain
1	0	768	U	Sidechain
1	0	795	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	867	A	Sidechain
1	0	881	C	Sidechain
1	0	919	U	Sidechain
1	0	952	G	Sidechain
2	9	65	A	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59041	0	29817	1161	0
2	9	2599	0	1325	86	0
3	A	1753	0	1766	148	0
4	B	2625	0	2533	200	0
5	C	1859	0	1816	160	0
6	D	1094	0	1085	138	0
7	E	1357	0	1266	77	0
8	F	890	0	843	79	0
9	G	240	0	231	22	0
10	H	1282	0	1292	95	0
11	I	519	0	500	63	0
12	J	1120	0	1098	80	0
13	K	992	0	1031	77	0
14	L	1118	0	1076	81	0
15	M	1558	0	1566	98	0
16	N	1445	0	1401	147	0
17	O	865	0	873	62	0
18	P	1136	0	1123	71	0
19	Q	735	0	729	37	0
20	R	1123	0	1099	69	0
21	S	641	0	605	39	0
22	T	950	0	923	99	0
23	U	410	0	364	31	0
24	V	499	0	511	44	0
25	W	1196	0	1137	120	0
26	X	654	0	653	57	0
27	Y	1130	0	1133	66	0
28	Z	578	0	539	39	0
29	1	431	0	426	36	0
30	2	421	0	437	35	0
31	3	755	0	728	31	0
32	0	107	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	74	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	9	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5866	0	0	246	0
37	1	63	0	0	8	0
37	2	32	0	0	2	0
37	3	69	0	0	8	0
37	9	143	0	0	12	0
37	A	119	0	0	21	0
37	B	148	0	0	31	0
37	C	180	0	0	34	0
37	D	46	0	0	17	0
37	E	45	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	F	27	0	0	8	0
37	G	19	0	0	2	0
37	H	69	0	0	12	0
37	I	9	0	0	5	0
37	J	57	0	0	8	0
37	K	54	0	0	10	0
37	L	84	0	0	17	0
37	M	130	0	0	10	0
37	N	64	0	0	22	0
37	O	45	0	0	11	0
37	P	64	0	0	10	0
37	Q	53	0	0	7	0
37	R	58	0	0	5	0
37	S	34	0	0	3	0
37	T	32	0	0	9	0
37	U	26	0	0	3	0
37	V	14	0	0	5	0
37	W	72	0	0	12	0
37	X	24	0	0	5	0
37	Y	104	0	0	15	0
37	Z	34	0	0	3	0
All	All	99031	0	59926	3232	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 21.

All (3232) 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)
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.66	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	0.95	1.08
1:0:1160:G:H5'	1:0:1161:A:H5'	1.13	1.07
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.36	1.04
29:1:25:LYS:HD2	30:2:49:GLU:H	1.20	1.03
13:K:10:GLN:NE2	13:K:10:GLN:H	1.58	1.02
1:0:871:G:H5'	1:0:871:G:H8	1.21	1.01
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.42	1.00
1:0:156:C:H5"	15:M:171:ARG:HD3	1.42	0.99
1:0:1559:A:H1'	37:0:5655:HOH:O	1.61	0.98
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.29	0.97
1:0:871:G:H5'	1:0:871:G:C8	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:381:G:H5”	37:0:4123:HOH:O	1.62	0.96
2:9:76:G:H3’	2:9:77:A:H5”	1.44	0.96
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.46	0.96
5:C:236:THR:HG22	5:C:239:ALA:N	1.80	0.96
1:0:1242:A:H5’	12:J:82:THR:HG23	1.44	0.96
30:2:20:ARG:HG3	30:2:20:ARG:HH11	1.29	0.95
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.48	0.95
2:9:6:C:H5”	16:N:37:ARG:NH1	1.82	0.95
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.45	0.95
28:Z:10:ARG:HA	37:Z:8715:HOH:O	1.67	0.95
13:K:10:GLN:HE21	13:K:10:GLN:N	1.66	0.94
1:0:2270:G:H4’	3:A:223:ARG:HH12	1.33	0.94
1:0:2717:C:H2’	1:0:2718:C:H5”	1.46	0.94
5:C:233:THR:HG22	5:C:234:VAL:H	1.33	0.94
1:0:396:U:H1’	37:0:7397:HOH:O	1.66	0.93
1:0:1474:C:H6	1:0:1474:C:H5’	1.34	0.93
5:C:76:ARG:HB3	5:C:76:ARG:HH11	1.30	0.93
4:B:202:VAL:HG11	4:B:301:VAL:HG13	1.51	0.92
1:0:541:C:H2’	1:0:542:A:H5”	1.51	0.92
1:0:1187:U:HO2’	1:0:1189:A:H2	1.03	0.92
3:A:81:GLN:HB2	3:A:92:ASN:ND2	1.85	0.92
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.51	0.92
18:P:115:SER:H	18:P:118:GLN:HE21	0.92	0.92
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.51	0.92
1:0:1160:G:C5’	1:0:1161:A:H5’	1.99	0.92
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.52	0.92
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.35	0.91
16:N:97:VAL:HG12	16:N:127:LEU:HD11	1.53	0.91
6:D:94:ALA:HB3	6:D:97:GLN:HE21	1.34	0.91
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.91
1:0:1160:G:H5’	1:0:1161:A:C5’	2.01	0.90
18:P:115:SER:H	18:P:118:GLN:NE2	1.69	0.90
11:I:95:LEU:HD22	11:I:99:GLN:HB3	1.49	0.90
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.52	0.90
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.53	0.90
4:B:238:ASN:HD22	4:B:240:GLY:H	0.92	0.90
14:L:79:ASP:HB3	37:L:8862:HOH:O	1.70	0.90
11:I:107:LYS:HD2	11:I:110:ASP:HB2	1.51	0.90
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.19	0.90
1:0:56:G:H5”	24:V:50:ARG:HH12	1.37	0.89
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:HG23	15:M:167:GLY:H	1.35	0.89
25:W:88:THR:HG22	25:W:89:ASP:H	1.36	0.89
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.72	0.88
3:A:35:GLY:O	3:A:36:ASP:HB3	1.72	0.88
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.55	0.88
1:0:2586:U:H3	1:0:2592:G:H22	1.20	0.87
1:0:1118:A:H8	1:0:1118:A:H3'	1.39	0.87
6:D:57:THR:HG23	6:D:63:ILE:HA	1.55	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.72	0.87
4:B:238:ASN:HD22	4:B:240:GLY:N	1.73	0.86
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.57	0.86
1:0:2717:C:C2'	1:0:2718:C:H5"	2.06	0.86
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.73	0.85
18:P:115:SER:N	18:P:118:GLN:HE21	1.74	0.85
3:A:85:SER:HA	37:A:8909:HOH:O	1.74	0.85
14:L:77:ALA:HB3	37:L:8833:HOH:O	1.75	0.85
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.85
4:B:238:ASN:ND2	4:B:240:GLY:H	1.74	0.85
12:J:105:LEU:HA	37:J:8866:HOH:O	1.77	0.85
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.56	0.85
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.57	0.85
1:0:182:G:H5'	37:0:4959:HOH:O	1.77	0.85
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.59	0.85
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.57	0.85
4:B:320:GLN:NE2	4:B:321:PRO:HD2	1.92	0.85
1:0:21:G:H5'	20:R:2:ILE:HA	1.58	0.84
1:0:870:G:H2'	1:0:871:G:H5"	1.57	0.84
10:H:41:LYS:HE2	10:H:45:ASP:HB3	1.59	0.84
10:H:168:VAL:HG13	37:H:213:HOH:O	1.76	0.84
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.58	0.84
8:F:96:ALA:HA	37:F:3111:HOH:O	1.78	0.84
16:N:23:ARG:HD3	37:N:8842:HOH:O	1.76	0.84
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.57	0.84
5:C:236:THR:HA	37:C:8660:HOH:O	1.77	0.83
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.25	0.83
5:C:236:THR:CG2	5:C:239:ALA:H	1.86	0.83
1:0:1118:A:H3'	1:0:1118:A:C8	2.13	0.83
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.58	0.83
12:J:107:ASN:ND2	12:J:109:TYR:H	1.76	0.83
8:F:61:MET:HB3	15:M:19:GLN:OE1	1.79	0.82
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.77	0.82
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.62	0.82
1:0:1118:A:H62	1:0:1244:U:H3	1.27	0.82
30:2:41:HIS:HD2	30:2:44:ARG:H	1.27	0.82
1:0:1205:U:H2'	1:0:1206:U:H5'	1.62	0.82
14:L:149:ARG:O	14:L:150:GLN:HB2	1.79	0.82
1:0:1834:C:H2'	1:0:1840:A:N6	1.94	0.82
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.59	0.82
4:B:98:THR:HG22	4:B:99:GLU:H	1.45	0.82
1:0:541:C:C2'	1:0:542:A:H5"	2.10	0.81
4:B:7:ARG:NH1	4:B:11:LEU:HD21	1.94	0.81
1:0:1184:C:H1'	37:0:7238:HOH:O	1.79	0.81
1:0:2506:A:HO2'	1:0:2507:G:H8	1.28	0.81
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.61	0.81
37:0:5022:HOH:O	13:K:39:GLY:HA2	1.80	0.81
24:V:39:ALA:H	24:V:40:PRO:HD2	1.46	0.81
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.61	0.81
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.60	0.81
1:0:1751:G:H2'	1:0:1752:G:H5"	1.60	0.81
6:D:25:MET:HE2	6:D:41:LEU:HG	1.63	0.81
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.61	0.81
16:N:151:ASP:O	16:N:154:LEU:HB2	1.81	0.81
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.63	0.81
6:D:136:ARG:HD2	6:D:155:HIS:O	1.80	0.80
1:0:542:A:H5'	1:0:542:A:H8	1.46	0.80
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.62	0.80
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.80
1:0:2908:A:H2'	1:0:2909:G:O4'	1.81	0.80
2:9:14:G:H5'	2:9:14:G:H8	1.47	0.80
2:9:56:A:H2'	2:9:57:A:H5"	1.64	0.80
4:B:41:PHE:HB3	4:B:190:MET:HE1	1.62	0.80
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.11	0.80
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.63	0.79
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.64	0.79
14:L:55:GLN:HA	14:L:58:GLN:HE21	1.47	0.79
18:P:115:SER:OG	18:P:118:GLN:HG3	1.82	0.79
9:G:64:ASN:HD22	9:G:64:ASN:N	1.79	0.79
1:0:2364:A:H5"	19:Q:15:LYS:HD3	1.64	0.79
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.46	0.79
5:C:140:VAL:HB	37:C:8660:HOH:O	1.82	0.79
37:0:5326:HOH:O	15:M:58:GLN:HG3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:22:ASN:ND2	21:S:68:LEU:HB2	1.98	0.79
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.97	0.79
5:C:2:GLN:HB3	37:C:8588:HOH:O	1.83	0.79
1:0:1116:U:H3	1:0:1246:A:H62	1.27	0.79
37:0:5256:HOH:O	9:G:12:ILE:HA	1.82	0.79
4:B:177:HIS:O	4:B:181:ILE:HG13	1.82	0.79
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.63	0.79
13:K:10:GLN:H	13:K:10:GLN:HE21	0.84	0.79
21:S:57:THR:HG22	21:S:59:ASP:H	1.47	0.79
1:0:877:G:H5'	1:0:878:G:OP1	1.83	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.78
1:0:1206:U:H5'	1:0:1206:U:H6	1.48	0.78
8:F:99:THR:HA	37:F:3461:HOH:O	1.82	0.78
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.64	0.78
16:N:151:ASP:OD1	16:N:154:LEU:HD13	1.84	0.78
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.49	0.78
37:C:8572:HOH:O	22:T:2:LYS:HE2	1.81	0.78
16:N:169:PRO:O	16:N:172:PHE:HB3	1.84	0.78
37:9:8671:HOH:O	16:N:147:ILE:HB	1.84	0.78
6:D:94:ALA:CB	6:D:97:GLN:HE21	1.96	0.78
6:D:104:PHE:HE2	6:D:132:VAL:HB	1.48	0.78
10:H:146:ALA:O	10:H:149:VAL:HG12	1.84	0.78
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.65	0.78
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.65	0.77
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.64	0.77
29:1:10:LYS:HG3	37:1:2979:HOH:O	1.84	0.77
1:0:272:A:H5'	1:0:273:G:OP2	1.83	0.77
3:A:121:ALA:O	3:A:124:VAL:HG22	1.84	0.77
10:H:165:ARG:HD3	37:H:238:HOH:O	1.84	0.77
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.64	0.77
16:N:80:SER:HB2	37:N:8832:HOH:O	1.83	0.77
26:X:43:VAL:HG12	26:X:44:ASP:H	1.49	0.77
1:0:21:G:C5'	20:R:2:ILE:HA	2.14	0.77
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.67	0.77
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.65	0.77
1:0:272:A:H3'	37:0:7298:HOH:O	1.85	0.77
6:D:99:ASP:CG	6:D:100:ASP:H	1.88	0.77
8:F:91:VAL:HG12	8:F:92:GLY:H	1.50	0.77
3:A:37:VAL:HG23	3:A:38:ILE:H	1.49	0.77
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.65	0.77
1:0:1474:C:H5'	1:0:1474:C:C6	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:0:7226:HOH:O	4:B:211:THR:HG21	1.85	0.76
2:9:92:G:H2'	2:9:93:A:C8	2.20	0.76
24:V:12:THR:HG22	24:V:15:GLU:CG	2.15	0.76
3:A:223:ARG:HG3	37:A:8892:HOH:O	1.85	0.76
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.50	0.76
27:Y:219:GLU:HG3	27:Y:220:GLU:N	1.99	0.76
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.84	0.76
27:Y:216:ARG:HD3	37:Y:8874:HOH:O	1.86	0.76
21:S:22:ASN:HD21	21:S:68:LEU:HB2	1.51	0.76
1:0:559:U:H6	1:0:559:U:H5'	1.50	0.76
37:0:4030:HOH:O	30:2:38:LYS:HE3	1.84	0.76
8:F:110:ASP:O	8:F:114:LYS:HG3	1.86	0.76
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.86	0.76
1:0:545:G:H5'	1:0:545:G:H8	1.50	0.75
1:0:1979:G:H2'	37:0:9091:HOH:O	1.85	0.75
1:0:2426:G:H1'	37:0:5876:HOH:O	1.87	0.75
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.68	0.75
5:C:16:VAL:HG12	5:C:17:ASP:H	1.52	0.75
5:C:25:PRO:HD2	37:C:8638:HOH:O	1.84	0.75
26:X:43:VAL:HG11	26:X:82:GLU:HA	1.66	0.75
1:0:1450:C:H4'	1:0:1451:C:OP2	1.85	0.75
1:0:1634:G:H3'	37:0:3693:HOH:O	1.85	0.75
1:0:2243:C:H5"	37:0:3549:HOH:O	1.86	0.75
1:0:282:C:H1'	1:0:368:C:N4	2.01	0.75
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.22	0.75
14:L:61:ALA:HA	37:L:8868:HOH:O	1.85	0.75
1:0:506:G:H22	1:0:509:A:H5'	1.51	0.75
1:0:1446:U:H2'	21:S:55:GLN:NE2	2.02	0.75
1:0:1593:C:H5'	18:P:116:SER:O	1.86	0.75
1:0:1919:A:H4'	37:0:4649:HOH:O	1.86	0.75
14:L:138:GLY:HA3	37:L:8857:HOH:O	1.86	0.75
1:0:130:C:H2'	37:0:9961:HOH:O	1.86	0.74
1:0:154:C:H2'	1:0:155:C:H6	1.52	0.74
6:D:174:VAL:HG12	37:D:6555:HOH:O	1.87	0.74
14:L:80:ASP:HB2	14:L:90:ARG:O	1.87	0.74
2:9:75:G:H1	2:9:106:U:H3	1.34	0.74
21:S:37:VAL:O	21:S:41:VAL:HG23	1.87	0.74
29:1:25:LYS:HD2	30:2:49:GLU:N	2.00	0.74
1:0:2578:G:H5'	1:0:2578:G:H8	1.52	0.74
1:0:2769:C:H2'	1:0:2770:G:O4'	1.87	0.74
6:D:99:ASP:HA	37:D:5675:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:56:ILE:O	24:V:60:GLN:HG3	1.88	0.74
1:0:821:U:H2'	1:0:822:C:H6	1.51	0.74
1:0:2748:G:H5'	37:0:7309:HOH:O	1.87	0.74
8:F:46:GLU:O	8:F:73:PRO:HD2	1.87	0.74
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.33	0.74
23:U:9:CYS:HA	23:U:52:THR:HG23	1.69	0.74
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.68	0.74
30:2:41:HIS:H	30:2:45:ASN:HD22	1.31	0.74
7:E:43:ASP:HA	37:E:5864:HOH:O	1.87	0.74
1:0:200:C:H2'	37:0:3243:HOH:O	1.87	0.74
1:0:100:C:H4'	22:T:16:LEU:HB2	1.67	0.74
20:R:129:ALA:O	20:R:130:MET:HB2	1.87	0.74
1:0:2004:U:H4'	37:0:5105:HOH:O	1.86	0.74
5:C:184:ARG:HG2	37:C:8673:HOH:O	1.88	0.74
6:D:99:ASP:HB3	6:D:103:ASN:H	1.53	0.74
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.17	0.74
1:0:541:C:H2'	1:0:542:A:C5'	2.18	0.74
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.69	0.74
21:S:43:GLU:HB3	37:S:8543:HOH:O	1.88	0.73
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.85	0.73
1:0:236:A:H4'	1:0:237:G:OP1	1.87	0.73
37:B:8852:HOH:O	12:J:104:TYR:HA	1.87	0.73
21:S:57:THR:HG22	21:S:59:ASP:N	2.03	0.73
1:0:794:U:H3	1:0:819:A:H61	1.35	0.73
16:N:119:GLN:O	16:N:123:ILE:HG13	1.89	0.73
1:0:544:G:H2'	1:0:545:G:H5"	1.70	0.73
1:0:1835:U:C5	1:0:1840:A:N7	2.55	0.73
4:B:179:LEU:O	4:B:183:GLU:HG2	1.87	0.73
9:G:23:ILE:O	9:G:27:ILE:HG13	1.88	0.73
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.71	0.73
25:W:88:THR:HB	37:W:6679:HOH:O	1.89	0.73
1:0:2332:A:H5'	6:D:56:ARG:HH22	1.53	0.72
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.71	0.72
12:J:45:VAL:HG23	12:J:130:VAL:O	1.89	0.72
1:0:2840:A:OP1	4:B:211:THR:HG23	1.88	0.72
1:0:2851:G:O2'	1:0:2852:A:H5'	1.88	0.72
1:0:2862:G:H4'	4:B:336:GLN:O	1.89	0.72
4:B:235:ARG:HA	37:B:8895:HOH:O	1.89	0.72
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.72	0.72
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.20	0.72
20:R:125:ARG:O	20:R:126:LYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.89	0.72
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.70	0.72
10:H:61:ARG:HH11	10:H:61:ARG:HG3	1.54	0.72
29:1:45:ARG:HB3	37:1:988:HOH:O	1.89	0.72
1:0:2524:G:H21	1:0:2526:C:N4	1.86	0.72
1:0:2812:A:H2	1:0:2814:A:H62	1.35	0.72
5:C:145:GLU:HG3	37:C:8578:HOH:O	1.88	0.72
16:N:132:ASN:O	16:N:135:VAL:HG12	1.88	0.72
25:W:130:HIS:O	25:W:136:GLY:HA3	1.90	0.72
1:0:944:G:H21	25:W:44:MET:CE	2.03	0.72
1:0:1234:U:N3	4:B:244:PRO:HB3	2.04	0.72
37:0:3789:HOH:O	5:C:188:ARG:HD3	1.89	0.72
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.54	0.72
1:0:558:C:H2'	1:0:559:U:H5'	1.71	0.72
5:C:127:ARG:HH21	5:C:225:PRO:HG2	1.55	0.72
25:W:82:GLU:HB2	37:W:2749:HOH:O	1.89	0.72
37:0:7197:HOH:O	22:T:9:LYS:HB2	1.89	0.71
5:C:242:GLU:HG3	37:C:8585:HOH:O	1.90	0.71
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.04	0.71
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.90	0.71
27:Y:141:THR:HG23	37:Y:8896:HOH:O	1.89	0.71
1:0:1080:C:H4'	1:0:1081:A:OP1	1.89	0.71
5:C:111:VAL:HB	37:C:8522:HOH:O	1.90	0.71
6:D:54:ALA:HB1	37:D:4069:HOH:O	1.89	0.71
8:F:91:VAL:HG12	8:F:92:GLY:N	2.04	0.71
1:0:1278:A:H4'	1:0:1279:U:C4	2.25	0.71
5:C:132:ASP:HB2	5:C:161:ASP:HB3	1.73	0.71
25:W:64:THR:O	25:W:68:THR:HG22	1.90	0.71
1:0:553:G:P	27:Y:204:ARG:HH22	2.13	0.71
17:O:42:GLU:HB2	37:O:2176:HOH:O	1.89	0.71
17:O:105:ASN:HD21	17:O:109:SER:H	1.39	0.71
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.20	0.71
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.16	0.71
8:F:58:GLU:HA	8:F:61:MET:HE2	1.72	0.71
1:0:506:G:H22	1:0:509:A:C5'	2.04	0.71
18:P:64:GLU:HG2	37:P:169:HOH:O	1.91	0.71
1:0:1594:C:OP2	18:P:120:ARG:HD2	1.91	0.71
1:0:1733:A:H4'	4:B:212:GLN:HA	1.73	0.71
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.06	0.71
9:G:64:ASN:HD22	9:G:64:ASN:H	1.38	0.71
22:T:106:GLU:HG3	37:T:4913:HOH:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1:PRO:O	4:B:2:GLN:HB2	1.90	0.71
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.55	0.71
30:2:20:ARG:HH11	30:2:20:ARG:CG	2.04	0.71
1:0:459:A:H4'	37:0:9260:HOH:O	1.90	0.70
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.24	0.70
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.55	0.70
5:C:236:THR:HG21	37:C:8578:HOH:O	1.90	0.70
24:V:44:GLY:O	24:V:48:GLU:HG2	1.91	0.70
4:B:305:ASP:O	4:B:306:LYS:HB2	1.89	0.70
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.57	0.70
1:0:285:A:H2'	1:0:286:U:O4'	1.90	0.70
1:0:902:G:N7	14:L:18:HIS:HD2	1.90	0.70
1:0:1120:U:H6	1:0:1120:U:H5'	1.55	0.70
1:0:2850:C:H6	1:0:2850:C:H5'	1.56	0.70
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.72	0.70
26:X:78:GLU:HG2	26:X:79:GLU:H	1.55	0.70
4:B:332:ASN:HB3	37:B:8861:HOH:O	1.91	0.70
1:0:447:A:P	22:T:1:SER:HB2	2.32	0.70
1:0:2506:A:O2'	1:0:2507:G:H8	1.73	0.70
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.74	0.70
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.57	0.70
18:P:115:SER:O	18:P:117:SER:N	2.23	0.70
1:0:1205:U:H2'	1:0:1206:U:C5'	2.21	0.70
1:0:1679:C:H5'	37:0:9135:HOH:O	1.90	0.70
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.74	0.70
22:T:48:VAL:HG13	22:T:97:ARG:O	1.92	0.70
2:9:73:A:H61	2:9:108:C:H42	1.39	0.70
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.38	0.70
1:0:1596:U:H2'	1:0:1598:A:OP2	1.92	0.70
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.27	0.70
1:0:88:G:H8	1:0:88:G:H5'	1.55	0.69
1:0:1118:A:H2'	1:0:1120:U:H5"	1.75	0.69
1:0:2291:A:C8	1:0:2309:C:H5'	2.26	0.69
4:B:36:PRO:HG3	4:B:169:GLY:H	1.56	0.69
12:J:19:MET:CE	12:J:132:LEU:HD11	2.22	0.69
1:0:1926:G:H2'	1:0:1927:A:C8	2.26	0.69
37:0:6135:HOH:O	4:B:298:LYS:HD3	1.91	0.69
2:9:56:A:C2'	2:9:57:A:H5"	2.21	0.69
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.22	0.69
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.74	0.69
7:E:6:GLU:HA	7:E:46:THR:HG22	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.21	0.69
1:0:2491:G:H1'	37:0:6645:HOH:O	1.92	0.69
9:G:64:ASN:H	9:G:64:ASN:ND2	1.91	0.69
16:N:152:GLU:C	16:N:154:LEU:H	1.92	0.69
17:O:32:ARG:HH21	17:O:35:LYS:CD	2.05	0.69
21:S:81:ILE:HG12	37:S:8536:HOH:O	1.91	0.69
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.28	0.69
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.28	0.69
1:0:2363:G:O2'	19:Q:11:ARG:HG3	1.93	0.69
1:0:2559:C:H4'	37:0:7025:HOH:O	1.92	0.69
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.07	0.69
15:M:46:LEU:HG	37:M:8919:HOH:O	1.92	0.69
22:T:28:SER:O	22:T:32:ARG:HG3	1.91	0.69
24:V:5:VAL:HG23	37:V:2271:HOH:O	1.93	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.75	0.69
1:0:839:C:H4'	1:0:840[A]:U:H5'	1.73	0.69
1:0:1119:G:N2	1:0:1246:A:C2	2.60	0.69
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.27	0.69
21:S:33:SER:OG	21:S:36:GLU:HG3	1.92	0.69
29:1:42:SER:HB2	37:1:354:HOH:O	1.92	0.69
1:0:839:C:H5"	1:0:840[B]:U:OP1	1.93	0.69
1:0:1130:U:H5'	37:0:7441:HOH:O	1.91	0.69
1:0:1589:G:N2	1:0:1605:G:H1'	2.07	0.69
2:9:35:C:H5"	37:9:8659:HOH:O	1.91	0.69
1:0:1180:U:H4'	11:I:86:GLU:HG2	1.74	0.69
24:V:12:THR:HG23	24:V:14:ALA:H	1.57	0.69
25:W:13:MET:HE1	25:W:18:GLN:HA	1.73	0.69
2:9:56:A:C3'	2:9:57:A:H5"	2.23	0.68
3:A:36:ASP:HB2	3:A:84:VAL:N	2.09	0.68
4:B:119:HIS:O	4:B:121:PRO:HD3	1.93	0.68
37:0:4504:HOH:O	28:Z:51:GLY:HA3	1.93	0.68
15:M:80:GLY:O	15:M:81:ARG:HD2	1.94	0.68
27:Y:133:HIS:HD2	37:Y:8886:HOH:O	1.76	0.68
1:0:1666:C:H2'	1:0:1667:A:H8	1.59	0.68
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.75	0.68
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.09	0.68
9:G:63:ARG:N	37:G:2569:HOH:O	2.26	0.68
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.57	0.68
25:W:39:ASP:HB2	37:W:3580:HOH:O	1.93	0.68
1:0:2392:C:H4'	37:Q:2875:HOH:O	1.91	0.68
12:J:52:GLN:HG3	12:J:53:ILE:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.75	0.68
1:0:1429:U:H1'	20:R:132:ARG:NH1	2.09	0.68
21:S:33:SER:O	21:S:37:VAL:HG23	1.94	0.68
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.76	0.68
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.75	0.68
1:0:1187:U:O2'	1:0:1189:A:H2	1.75	0.68
1:0:2502:C:C2'	1:0:2503:A:H5'	2.22	0.68
4:B:152:PRO:HD2	37:B:8931:HOH:O	1.92	0.68
10:H:12:ILE:HD12	10:H:57:THR:HG22	1.76	0.68
20:R:62:HIS:NE2	37:R:8831:HOH:O	2.26	0.68
1:0:2570:G:H5"	37:0:4714:HOH:O	1.93	0.67
2:9:6:C:H5"	16:N:37:ARG:HH12	1.57	0.67
27:Y:212:ARG:HD2	37:Y:8909:HOH:O	1.94	0.67
1:0:1741:U:H5'	1:0:1742:A:OP1	1.94	0.67
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.75	0.67
6:D:63:ILE:HG13	6:D:64:ARG:N	2.08	0.67
11:I:68:PRO:HB2	11:I:69:PRO:HD2	1.76	0.67
14:L:104:ASP:O	14:L:105:TYR:HB3	1.93	0.67
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.75	0.67
17:O:44:ASN:OD1	17:O:65:LEU:HB2	1.93	0.67
22:T:43:ASN:HD22	22:T:108:ARG:CZ	2.07	0.67
31:3:65:THR:HG22	31:3:67:LEU:HG	1.76	0.67
4:B:198:GLU:HA	37:B:8958:HOH:O	1.93	0.67
4:B:297:VAL:HB	37:B:8905:HOH:O	1.94	0.67
5:C:154:VAL:O	5:C:158:GLU:HG3	1.95	0.67
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.60	0.67
1:0:583:C:H2'	1:0:584:U:H6	1.60	0.67
1:0:870:G:C2'	1:0:871:G:H5"	2.23	0.67
17:O:49:GLU:OE1	17:O:72:LYS:HG3	1.94	0.67
26:X:43:VAL:HG12	26:X:44:ASP:N	2.08	0.67
4:B:84:LEU:HD23	4:B:178:ALA:HB1	1.77	0.67
12:J:74:ARG:O	12:J:78:ILE:HG12	1.95	0.67
15:M:28:GLN:O	15:M:32:ARG:HG3	1.94	0.67
1:0:1636:G:O2'	1:0:1637:A:H5'	1.94	0.67
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.76	0.67
24:V:64:GLY:O	24:V:65:ASP:HB2	1.94	0.67
3:A:5:GLN:HB3	37:A:8894:HOH:O	1.94	0.67
8:F:27:GLY:HA3	8:F:101:ALA:O	1.95	0.67
1:0:814:G:H4'	37:0:9934:HOH:O	1.95	0.67
1:0:2346:C:O2'	6:D:52:THR:HG21	1.95	0.67
1:0:2526:C:O2'	1:0:2527:U:H5'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:16:VAL:HG12	5:C:17:ASP:N	2.10	0.67
14:L:148:GLU:HA	37:L:8876:HOH:O	1.95	0.67
1:0:840[B]:U:H5'	37:0:4709:HOH:O	1.95	0.67
1:0:1419:U:H2'	1:0:1685:A:C2	2.30	0.67
2:9:14:G:H5'	2:9:14:G:C8	2.28	0.67
17:O:87:THR:O	17:O:91:GLN:HG3	1.95	0.67
1:0:136:C:H2'	1:0:137:U:O4'	1.94	0.66
1:0:308:U:H5'	1:0:309:C:OP1	1.94	0.66
1:0:2637:A:H5'	37:0:9086:HOH:O	1.94	0.66
4:B:86:ALA:HA	37:B:8880:HOH:O	1.94	0.66
8:F:79:GLN:HB2	8:F:82:ASP:OD2	1.96	0.66
20:R:39:THR:HB	20:R:42:GLU:HG3	1.76	0.66
1:0:1043:C:H2'	37:0:7091:HOH:O	1.94	0.66
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.24	0.66
1:0:1964:U:H2'	1:0:1964:U:O2	1.94	0.66
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.30	0.66
11:I:111:LEU:HD22	11:I:122:GLU:OE1	1.95	0.66
2:9:64:C:H2'	2:9:65:A:H5'	1.78	0.66
10:H:59:GLN:HE21	10:H:129:ARG:NE	1.91	0.66
1:0:21:G:H4'	20:R:2:ILE:HG22	1.78	0.66
1:0:1181:A:H2'	1:0:1182:C:H5'	1.76	0.66
7:E:11:VAL:HG12	7:E:12:ASP:N	2.10	0.66
10:H:26:ILE:HA	10:H:123:ILE:HG21	1.77	0.66
11:I:94:ASP:OD1	11:I:133:THR:HB	1.96	0.66
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.78	0.66
16:N:154:LEU:O	16:N:155:GLU:HB3	1.95	0.66
25:W:38:THR:HG22	25:W:39:ASP:N	2.09	0.66
1:0:1926:G:H2'	1:0:1927:A:H8	1.60	0.66
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.31	0.66
10:H:43:ALA:O	10:H:170:ARG:NH1	2.28	0.66
13:K:22:ASP:HB2	37:K:5264:HOH:O	1.96	0.66
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.77	0.66
1:0:1589:G:H22	1:0:1605:G:H1'	1.60	0.66
4:B:98:THR:HG22	4:B:99:GLU:N	2.10	0.66
15:M:164:THR:HG23	15:M:167:GLY:N	2.10	0.66
19:Q:26:PRO:O	19:Q:30:VAL:HG23	1.95	0.66
23:U:17:THR:HG22	23:U:18:GLY:N	2.10	0.66
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.26	0.66
30:2:40:ARG:CD	30:2:47:THR:HG22	2.24	0.66
3:A:88:ILE:O	3:A:88:ILE:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:76:ARG:HH11	5:C:76:ARG:CB	2.08	0.66
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.76	0.66
18:P:143:ALA:HA	37:P:193:HOH:O	1.95	0.66
1:0:1362:U:H5'	37:0:3068:HOH:O	1.96	0.66
10:H:12:ILE:O	10:H:12:ILE:HG22	1.96	0.66
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.59	0.66
23:U:52:THR:HG22	23:U:54:THR:H	1.60	0.66
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.78	0.66
1:0:338:C:H4'	5:C:174:ILE:CD1	2.26	0.65
1:0:657:G:H2'	1:0:658:C:H6	1.61	0.65
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.78	0.65
1:0:111:C:O2'	29:1:20:ARG:HG2	1.96	0.65
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.65
1:0:1116:U:O2'	1:0:1118:A:H2	1.80	0.65
1:0:1319:G:H1'	37:0:4492:HOH:O	1.95	0.65
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.79	0.65
1:0:2053:G:H4'	20:R:136:TRP:CE3	2.31	0.65
1:0:2301:A:H5"	1:0:2302:A:H5'	1.78	0.65
15:M:65:VAL:HG21	15:M:105:ALA:HB2	1.78	0.65
1:0:1790:C:H2'	1:0:1791:U:H6	1.60	0.65
1:0:1909:A:H2'	1:0:1910:A:C8	2.31	0.65
3:A:81:GLN:HB2	3:A:92:ASN:HD21	1.62	0.65
5:C:236:THR:H	5:C:239:ALA:HB3	1.61	0.65
16:N:4:PRO:HD2	37:N:8854:HOH:O	1.94	0.65
6:D:21:VAL:HG13	6:D:132:VAL:HG22	1.76	0.65
6:D:166:ILE:HB	37:D:6326:HOH:O	1.96	0.65
24:V:27:LEU:HA	24:V:49:LEU:HD13	1.79	0.65
1:0:2504:A:H4'	10:H:74:ARG:HH11	1.61	0.65
5:C:246:ARG:HB3	5:C:246:ARG:HH11	1.59	0.65
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.06	0.65
16:N:166:ALA:HA	37:N:8824:HOH:O	1.95	0.65
1:0:450:C:OP1	5:C:184:ARG:NH2	2.30	0.65
16:N:37:ARG:HD3	35:N:8807:CL:CL	2.33	0.65
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.77	0.65
20:R:72:VAL:HG11	20:R:75:TRP:HB3	1.78	0.65
1:0:1525:G:H2'	1:0:1526:A:C8	2.32	0.65
1:0:1657:A:H2'	1:0:1658:A:C8	2.32	0.65
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.79	0.65
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.78	0.65
17:O:73:ASP:HA	17:O:92:VAL:O	1.97	0.65
1:0:657:G:H2'	1:0:658:C:C6	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:17:ARG:HG2	6:D:135:VAL:O	1.97	0.65
1:0:285:A:C2	1:0:368:C:H4'	2.31	0.65
1:0:1701:A:H4'	1:0:1702:U:H5"	1.79	0.65
3:A:200:PRO:HD3	37:A:8818:HOH:O	1.95	0.65
1:0:157:G:H4'	15:M:95:LYS:HE3	1.77	0.64
1:0:199:A:H5"	37:0:3331:HOH:O	1.97	0.64
1:0:246:G:H5'	37:0:5368:HOH:O	1.97	0.64
2:9:54:A:O2'	2:9:55:U:H5'	1.96	0.64
7:E:138:ILE:HG22	37:E:6457:HOH:O	1.96	0.64
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.12	0.64
14:L:114:VAL:HG11	37:L:8877:HOH:O	1.96	0.64
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.97	0.64
1:0:20:G:H21	20:R:117:HIS:HD2	1.44	0.64
1:0:1428:C:O2'	20:R:132:ARG:HB2	1.96	0.64
1:0:2272:G:H5'	3:A:223:ARG:HB2	1.77	0.64
1:0:2679:G:H2'	1:0:2681:A:OP2	1.97	0.64
4:B:51:VAL:CG1	4:B:53:LEU:HD13	2.26	0.64
9:G:16:LYS:O	9:G:20:VAL:HG23	1.98	0.64
25:W:52:VAL:HG22	25:W:53:ALA:H	1.61	0.64
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.79	0.64
10:H:174:LEU:HA	37:H:225:HOH:O	1.97	0.64
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.79	0.64
1:0:544:G:C2'	1:0:545:G:H5"	2.28	0.64
1:0:1377:C:H5'	1:0:1377:C:H6	1.63	0.64
3:A:94:LEU:HD23	3:A:94:LEU:N	2.12	0.64
12:J:126:ASN:HA	35:J:8801:CL:CL	2.35	0.64
14:L:143:THR:HG22	14:L:145:LEU:H	1.61	0.64
5:C:107:ARG:NE	37:C:8666:HOH:O	2.29	0.64
1:0:447:A:OP1	22:T:2:LYS:HG2	1.98	0.64
1:0:1687:C:O2	29:1:9:GLY:HA2	1.97	0.64
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.13	0.64
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.28	0.64
4:B:62:ARG:HA	4:B:65:MET:HE3	1.80	0.64
4:B:83:ALA:HA	4:B:100:VAL:O	1.96	0.64
11:I:118:ASN:HA	11:I:121:LYS:CD	2.27	0.64
15:M:134:ILE:O	15:M:136:PRO:HD3	1.98	0.64
24:V:33:VAL:HG12	24:V:38:GLY:HA3	1.78	0.64
25:W:110:GLN:HA	25:W:110:GLN:HE21	1.62	0.64
26:X:20:GLU:OE1	26:X:21:PRO:HD2	1.97	0.64
1:0:1181:A:H5'	11:I:89:GLU:OE2	1.97	0.64
11:I:80:PHE:CD2	11:I:92:VAL:HG12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.79	0.64
3:A:33:GLU:O	3:A:34:ASP:HB2	1.95	0.64
4:B:162:MET:CE	4:B:308:LEU:HD21	2.27	0.64
5:C:14:GLY:O	5:C:15:GLU:HB3	1.97	0.64
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.80	0.64
20:R:40:ALA:O	20:R:44:VAL:HG23	1.98	0.64
25:W:59:GLN:HE22	25:W:97:ALA:HB3	1.63	0.64
25:W:110:GLN:HA	25:W:110:GLN:NE2	2.13	0.64
1:0:621:C:H5'	27:Y:132:ASP:OD2	1.98	0.63
1:0:1804:A:H2'	1:0:1805:G:C8	2.33	0.63
2:9:1:U:H4'	2:9:3:A:OP1	1.99	0.63
19:Q:66:LYS:HB2	19:Q:70:ALA:O	1.98	0.63
37:0:6147:HOH:O	20:R:33:ARG:HG3	1.97	0.63
3:A:36:ASP:HB2	3:A:85:SER:H	1.63	0.63
20:R:53:GLY:HA2	20:R:80:TYR:CD2	2.33	0.63
29:1:25:LYS:O	29:1:25:LYS:HG2	1.97	0.63
1:0:1804:A:H2'	1:0:1805:G:H8	1.63	0.63
6:D:63:ILE:HG13	6:D:64:ARG:H	1.60	0.63
16:N:165:ALA:HA	37:N:8821:HOH:O	1.96	0.63
25:W:60:GLU:HG2	37:W:705:HOH:O	1.98	0.63
28:Z:56:GLN:HG3	28:Z:62:TYR:O	1.98	0.63
1:0:56:G:H5"	24:V:50:ARG:NH1	2.11	0.63
1:0:1116:U:HO2'	1:0:1118:A:H2	1.44	0.63
25:W:52:VAL:HG22	25:W:53:ALA:N	2.13	0.63
1:0:653:U:H5"	37:O:7674:HOH:O	1.96	0.63
1:0:2073:G:OP2	1:0:2490:A:H5'	1.99	0.63
1:0:2681:A:H4'	1:0:2682:C:H5'	1.80	0.63
10:H:49:GLN:HB3	10:H:170:ARG:CG	2.29	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.80	0.63
1:0:1506:U:H6	1:0:1506:U:H5'	1.64	0.63
1:0:2827:A:H2'	1:0:2828:G:O4'	1.99	0.63
9:G:71:LEU:C	9:G:73:ASP:H	2.00	0.63
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.33	0.63
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.99	0.63
1:0:1603:A:H5'	1:0:1605:G:O4'	1.99	0.63
4:B:24:PRO:O	4:B:25:ARG:HD3	1.98	0.63
4:B:66:GLU:OE1	4:B:328:ARG:HD2	1.98	0.63
29:1:1:THR:HB	37:1:6858:HOH:O	1.99	0.63
1:0:584:U:H3'	37:0:5879:HOH:O	1.98	0.63
1:0:753:U:H3'	37:0:5320:HOH:O	1.99	0.63
1:0:1168:C:H5'	11:I:83:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.81	0.63
5:C:237:GLU:HB2	37:C:8640:HOH:O	1.97	0.63
14:L:140:VAL:HG23	37:L:8860:HOH:O	1.97	0.63
20:R:99:ALA:HB1	20:R:109:MET:HE2	1.80	0.63
22:T:99:THR:O	22:T:100:ASP:HB2	1.98	0.63
1:0:69:A:H5'	1:0:69:A:H8	1.64	0.62
1:0:1197:G:H21	1:0:1202:A:H62	1.44	0.62
1:0:69:A:H5'	1:0:69:A:C8	2.34	0.62
1:0:800:G:H4'	37:0:6831:HOH:O	1.98	0.62
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.26	0.62
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.27	0.62
1:0:1118:A:C8	1:0:1118:A:C3'	2.78	0.62
1:0:2459:G:H3'	37:0:6782:HOH:O	1.97	0.62
2:9:48:C:H4'	16:N:141:ARG:HH21	1.64	0.62
7:E:166:VAL:HG12	37:E:3134:HOH:O	1.98	0.62
14:L:90:ARG:HA	14:L:119:THR:HB	1.81	0.62
1:0:1221:G:H8	37:0:5773:HOH:O	1.82	0.62
1:0:1632:A:H2'	1:0:1633:C:H5'	1.82	0.62
5:C:3:ALA:HA	37:C:8581:HOH:O	1.98	0.62
7:E:37:ASP:OD1	12:J:125:SER:HB3	1.99	0.62
1:0:694:A:H2'	1:0:695:C:H5'	1.81	0.62
1:0:944:G:H21	25:W:44:MET:HE2	1.63	0.62
14:L:133:VAL:HB	37:L:8860:HOH:O	1.98	0.62
1:0:2256:G:O2'	1:0:2257:G:H5'	2.00	0.62
1:0:2332:A:H5'	6:D:56:ARG:NH2	2.15	0.62
3:A:43:VAL:O	3:A:76:VAL:HG13	2.00	0.62
8:F:21:GLU:HA	8:F:24:ARG:HD3	1.81	0.62
30:2:49:GLU:HB2	37:2:719:HOH:O	1.98	0.62
1:0:969:G:H1	1:0:999:C:N4	1.97	0.62
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.63	0.62
12:J:6:PHE:HB3	12:J:109:TYR:OH	1.99	0.62
13:K:55:VAL:HG12	13:K:56:SER:N	2.15	0.62
21:S:45:TYR:HE2	21:S:81:ILE:HD13	1.65	0.62
22:T:71:VAL:HG13	22:T:91:LEU:O	2.00	0.62
1:0:1285:U:H4'	25:W:74:GLU:OE1	2.00	0.62
29:1:25:LYS:CD	30:2:49:GLU:H	2.03	0.62
1:0:684:G:H5"	37:0:3862:HOH:O	1.99	0.62
1:0:1279:U:O2	1:0:1279:U:H2'	2.00	0.62
6:D:159:PRO:O	6:D:163:VAL:HG23	1.99	0.62
1:0:1528:A:H2'	1:0:1529:G:O4'	1.99	0.62
1:0:2346:C:H6	1:0:2346:C:O5'	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.82	0.62
8:F:107:ASP:O	8:F:111:ILE:HG13	2.00	0.62
16:N:128:ASP:HA	37:N:8858:HOH:O	2.00	0.62
23:U:9:CYS:HA	23:U:52:THR:CG2	2.30	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.35	0.61
1:0:2897:C:H2'	1:0:2898:G:H8	1.65	0.61
3:A:194:MET:CE	3:A:199:HIS:HB2	2.29	0.61
4:B:225:GLY:HA3	37:B:8866:HOH:O	1.99	0.61
7:E:93:MET:O	7:E:94:GLN:HG3	1.99	0.61
17:O:32:ARG:HB2	37:O:4656:HOH:O	1.98	0.61
4:B:149:ASP:HB2	37:B:8881:HOH:O	2.00	0.61
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.82	0.61
8:F:38:LYS:NZ	15:M:3:SER:HA	2.14	0.61
13:K:101:ASN:HA	37:K:6456:HOH:O	2.00	0.61
22:T:26:THR:HA	22:T:39:ASN:HB3	1.81	0.61
1:0:154:C:H2'	1:0:155:C:C6	2.33	0.61
37:0:6651:HOH:O	15:M:178:LYS:HB2	2.01	0.61
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.29	0.61
25:W:73:LEU:O	25:W:74:GLU:HG3	2.01	0.61
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.15	0.61
1:0:1159:G:H21	1:0:1189:A:H8	1.48	0.61
1:0:1164:U:H3	1:0:1192:A:H2	1.48	0.61
1:0:1688:G:H4'	29:1:8:GLN:HG3	1.83	0.61
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.82	0.61
4:B:51:VAL:HG22	4:B:330:VAL:HG22	1.81	0.61
4:B:54:VAL:HB	37:B:8913:HOH:O	2.00	0.61
14:L:136:ALA:HB3	37:L:8877:HOH:O	1.99	0.61
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.81	0.61
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.30	0.61
1:0:1008:C:H5"	10:H:19:ARG:HH12	1.65	0.61
1:0:2488:A:H61	1:0:2534:C:H42	1.48	0.61
3:A:211:LYS:HB2	37:A:8914:HOH:O	2.00	0.61
14:L:133:VAL:HA	37:L:8877:HOH:O	2.00	0.61
4:B:313:PRO:HA	37:B:8896:HOH:O	2.01	0.61
7:E:132:THR:HB	37:E:2227:HOH:O	2.00	0.61
10:H:30:LYS:H	10:H:62:HIS:CD2	2.18	0.61
10:H:88:MET:HA	10:H:139:ALA:HA	1.83	0.61
11:I:127:CYS:C	11:I:129:SER:H	2.03	0.61
25:W:125:HIS:HD2	25:W:127:GLY:H	1.47	0.61
1:0:290:C:H2'	1:0:291:C:H6	1.64	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2895:C:H2'	37:0:9379:HOH:O	2.00	0.61
37:0:3868:HOH:O	15:M:97:ILE:HB	2.00	0.61
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.29	0.61
7:E:118:ILE:HG23	7:E:144:THR:HG21	1.82	0.61
2:9:34:A:H2'	2:9:35:C:O4'	2.00	0.61
6:D:146:LYS:HE2	16:N:107:ASN:ND2	2.16	0.61
1:0:447:A:OP2	22:T:1:SER:HB2	2.00	0.61
1:0:856:G:H2'	37:0:5225:HOH:O	2.00	0.61
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.83	0.61
4:B:129:ARG:O	4:B:133:GLU:HG3	2.00	0.61
23:U:9:CYS:CA	23:U:52:THR:HG23	2.29	0.61
26:X:31:ILE:O	26:X:35:GLU:HG3	1.99	0.61
6:D:55:LYS:O	6:D:56:ARG:HB2	2.01	0.60
13:K:49:LEU:HD21	13:K:74:VAL:O	2.00	0.60
16:N:110:THR:HG22	37:N:8848:HOH:O	2.01	0.60
16:N:43:VAL:O	16:N:84:THR:HG21	2.01	0.60
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.66	0.60
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.16	0.60
1:0:1422:U:H2'	1:0:1423:C:C6	2.37	0.60
1:0:1691:A:H5"	37:0:9946:HOH:O	2.01	0.60
1:0:2421:G:H3'	1:0:2422:U:H5"	1.83	0.60
1:0:2502:C:H2'	1:0:2503:A:H5'	1.83	0.60
16:N:149:GLU:HA	16:N:152:GLU:HB2	1.83	0.60
21:S:73:ASP:O	21:S:77:VAL:HG23	2.01	0.60
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.35	0.60
1:0:2094:G:H4'	4:B:245:SER:HB3	1.82	0.60
3:A:105:VAL:HG13	3:A:155:THR:O	2.02	0.60
4:B:162:MET:HG3	4:B:310:ARG:CD	2.29	0.60
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.65	0.60
19:Q:28:ARG:HG2	37:Q:4350:HOH:O	2.00	0.60
1:0:506:G:H5'	37:0:5722:HOH:O	2.00	0.60
1:0:714:U:H3'	37:0:6721:HOH:O	2.00	0.60
1:0:2690:U:O2'	7:E:111:LYS:HE3	2.01	0.60
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.84	0.60
7:E:172:PRO:HB3	37:E:6931:HOH:O	2.02	0.60
12:J:133:GLY:O	12:J:137:GLU:HG3	2.01	0.60
14:L:134:GLU:HG3	37:L:8860:HOH:O	2.01	0.60
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.01	0.60
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.67	0.60
1:0:545:G:H5'	1:0:545:G:C8	2.34	0.60
1:0:1311:G:O6	5:C:173:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:140:LEU:HA	37:B:8880:HOH:O	2.01	0.60
4:B:279:THR:OG1	4:B:290:VAL:HB	2.01	0.60
7:E:7:ILE:HD11	7:E:11:VAL:C	2.22	0.60
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.31	0.60
10:H:66:GLU:HA	37:H:235:HOH:O	2.01	0.60
2:9:114:G:O6	16:N:11:ARG:HD3	2.01	0.60
5:C:20:ASP:HB2	37:C:8601:HOH:O	2.00	0.60
6:D:40:ILE:O	6:D:44:ILE:HG22	2.02	0.60
7:E:125:GLU:HB2	7:E:132:THR:CG2	2.30	0.60
1:0:709:G:O2'	17:O:25:VAL:HG12	2.02	0.60
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.16	0.60
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.83	0.60
8:F:56:PRO:CG	15:M:44:THR:HA	2.31	0.60
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.83	0.60
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.60
29:1:28:HIS:HD2	29:1:30:LYS:H	1.49	0.60
1:0:1803:C:H2'	1:0:1804:A:C8	2.36	0.60
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.37	0.60
4:B:132:HIS:HB2	4:B:137:LEU:CD2	2.32	0.60
6:D:25:MET:CE	6:D:41:LEU:HG	2.31	0.60
16:N:154:LEU:HD12	16:N:156:GLU:O	2.01	0.60
1:0:354:A:H2'	1:0:355:C:C6	2.36	0.59
1:0:1523:G:H2'	1:0:1524:U:O4'	2.02	0.59
1:0:1878:G:H1'	37:0:5905:HOH:O	2.02	0.59
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.84	0.59
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.37	0.59
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.02	0.59
29:1:28:HIS:O	29:1:32:LYS:N	2.35	0.59
1:0:1213:C:O2'	1:0:1214:G:H5'	2.01	0.59
1:0:1535:G:H2'	1:0:1536:C:C6	2.37	0.59
4:B:55:ASN:ND2	4:B:67:GLU:OE2	2.35	0.59
8:F:100:ASP:HB3	37:F:5691:HOH:O	2.01	0.59
12:J:52:GLN:HG3	12:J:53:ILE:H	1.65	0.59
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.83	0.59
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.50	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
1:0:1189:A:H1'	1:0:1209:C:O4'	2.02	0.59
11:I:120:ALA:O	11:I:124:VAL:HG23	2.02	0.59
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.17	0.59
14:L:94:ARG:HA	14:L:106:VAL:HG21	1.84	0.59
15:M:60:VAL:C	15:M:61:ILE:HD12	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.67	0.59
25:W:151:GLU:O	25:W:154:ARG:HB3	2.02	0.59
1:0:2719:A:C2	4:B:70:PRO:HG3	2.37	0.59
1:0:2769:C:O2'	1:0:2770:G:H5'	2.03	0.59
2:9:38:A:H2'	2:9:39:U:C6	2.37	0.59
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.03	0.59
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.17	0.59
1:0:1342:C:C2'	1:0:1343:C:H5'	2.32	0.59
4:B:307:ARG:HH11	4:B:307:ARG:HB2	1.66	0.59
13:K:37:TYR:HB3	37:K:7169:HOH:O	2.02	0.59
28:Z:46:ARG:CD	28:Z:59:TYR:HB2	2.29	0.59
1:0:671:A:O2'	1:0:672:G:H2'	2.01	0.59
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.85	0.59
11:I:108:HIS:N	11:I:109:PRO:HD2	2.17	0.59
16:N:113:SER:HB2	37:N:8856:HOH:O	2.01	0.59
22:T:24:ARG:HG2	22:T:24:ARG:HH11	1.66	0.59
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.85	0.59
27:Y:130:ARG:HB2	27:Y:142:SER:O	2.01	0.59
1:0:87:C:H2'	30:2:28:LYS:O	2.02	0.59
1:0:2740:G:H2'	1:0:2741:A:O4'	2.03	0.59
4:B:85:ARG:NH1	37:B:8935:HOH:O	2.36	0.59
17:O:88:LYS:HB3	37:O:7061:HOH:O	2.01	0.59
22:T:87:VAL:HB	37:T:5545:HOH:O	2.03	0.59
1:0:871:G:C8	1:0:871:G:C5'	2.76	0.59
1:0:1189:A:H3'	37:0:7449:HOH:O	2.03	0.59
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.03	0.59
2:9:13:A:O2'	2:9:14:G:H5"	2.02	0.59
6:D:101:THR:O	6:D:101:THR:HG22	2.03	0.59
12:J:39:VAL:HG12	12:J:40:ASN:CG	2.23	0.59
13:K:113:ILE:HD12	13:K:128:ALA:HB2	1.83	0.59
24:V:13:PRO:O	24:V:17:GLU:HG3	2.02	0.59
1:0:837:U:H4'	37:0:3192:HOH:O	2.02	0.59
5:C:170:ASP:O	5:C:171:GLU:HG3	2.03	0.59
6:D:50:VAL:O	6:D:71:ALA:HA	2.03	0.59
25:W:65:VAL:HA	25:W:68:THR:HG22	1.83	0.59
1:0:711:G:H1'	37:0:6868:HOH:O	2.03	0.59
6:D:86:THR:C	6:D:89:PRO:HD2	2.22	0.59
10:H:49:GLN:HB3	10:H:170:ARG:HG3	1.84	0.59
12:J:90:LYS:HB2	35:J:8802:CL:CL	2.39	0.59
13:K:65:ARG:HD3	37:K:5358:HOH:O	2.02	0.59
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:H4'	1.83	0.58
1:0:1874:U:OP1	3:A:51:ARG:HD2	2.03	0.58
1:0:2716:G:H5"	4:B:206:THR:HG21	1.85	0.58
3:A:134:ASN:O	3:A:150:PRO:HD3	2.02	0.58
14:L:143:THR:HG22	14:L:144:ASP:N	2.18	0.58
1:0:1537:C:H1'	37:0:6368:HOH:O	2.02	0.58
1:0:1666:C:H2'	1:0:1667:A:C8	2.37	0.58
1:0:2880:A:H2'	1:0:2881:C:H5'	1.85	0.58
4:B:267:LYS:HE3	4:B:300:SER:O	2.03	0.58
5:C:3:ALA:O	5:C:15:GLU:HB2	2.03	0.58
10:H:57:THR:HG23	10:H:131:GLN:HA	1.85	0.58
17:O:105:ASN:ND2	17:O:109:SER:H	2.00	0.58
20:R:39:THR:HG23	20:R:107:GLU:O	2.02	0.58
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.18	0.58
1:0:80:A:H3'	22:T:43:ASN:OD1	2.02	0.58
2:9:64:C:C2'	2:9:65:A:H5'	2.34	0.58
4:B:51:VAL:HG12	4:B:53:LEU:HD13	1.83	0.58
7:E:10:ASP:HA	37:E:6017:HOH:O	2.03	0.58
15:M:164:THR:CG2	15:M:167:GLY:H	2.10	0.58
16:N:163:PHE:O	16:N:164:ASP:O	2.20	0.58
25:W:7:LEU:HD12	25:W:53:ALA:HB2	1.85	0.58
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.02	0.58
30:2:48:ASP:O	30:2:49:GLU:HB2	2.02	0.58
1:0:1500:U:P	18:P:41:ARG:HH22	2.26	0.58
1:0:1735:C:OP2	4:B:234:ARG:HG3	2.03	0.58
1:0:1778:A:H2'	1:0:1779:A:H5'	1.84	0.58
1:0:1850:U:H2'	1:0:1851:G:H8	1.68	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.04	0.58
37:0:9986:HOH:O	15:M:9:ARG:HG3	2.04	0.58
3:A:199:HIS:CD2	3:A:201:PHE:H	2.21	0.58
5:C:133:ARG:HE	5:C:138:VAL:HG22	1.69	0.58
25:W:1:MET:H2	25:W:37:GLU:HG3	1.68	0.58
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.02	0.58
37:0:3784:HOH:O	22:T:82:THR:HA	2.02	0.58
4:B:264:GLU:CG	4:B:267:LYS:HE2	2.24	0.58
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.86	0.58
8:F:28:ALA:CB	8:F:99:THR:HG23	2.34	0.58
8:F:56:PRO:HG2	15:M:44:THR:HA	1.85	0.58
10:H:42:ASP:HB2	10:H:45:ASP:OD1	2.04	0.58
1:0:1641:A:H2'	1:0:1642:A:H5'	1.84	0.58
1:0:2053:G:OP1	20:R:138:SER:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:275:GLY:O	4:B:291:ASP:HA	2.03	0.58
4:B:329:TYR:HE2	23:U:15:PRO:HG2	1.69	0.58
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.86	0.58
7:E:125:GLU:HB2	7:E:132:THR:HG23	1.86	0.58
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.36	0.58
17:O:78:ALA:O	17:O:98:LEU:HD13	2.04	0.58
22:T:48:VAL:HG13	22:T:97:ARG:C	2.23	0.58
3:A:8:ARG:HG2	37:A:8849:HOH:O	2.02	0.58
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.04	0.58
10:H:44:ASP:HA	10:H:170:ARG:HH12	1.68	0.58
1:0:419:A:H1'	1:0:1921:A:C2	2.38	0.58
1:0:1060:C:H6	1:0:1060:C:H5'	1.69	0.58
1:0:1183:C:N4	1:0:1184:C:H41	2.02	0.58
1:0:2524:G:H21	1:0:2526:C:H41	1.52	0.58
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.04	0.58
11:I:118:ASN:HA	11:I:121:LYS:HD2	1.85	0.58
15:M:57:LYS:NZ	15:M:144:ASP:HB2	2.19	0.58
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.04	0.58
1:0:841:A:P	37:0:6689:HOH:O	2.61	0.58
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.58
5:C:2:GLN:HA	5:C:17:ASP:HA	1.86	0.58
1:0:214:U:H5'	37:0:5924:HOH:O	2.03	0.57
1:0:796:A:HO2'	28:Z:10:ARG:N	2.02	0.57
1:0:1624:A:H5'	1:0:1626:A:O4'	2.04	0.57
3:A:179:MET:HG2	3:A:186:TRP:CB	2.34	0.57
4:B:144:THR:HB	37:B:8925:HOH:O	2.04	0.57
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.87	0.57
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.34	0.57
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.52	0.57
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.38	0.57
1:0:282:C:H2'	1:0:283:U:O4'	2.05	0.57
1:0:960:G:H3'	1:0:960:G:N3	2.19	0.57
1:0:1561:U:H5'	37:0:7201:HOH:O	2.04	0.57
4:B:22:GLU:HG2	37:B:8851:HOH:O	2.04	0.57
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.04	0.57
4:B:62:ARG:HG2	4:B:65:MET:HE3	1.86	0.57
1:0:1015:C:H2'	1:0:1016:U:H6	1.70	0.57
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.86	0.57
1:0:2467:A:H2'	37:0:5254:HOH:O	2.03	0.57
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.87	0.57
8:F:19:ALA:O	8:F:22:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:27:LEU:HD22	16:N:50:LEU:HD22	1.86	0.57
27:Y:115:ARG:NE	37:Y:8857:HOH:O	2.37	0.57
1:0:316:A:N3	1:0:336:G:O2'	2.36	0.57
1:0:1201:C:H2'	1:0:1202:A:H5'	1.87	0.57
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.85	0.57
23:U:14:GLU:O	23:U:17:THR:HB	2.05	0.57
1:0:657:G:OP1	5:C:27:ARG:NH2	2.37	0.57
2:9:48:C:H4'	16:N:141:ARG:NH2	2.18	0.57
20:R:125:ARG:HH12	20:R:134:SER:HB2	1.70	0.57
24:V:64:GLY:O	24:V:65:ASP:CB	2.53	0.57
26:X:25:ARG:NH1	37:X:3861:HOH:O	2.38	0.57
28:Z:46:ARG:O	28:Z:57:CYS:HA	2.05	0.57
1:0:232:A:H4'	37:0:5867:HOH:O	2.05	0.57
1:0:583:C:H2'	1:0:584:U:C6	2.40	0.57
1:0:585:C:H6	37:0:5879:HOH:O	1.88	0.57
1:0:2338:G:OP1	6:D:97:GLN:HG2	2.05	0.57
11:I:108:HIS:N	11:I:109:PRO:CD	2.67	0.57
12:J:19:MET:CE	12:J:132:LEU:HD21	2.34	0.57
1:0:263:U:C4	8:F:54:VAL:HG13	2.38	0.57
1:0:2751:C:H3'	37:0:7037:HOH:O	2.03	0.57
3:A:153:ARG:HD3	37:A:8826:HOH:O	2.05	0.57
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.30	0.57
4:B:27:ASN:HD22	4:B:27:ASN:H	1.51	0.57
10:H:29:SER:HA	10:H:62:HIS:HD2	1.70	0.57
30:2:39:ARG:HG2	37:2:3143:HOH:O	2.05	0.57
1:0:702:G:O2'	1:0:703:G:H5'	2.05	0.57
1:0:1164:U:C1'	1:0:1166:A:H5'	2.34	0.57
1:0:2344:G:H2'	1:0:2344:G:N3	2.19	0.57
1:0:2472:C:O2'	1:0:2634:G:H4'	2.04	0.57
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.70	0.57
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.05	0.57
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.05	0.57
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.03	0.57
17:O:32:ARG:NH2	17:O:35:LYS:HD2	2.20	0.57
24:V:42:ASN:HB3	37:V:7247:HOH:O	2.03	0.57
26:X:18:ARG:NH1	37:X:4132:HOH:O	2.37	0.57
1:0:732:C:H2'	1:0:733:U:H6	1.70	0.57
1:0:1751:G:C2'	1:0:1752:G:H5"	2.34	0.57
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.05	0.57
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.57
12:J:105:LEU:HD23	37:J:8866:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:170:GLU:HA	16:N:173:ASP:OD2	2.04	0.57
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.70	0.57
1:0:1508:C:H5'	21:S:21:GLN:NE2	2.20	0.57
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.57
8:F:22:VAL:HG23	8:F:104:ALA:HB2	1.87	0.57
24:V:49:LEU:O	24:V:53:ILE:HG13	2.04	0.57
1:0:120:A:H2'	1:0:120:A:N3	2.20	0.56
1:0:558:C:O2'	1:0:559:U:H5"	2.05	0.56
1:0:2737:C:OP2	18:P:61:ARG:NH2	2.37	0.56
37:0:3401:HOH:O	3:A:236:GLY:HA3	2.03	0.56
2:9:11:A:P	19:Q:19:ARG:HH21	2.28	0.56
2:9:69:U:OP1	16:N:4:PRO:HG3	2.04	0.56
6:D:36:ASN:HA	37:D:7500:HOH:O	2.05	0.56
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.87	0.56
7:E:84:MET:HG2	7:E:168:ILE:HD13	1.86	0.56
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.20	0.56
1:0:1333:U:H2'	1:0:1334:C:C6	2.41	0.56
1:0:1711:A:O2'	1:0:1712:A:H5'	2.05	0.56
1:0:2359:G:H3'	37:0:5484:HOH:O	2.05	0.56
6:D:21:VAL:HA	6:D:131:THR:O	2.05	0.56
6:D:54:ALA:HB2	6:D:69:ILE:CD1	2.30	0.56
10:H:49:GLN:NE2	10:H:140:TYR:HE2	2.00	0.56
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.71	0.56
14:L:149:ARG:O	14:L:150:GLN:CB	2.52	0.56
18:P:134:VAL:O	18:P:137:LEU:HB3	2.04	0.56
21:S:19:ASP:O	21:S:20:PHE:HD2	1.88	0.56
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.40	0.56
1:0:1164:U:O4'	1:0:1166:A:H5'	2.05	0.56
1:0:1834:C:H2'	1:0:1840:A:H62	1.67	0.56
1:0:1971:G:H2'	37:0:3091:HOH:O	2.04	0.56
3:A:101:GLU:O	3:A:103:VAL:HG23	2.06	0.56
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.39	0.56
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.87	0.56
8:F:48:VAL:HG23	8:F:74:PHE:HB3	1.86	0.56
12:J:74:ARG:HD3	37:J:8859:HOH:O	2.04	0.56
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.34	0.56
17:O:41:ALA:HA	37:O:5104:HOH:O	2.06	0.56
23:U:52:THR:HG22	23:U:54:THR:N	2.20	0.56
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.41	0.56
1:0:2715:G:N2	4:B:264:GLU:OE1	2.36	0.56
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.20	0.56
5:C:136:VAL:HA	5:C:137:PRO:C	2.25	0.56
10:H:69:ARG:HB3	37:H:235:HOH:O	2.05	0.56
11:I:80:PHE:HB2	11:I:93:ALA:HB2	1.88	0.56
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.36	0.56
12:J:107:ASN:C	12:J:107:ASN:HD22	2.08	0.56
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.87	0.56
1:0:1180:U:H2'	1:0:1181:A:C8	2.39	0.56
1:0:1701:A:H4'	1:0:1702:U:C5'	2.36	0.56
1:0:2816:A:H4'	37:0:3702:HOH:O	2.05	0.56
2:9:49:G:H5"	37:9:8671:HOH:O	2.04	0.56
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.18	0.56
4:B:294:TYR:HE2	37:B:8951:HOH:O	1.87	0.56
6:D:64:ARG:NE	6:D:67:ASP:HB3	2.20	0.56
8:F:57:GLU:HB2	15:M:23:LEU:HD11	1.88	0.56
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.19	0.56
15:M:99:ARG:HG2	37:M:8857:HOH:O	2.05	0.56
17:O:27:GLY:O	17:O:31:GLU:HG3	2.06	0.56
1:0:797:A:C4'	28:Z:10:ARG:N	2.68	0.56
1:0:922:A:N7	1:0:2281:C:H5'	2.21	0.56
2:9:44:A:O4'	6:D:76:ARG:NE	2.37	0.56
3:A:199:HIS:HD2	3:A:201:PHE:H	1.54	0.56
8:F:56:PRO:HG2	15:M:43:PRO:O	2.05	0.56
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.87	0.56
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.88	0.56
1:0:1477:C:H5'	1:0:1868:G:C5'	2.36	0.56
1:0:1504:A:H5"	37:0:5392:HOH:O	2.06	0.56
1:0:2661:U:H3	1:0:2812:A:H62	1.52	0.56
12:J:19:MET:HE2	12:J:79:PHE:HA	1.87	0.56
12:J:92:GLN:HB3	37:J:8829:HOH:O	2.06	0.56
20:R:125:ARG:HA	20:R:140:GLN:OE1	2.06	0.56
1:0:638:C:H2'	1:0:639:A:C8	2.41	0.56
1:0:820:G:C6	3:A:171:LYS:HB2	2.40	0.56
1:0:1299:G:O6	14:L:6:ARG:HD3	2.06	0.56
1:0:1702:U:H5'	37:0:3224:HOH:O	2.05	0.56
1:0:2256:G:C2'	1:0:2257:G:H5'	2.36	0.56
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.13	0.56
12:J:41:ALA:HB3	37:J:8866:HOH:O	2.05	0.56
14:L:115:ARG:O	14:L:116:HIS:ND1	2.39	0.56
17:O:32:ARG:HD2	37:O:3240:HOH:O	2.05	0.56
1:0:31:C:H4'	37:0:7197:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1176:C:H1'	37:0:3728:HOH:O	2.06	0.56
1:0:2265:U:H2'	1:0:2266:A:C8	2.41	0.56
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.40	0.56
1:0:2768:A:O2'	1:0:2769:C:H5'	2.05	0.56
6:D:23:VAL:HG23	6:D:23:VAL:O	2.06	0.56
14:L:73:VAL:HG21	14:L:116:HIS:HD2	1.67	0.56
1:0:282:C:O2'	1:0:283:U:H5'	2.06	0.55
1:0:793:A:H5"	18:P:83:LYS:HG2	1.87	0.55
4:B:202:VAL:HG11	4:B:301:VAL:CG1	2.32	0.55
5:C:139:VAL:HG13	37:C:8657:HOH:O	2.06	0.55
13:K:34:VAL:HB	37:K:7169:HOH:O	2.05	0.55
13:K:113:ILE:HG22	13:K:114:ALA:O	2.04	0.55
16:N:13:ARG:NH1	16:N:13:ARG:O	2.38	0.55
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.06	0.55
20:R:91:LEU:HD22	20:R:143:VAL:HG22	1.88	0.55
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.46	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.55
1:0:2831:C:H2'	1:0:2832:C:H5'	1.88	0.55
5:C:7:ASP:O	5:C:9:ASP:N	2.38	0.55
5:C:165:ASP:OD2	5:C:191:SER:HB2	2.06	0.55
6:D:170:TYR:O	6:D:171:ASP:HB3	2.05	0.55
10:H:72:ALA:HB2	10:H:156:ALA:HB2	1.88	0.55
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.01	0.55
31:3:16:GLU:HB2	37:3:8864:HOH:O	2.06	0.55
37:0:3554:HOH:O	22:T:9:LYS:HD3	2.06	0.55
4:B:109:LEU:HD11	4:B:113:LEU:HD12	1.87	0.55
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.71	0.55
10:H:61:ARG:HG3	10:H:61:ARG:NH1	2.20	0.55
26:X:78:GLU:HG2	26:X:79:GLU:N	2.22	0.55
1:0:263:U:O4	8:F:54:VAL:HG13	2.06	0.55
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.89	0.55
5:C:5:ILE:HG22	5:C:6:TYR:N	2.22	0.55
8:F:12:LEU:HD23	8:F:12:LEU:O	2.06	0.55
16:N:22:GLN:HG2	16:N:26:LEU:CD2	2.36	0.55
16:N:170:GLU:O	16:N:174:GLU:HG3	2.07	0.55
1:0:280:C:H2'	1:0:281:U:O4'	2.07	0.55
1:0:558:C:H5'	37:0:5056:HOH:O	2.07	0.55
1:0:1702:U:H5"	37:0:6988:HOH:O	2.05	0.55
1:0:1826:C:H3'	37:0:7325:HOH:O	2.06	0.55
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.05	0.55
2:9:6:C:OP1	16:N:37:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:132:HIS:CE1	4:B:171:VAL:HG23	2.41	0.55
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.36	0.55
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.09	0.55
16:N:37:ARG:NH2	37:N:8830:HOH:O	2.39	0.55
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.06	0.55
22:T:99:THR:O	22:T:100:ASP:CB	2.54	0.55
5:C:37:ALA:O	5:C:41:ASN:ND2	2.39	0.55
5:C:240:LEU:HD23	5:C:240:LEU:O	2.06	0.55
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.37	0.55
11:I:96:SER:H	11:I:99:GLN:HB2	1.71	0.55
20:R:39:THR:HG22	20:R:42:GLU:H	1.72	0.55
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.06	0.55
25:W:65:VAL:HA	25:W:68:THR:CG2	2.36	0.55
1:0:1058:A:H2'	1:0:1060:C:H5"	1.87	0.55
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.87	0.55
8:F:69:GLU:O	8:F:70:LYS:HG2	2.07	0.55
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.71	0.55
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.89	0.55
21:S:57:THR:C	21:S:59:ASP:H	2.10	0.55
22:T:101:LEU:HB2	22:T:103:LEU:HD21	1.87	0.55
25:W:77:ALA:HA	37:W:6694:HOH:O	2.06	0.55
1:0:797:A:H4'	28:Z:10:ARG:N	2.22	0.55
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.71	0.55
4:B:145:HIS:HD2	4:B:146:THR:O	1.90	0.55
15:M:96:ASP:OD1	15:M:99:ARG:HD3	2.06	0.55
15:M:190:ASN:HB2	37:M:8820:HOH:O	2.07	0.55
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.07	0.55
1:0:1044:C:H5	37:0:6383:HOH:O	1.89	0.55
1:0:1593:C:OP1	18:P:117:SER:HB3	2.06	0.55
1:0:1756:G:H1'	37:0:6047:HOH:O	2.07	0.55
1:0:2769:C:C2'	1:0:2770:G:H5'	2.37	0.55
7:E:18:LEU:HD13	7:E:34:TRP:CD1	2.42	0.55
8:F:111:ILE:O	8:F:115:VAL:HG23	2.06	0.55
12:J:95:ARG:O	12:J:99:GLU:HB2	2.07	0.55
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.35	0.55
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.37	0.55
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.06	0.55
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.55	0.55
1:0:1116:U:H3	1:0:1246:A:N6	2.02	0.55
1:0:1189:A:H1'	1:0:1209:C:C1'	2.37	0.55
1:0:2111:G:H1'	37:0:8867:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.19	0.55
4:B:171:VAL:O	4:B:175:LEU:HB2	2.07	0.55
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.42	0.55
1:0:945:U:H2'	1:0:946:C:C6	2.43	0.54
1:0:2361:A:H5'	37:0:4877:HOH:O	2.05	0.54
1:0:2415:A:O2'	16:N:29:SER:HB3	2.07	0.54
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.88	0.54
13:K:49:LEU:HD23	13:K:73:VAL:O	2.07	0.54
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.39	0.54
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.36	0.54
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.04	0.54
25:W:88:THR:HG22	25:W:89:ASP:N	2.15	0.54
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
1:0:449:A:N7	5:C:43:LYS:HG2	2.22	0.54
1:0:1701:A:H5'	37:0:6068:HOH:O	2.07	0.54
1:0:2546:U:H4'	37:B:8886:HOH:O	2.06	0.54
1:0:2755:G:H1'	37:0:4482:HOH:O	2.07	0.54
3:A:37:VAL:HG23	3:A:38:ILE:N	2.21	0.54
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.38	0.54
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.43	0.54
17:O:52:ALA:HB1	17:O:74:VAL:HG11	1.90	0.54
1:0:544:G:C3'	1:0:545:G:H5"	2.37	0.54
1:0:1168:C:H5"	11:I:83:GLY:H	1.72	0.54
1:0:1342:C:O2'	1:0:1343:C:H5'	2.07	0.54
1:0:2316:G:H4'	37:0:5876:HOH:O	2.08	0.54
1:0:2793:A:H5'	37:0:4360:HOH:O	2.08	0.54
10:H:49:GLN:HB2	10:H:170:ARG:HD2	1.89	0.54
12:J:107:ASN:HD22	12:J:108:PRO:N	2.05	0.54
20:R:9:ASP:O	20:R:13:THR:HG22	2.06	0.54
1:0:732:C:H2'	1:0:733:U:C6	2.43	0.54
1:0:2469:A:H1'	37:0:3045:HOH:O	2.06	0.54
1:0:2604:A:H5'	37:0:5579:HOH:O	2.06	0.54
3:A:140:LEU:HB3	3:A:141:PRO:HD2	1.88	0.54
8:F:21:GLU:O	8:F:24:ARG:HG2	2.07	0.54
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.38	0.54
20:R:22:GLN:CG	20:R:140:GLN:HE21	2.21	0.54
22:T:25:ALA:O	22:T:39:ASN:HB2	2.08	0.54
22:T:55:PHE:CD2	22:T:77:VAL:HG13	2.42	0.54
1:0:111:C:H2'	1:0:112:G:O4'	2.08	0.54
4:B:140:LEU:HD23	37:B:8880:HOH:O	2.06	0.54
8:F:30:LYS:HA	37:F:5719:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:38:LYS:HD2	16:N:114:LYS:HE3	1.88	0.54
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.90	0.54
1:0:1882:C:H4'	37:0:4269:HOH:O	2.08	0.54
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.91	0.54
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.08	0.54
1:0:2504:A:H2'	1:0:2505:G:O4'	2.08	0.54
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.73	0.54
1:0:399:C:H5'	15:M:179:GLY:O	2.08	0.54
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.89	0.54
3:A:194:MET:HE2	3:A:199:HIS:HB2	1.89	0.54
5:C:21:VAL:HG23	5:C:22:PHE:CD1	2.42	0.54
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.08	0.54
10:H:135:GLN:HG3	37:H:236:HOH:O	2.07	0.54
16:N:72:GLU:HB3	16:N:171:HIS:HE1	1.73	0.54
18:P:16:VAL:HG12	18:P:17:GLY:N	2.22	0.54
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.38	0.54
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.89	0.54
21:S:52:VAL:HG22	21:S:66:VAL:HG22	1.89	0.54
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.38	0.54
26:X:70:ILE:HG23	26:X:70:ILE:O	2.08	0.54
29:1:28:HIS:ND1	29:1:31:LYS:HE2	2.22	0.54
1:0:947:U:O2'	1:0:948:G:H5'	2.07	0.54
1:0:1617:C:C4	1:0:1643:C:H4'	2.43	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.54
1:0:1972:U:H2'	1:0:1973:A:H5'	1.90	0.54
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.54
2:9:122:C:H5'	37:9:8628:HOH:O	2.07	0.54
4:B:82:VAL:O	4:B:82:VAL:HG12	2.06	0.54
11:I:113:SER:CB	11:I:118:ASN:HB2	2.38	0.54
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.90	0.54
1:0:542:A:H2'	1:0:543:G:O4'	2.08	0.54
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.08	0.54
1:0:2824:C:H5"	1:0:2825:C:H5'	1.90	0.54
37:0:6155:HOH:O	29:1:30:LYS:HE2	2.08	0.54
6:D:154:LYS:H	6:D:154:LYS:HD2	1.71	0.54
10:H:100:GLU:HB3	10:H:124:VAL:HG11	1.88	0.54
15:M:107:ARG:HD2	37:M:8875:HOH:O	2.08	0.54
23:U:17:THR:CG2	23:U:18:GLY:N	2.71	0.54
24:V:4:HIS:O	24:V:8:ILE:HG13	2.07	0.54
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.88	0.54
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:819:A:HO2'	1:0:821:U:H6	1.56	0.54
1:0:1701:A:H5"	1:0:1702:U:H3'	1.90	0.54
3:A:86:ALA:HB1	3:A:92:ASN:HD22	1.72	0.54
4:B:7:ARG:CZ	4:B:11:LEU:HD21	2.38	0.54
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.88	0.54
5:C:26:VAL:N	37:C:8558:HOH:O	2.41	0.54
27:Y:234:VAL:HG12	27:Y:235:GLU:H	1.73	0.54
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.56	0.54
1:0:1614:G:H2'	37:0:4429:HOH:O	2.07	0.53
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	0.53
2:9:76:G:C3'	2:9:77:A:H5"	2.29	0.53
5:C:95:GLU:HG3	37:C:8684:HOH:O	2.06	0.53
6:D:95:THR:OG1	6:D:174:VAL:HG13	2.08	0.53
13:K:75:ARG:NH2	37:K:4172:HOH:O	2.41	0.53
16:N:64:SER:C	16:N:66:LEU:H	2.11	0.53
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.73	0.53
26:X:87:ALA:O	26:X:88:GLU:CB	2.56	0.53
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.43	0.53
12:J:130:VAL:HG11	12:J:135:ILE:HG13	1.90	0.53
25:W:1:MET:N	25:W:37:GLU:HG3	2.22	0.53
30:2:41:HIS:CD2	30:2:44:ARG:H	2.17	0.53
1:0:324:G:O2'	1:0:325:U:H5'	2.08	0.53
1:0:542:A:H5'	1:0:542:A:C8	2.35	0.53
1:0:719:C:O2'	17:O:112:ARG:NH2	2.41	0.53
1:0:2036:C:O4'	13:K:44:LEU:HG	2.08	0.53
1:0:2597:U:H2'	1:0:2598:U:H5'	1.89	0.53
3:A:107:ASN:N	3:A:119:ALA:O	2.38	0.53
5:C:1:MET:HG2	5:C:2:GLN:H	1.73	0.53
5:C:218:VAL:HG12	37:C:8633:HOH:O	2.07	0.53
11:I:119:ALA:O	11:I:123:VAL:HG23	2.07	0.53
20:R:47:LEU:O	20:R:51:ILE:HG13	2.09	0.53
22:T:48:VAL:HG12	22:T:49:GLU:N	2.23	0.53
22:T:51:LEU:HD11	22:T:97:ARG:HB2	1.91	0.53
1:0:88:G:H1'	37:0:6850:HOH:O	2.08	0.53
1:0:870:G:OP2	3:A:3:ARG:HD3	2.09	0.53
1:0:1505:U:H6	1:0:1505:U:H5'	1.71	0.53
1:0:2237:G:H1'	37:0:4653:HOH:O	2.08	0.53
1:0:2252:A:C5	1:0:2253:G:H1'	2.44	0.53
4:B:7:ARG:HD3	4:B:9:GLY:O	2.08	0.53
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.91	0.53
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:79:GLU:C	10:H:80:LEU:HD23	2.29	0.53
17:O:44:ASN:HB3	17:O:67:SER:O	2.08	0.53
1:0:67:A:H5"	1:0:69:A:C8	2.43	0.53
1:0:677:C:H4'	5:C:246:ARG:NH2	2.23	0.53
1:0:1185:U:H5'	37:0:7238:HOH:O	2.08	0.53
1:0:1334:C:H2'	1:0:1335:C:H6	1.74	0.53
1:0:1632:A:C2'	1:0:1633:C:H5'	2.39	0.53
1:0:2314:G:C2'	1:0:2315:C:H5'	2.39	0.53
1:0:2578:G:H5'	1:0:2578:G:C8	2.40	0.53
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.89	0.53
22:T:55:PHE:HB2	37:T:6384:HOH:O	2.08	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.09	0.53
26:X:85:VAL:HG12	26:X:86:GLU:N	2.23	0.53
31:3:30:GLN:HB3	37:3:8852:HOH:O	2.08	0.53
1:0:635:A:H2'	1:0:636:G:H5"	1.89	0.53
1:0:2276:U:H2'	1:0:2277:U:C6	2.43	0.53
3:A:36:ASP:CB	3:A:85:SER:H	2.22	0.53
3:A:121:ALA:H	3:A:124:VAL:CG2	2.20	0.53
6:D:44:ILE:O	6:D:44:ILE:HG12	2.08	0.53
6:D:55:LYS:O	6:D:56:ARG:CB	2.56	0.53
9:G:23:ILE:HG22	9:G:27:ILE:HD11	1.90	0.53
14:L:17:SER:C	14:L:19:LYS:H	2.12	0.53
20:R:39:THR:HB	20:R:42:GLU:CG	2.38	0.53
1:0:290:C:H2'	1:0:291:C:C6	2.43	0.53
1:0:338:C:H5"	37:0:3599:HOH:O	2.08	0.53
1:0:2672:C:OP2	4:B:25:ARG:NH1	2.40	0.53
1:0:2748:G:H2'	37:0:7309:HOH:O	2.08	0.53
7:E:80:TRP:O	7:E:134:SER:HA	2.08	0.53
9:G:19:GLU:HG2	9:G:66:LEU:HD12	1.90	0.53
10:H:27:PRO:HD3	10:H:123:ILE:CG2	2.39	0.53
10:H:114:ASP:HB2	37:H:199:HOH:O	2.07	0.53
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	0.53
17:O:38:ARG:NH1	37:O:7674:HOH:O	2.42	0.53
21:S:7:HIS:CD2	21:S:27:ALA:HB3	2.44	0.53
23:U:6:CYS:C	23:U:8:TYR:H	2.12	0.53
1:0:656:G:H5'	17:O:3:THR:HB	1.91	0.53
1:0:2533:C:H5'	1:0:2533:C:H6	1.74	0.53
1:0:2896:A:H5"	37:0:5883:HOH:O	2.08	0.53
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.90	0.53
5:C:198:ASP:C	5:C:199:GLU:HG3	2.29	0.53
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.22	0.53
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.44	0.53
28:Z:73:THR:O	28:Z:76:GLY:N	2.42	0.53
1:0:122:C:H5"	37:0:3387:HOH:O	2.08	0.53
1:0:1120:U:H5'	1:0:1120:U:C6	2.40	0.53
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.53
1:0:1527:A:H1'	1:0:1528:A:C8	2.43	0.53
1:0:1762:C:H4'	37:0:4456:HOH:O	2.08	0.53
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.91	0.53
1:0:2028:U:H2'	1:0:2029:C:C6	2.43	0.53
4:B:150:ALA:O	4:B:152:PRO:HD3	2.09	0.53
6:D:99:ASP:CG	6:D:100:ASP:N	2.59	0.53
10:H:30:LYS:H	10:H:62:HIS:HD2	1.55	0.53
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.24	0.53
29:1:10:LYS:N	37:1:2979:HOH:O	2.41	0.53
1:0:1790:C:H2'	1:0:1791:U:C6	2.43	0.53
1:0:2405:C:H5'	37:0:6375:HOH:O	2.08	0.53
1:0:2445:U:H2'	1:0:2446:G:C8	2.44	0.53
1:0:2786:G:H2'	37:0:6957:HOH:O	2.08	0.53
1:0:2798:G:H3'	37:0:4196:HOH:O	2.08	0.53
4:B:51:VAL:HG13	4:B:327:VAL:HG13	1.92	0.53
11:I:95:LEU:HD23	11:I:99:GLN:OE1	2.08	0.53
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.91	0.53
24:V:16:ARG:HB2	37:V:874:HOH:O	2.09	0.53
26:X:87:ALA:O	26:X:88:GLU:HB3	2.09	0.53
27:Y:203:VAL:HG22	37:Y:8875:HOH:O	2.09	0.53
1:0:138:U:OP2	1:0:139:C:H5	1.92	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.74	0.52
1:0:1391:G:H2'	1:0:1392:A:H5'	1.91	0.52
37:0:5256:HOH:O	9:G:12:ILE:HG23	2.10	0.52
37:0:6839:HOH:O	20:R:33:ARG:HD3	2.08	0.52
15:M:152:ALA:HB1	37:M:8941:HOH:O	2.07	0.52
1:0:660:A:H4'	1:0:661:G:O5'	2.09	0.52
1:0:1268:C:H2'	1:0:1269:G:H8	1.74	0.52
1:0:1477:C:H5'	1:0:1868:G:H5"	1.92	0.52
3:A:69:LEU:HB3	37:A:8871:HOH:O	2.08	0.52
4:B:253:GLN:HA	37:B:8924:HOH:O	2.10	0.52
31:3:69:TYR:O	31:3:77:ALA:HA	2.09	0.52
1:0:1119:G:H5'	12:J:52:GLN:HE21	1.74	0.52
1:0:1815:A:H2'	1:0:1816:C:O4'	2.09	0.52
1:0:1882:C:O2'	1:0:2012:U:OP2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.91	0.52
12:J:127:ILE:N	35:J:8801:CL:CL	2.75	0.52
16:N:86:LEU:O	16:N:90:LEU:HG	2.10	0.52
20:R:13:THR:HG23	37:R:8856:HOH:O	2.08	0.52
20:R:82:GLU:O	20:R:86:LYS:HG3	2.09	0.52
23:U:23:HIS:HB2	23:U:27:ALA:HB3	1.90	0.52
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.45	0.52
1:0:513:A:N3	37:0:3459:HOH:O	2.33	0.52
1:0:2910:A:H5"	37:0:3932:HOH:O	2.09	0.52
37:0:7477:HOH:O	5:C:94:THR:HG21	2.09	0.52
4:B:254:GLN:HG2	4:B:255:GLY:N	2.24	0.52
5:C:34:ALA:HA	5:C:102:LEU:CD2	2.39	0.52
5:C:236:THR:O	5:C:237:GLU:C	2.47	0.52
6:D:146:LYS:CE	16:N:107:ASN:HD21	2.21	0.52
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.39	0.52
11:I:117:THR:O	11:I:121:LYS:HG3	2.09	0.52
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.52
1:0:440:C:O2'	1:0:441:A:H5'	2.09	0.52
1:0:536:A:H3'	37:0:4850:HOH:O	2.10	0.52
1:0:2015:A:H2'	1:0:2016:U:O4'	2.08	0.52
1:0:2776:A:H2'	1:0:2777:G:O4'	2.09	0.52
2:9:29:C:H2'	2:9:30:C:H5'	1.91	0.52
5:C:84:VAL:O	5:C:85:LYS:HB2	2.09	0.52
8:F:34:ASN:HA	15:M:4:ALA:HB2	1.92	0.52
16:N:58:LEU:N	16:N:58:LEU:HD12	2.24	0.52
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.24	0.52
26:X:69:LYS:O	26:X:70:ILE:HB	2.10	0.52
27:Y:180:SER:HA	37:Y:8844:HOH:O	2.08	0.52
31:3:42:ARG:HB2	31:3:42:ARG:HH11	1.75	0.52
1:0:1741:U:O2'	1:0:2723:G:H4'	2.10	0.52
1:0:1762:C:H2'	1:0:1763:C:H6	1.75	0.52
3:A:52:SER:HB2	3:A:164:ARG:HH11	1.74	0.52
4:B:53:LEU:HD12	4:B:327:VAL:HA	1.91	0.52
5:C:26:VAL:HG21	5:C:123:LEU:HD11	1.91	0.52
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.25	0.52
5:C:219:ASN:O	5:C:222:ASP:OD1	2.28	0.52
6:D:84:LEU:C	6:D:86:THR:H	2.13	0.52
19:Q:28:ARG:HD3	19:Q:92:ARG:HH12	1.73	0.52
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.92	0.52
1:0:2768:A:H2'	1:0:2769:C:O4'	2.09	0.52
4:B:223:ARG:HG3	4:B:232:TRP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:131:PHE:CD2	5:C:232:LEU:HD22	2.45	0.52
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.44	0.52
17:O:49:GLU:HG2	37:O:5191:HOH:O	2.09	0.52
25:W:48:VAL:O	25:W:48:VAL:HG12	2.10	0.52
26:X:80:GLU:O	26:X:80:GLU:HG2	2.08	0.52
1:0:625:U:H5'	37:0:9987:HOH:O	2.10	0.52
1:0:820:G:C5	3:A:171:LYS:HB2	2.44	0.52
1:0:821:U:H2'	1:0:822:C:C6	2.39	0.52
1:0:1187:U:H2'	37:0:6675:HOH:O	2.09	0.52
1:0:2478:U:O2'	1:0:2479:A:H5'	2.09	0.52
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.92	0.52
1:0:2837:U:H2'	37:0:6615:HOH:O	2.10	0.52
4:B:82:VAL:HG12	4:B:101:TRP:CE3	2.45	0.52
5:C:235:PHE:CE2	5:C:243:VAL:HG21	2.44	0.52
16:N:159:TYR:HB2	37:N:8828:HOH:O	2.09	0.52
21:S:50:GLU:CG	21:S:69:SER:HA	2.40	0.52
22:T:23:VAL:C	22:T:93:THR:HG21	2.30	0.52
22:T:41:ARG:NH1	22:T:42:VAL:O	2.43	0.52
1:0:289:G:O2'	1:0:290:C:H5'	2.09	0.52
1:0:1495:C:H1'	1:0:1573:A:H1'	1.91	0.52
1:0:1771:U:O2'	1:0:1773:G:N7	2.38	0.52
6:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.54	0.52
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.90	0.52
7:E:77:THR:OG1	7:E:78:GLU:N	2.42	0.52
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.90	0.52
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.91	0.52
28:Z:46:ARG:HA	37:Z:8730:HOH:O	2.10	0.52
1:0:1441:G:H5'	20:R:130:MET:HE2	1.92	0.52
1:0:2064:U:H4'	1:0:2653:A:OP1	2.09	0.52
1:0:2256:G:H2'	1:0:2257:G:C5'	2.40	0.52
1:0:2443:C:H3'	37:0:3275:HOH:O	2.09	0.52
1:0:2481:G:C3'	1:0:2482:G:H5"	2.40	0.52
3:A:103:VAL:O	3:A:105:VAL:HG23	2.10	0.52
14:L:142:LEU:HG	14:L:146:GLY:HA3	1.92	0.52
16:N:82:TYR:C	16:N:82:TYR:CD2	2.84	0.52
18:P:127:GLY:HA3	37:P:152:HOH:O	2.08	0.52
1:0:685:C:O2	1:0:748:C:H4'	2.09	0.51
1:0:1398:G:H2'	1:0:1399:A:C8	2.46	0.51
1:0:1428:C:O2	20:R:132:ARG:HD3	2.10	0.51
4:B:72:THR:HB	37:B:8905:HOH:O	2.09	0.51
5:C:21:VAL:C	5:C:23:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:114:ALA:HB1	5:C:223:LEU:HB3	1.91	0.51
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.25	0.51
27:Y:196:VAL:HG13	27:Y:201:GLU:HG3	1.91	0.51
1:0:2629:C:H41	3:A:206:ARG:HH21	1.56	0.51
2:9:57:A:O2'	6:D:152:PRO:HD2	2.10	0.51
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.10	0.51
3:A:84:VAL:O	3:A:98:GLU:HG3	2.10	0.51
4:B:43:GLY:HA3	4:B:76:THR:HG22	1.92	0.51
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.40	0.51
7:E:103:VAL:HG22	7:E:115:ARG:HB3	1.92	0.51
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.39	0.51
27:Y:205:ILE:O	27:Y:206:ALA:C	2.49	0.51
1:0:74:G:H1'	37:0:9872:HOH:O	2.09	0.51
1:0:100:C:C4'	22:T:16:LEU:HB2	2.39	0.51
1:0:188:C:H5"	15:M:163:LEU:HD21	1.91	0.51
1:0:396:U:OP2	31:3:38:ARG:HD2	2.10	0.51
1:0:1120:U:H6	1:0:1120:U:C5'	2.22	0.51
6:D:138:GLY:N	37:D:7597:HOH:O	2.42	0.51
6:D:140:ARG:O	6:D:144:ARG:HG2	2.11	0.51
10:H:157:TYR:HD1	10:H:157:TYR:C	2.14	0.51
16:N:152:GLU:OE1	16:N:152:GLU:HA	2.10	0.51
31:3:70:ARG:HD3	37:3:8868:HOH:O	2.09	0.51
1:0:138:U:H5"	1:0:139:C:OP2	2.10	0.51
1:0:2420:G:O2'	1:0:2421:G:H5'	2.10	0.51
1:0:2815:G:N7	12:J:80:LYS:NZ	2.59	0.51
3:A:53:ALA:HB3	37:A:8898:HOH:O	2.10	0.51
4:B:48:MET:N	37:B:8858:HOH:O	2.44	0.51
10:H:157:TYR:C	10:H:157:TYR:CD1	2.83	0.51
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.93	0.51
1:0:318:U:O2'	1:0:338:C:H2'	2.11	0.51
1:0:736:A:H2'	1:0:737:A:O4'	2.10	0.51
1:0:1703:G:H21	18:P:57:ASN:HD21	1.57	0.51
1:0:1734:C:OP1	4:B:234:ARG:HD3	2.11	0.51
1:0:2768:A:H5"	37:0:4229:HOH:O	2.11	0.51
12:J:108:PRO:HG2	12:J:109:TYR:HD1	1.75	0.51
16:N:47:LEU:HD11	16:N:97:VAL:HG11	1.93	0.51
24:V:39:ALA:C	24:V:41:GLU:H	2.14	0.51
1:0:105:G:O2'	1:0:106:A:H5'	2.10	0.51
1:0:581:G:O2'	1:0:582:U:H5'	2.11	0.51
1:0:746:A:C6	17:O:65:LEU:HD13	2.46	0.51
1:0:1029:U:O2'	1:0:1273:C:OP1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1215:A:O3'	1:0:1216:G:H4'	2.11	0.51
1:0:1562:C:N4	37:0:5655:HOH:O	2.44	0.51
1:0:1973:A:H2'	1:0:1974:G:O4'	2.10	0.51
1:0:2597:U:H5"	37:0:3625:HOH:O	2.11	0.51
14:L:104:ASP:O	14:L:105:TYR:CB	2.58	0.51
21:S:32:ALA:HA	21:S:36:GLU:OE1	2.10	0.51
25:W:11:VAL:O	25:W:12:ASN:HB2	2.11	0.51
31:3:65:THR:CG2	31:3:67:LEU:HG	2.39	0.51
1:0:453:A:H4'	1:0:455:A:N7	2.26	0.51
1:0:1072:G:OP2	27:Y:154:ARG:NH2	2.40	0.51
1:0:1313:A:H5'	27:Y:208:LYS:O	2.11	0.51
3:A:9:ARG:HG2	3:A:16:PHE:CD2	2.45	0.51
4:B:66:GLU:O	4:B:67:GLU:HG3	2.11	0.51
5:C:127:ARG:HD2	5:C:229:PRO:O	2.11	0.51
7:E:149:GLU:OE1	7:E:167:TYR:HA	2.11	0.51
19:Q:26:PRO:HG3	37:Q:2847:HOH:O	2.11	0.51
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.92	0.51
37:0:3089:HOH:O	13:K:9:THR:HA	2.10	0.51
5:C:107:ARG:CZ	37:C:8666:HOH:O	2.59	0.51
7:E:20:ILE:O	7:E:30:THR:HA	2.10	0.51
9:G:71:LEU:C	9:G:73:ASP:N	2.65	0.51
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.26	0.51
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.93	0.51
22:T:73:HIS:HD2	22:T:88:PRO:CG	2.24	0.51
23:U:30:HIS:HD2	37:U:6215:HOH:O	1.93	0.51
1:0:243:A:H61	1:0:269:G:H1'	1.76	0.51
1:0:1439:C:OP1	30:2:41:HIS:HE1	1.93	0.51
7:E:84:MET:HE3	7:E:131:LEU:HD13	1.92	0.51
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.40	0.51
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.34	0.51
15:M:122:GLN:HG3	15:M:122:GLN:O	2.11	0.51
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.29	0.51
25:W:7:LEU:CD1	25:W:53:ALA:HB2	2.41	0.51
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.93	0.51
1:0:226:A:H1'	1:0:393:G:C5	2.46	0.51
1:0:1761:U:H5'	18:P:81:LYS:O	2.11	0.51
1:0:1882:C:H2'	1:0:1883:U:H6	1.76	0.51
4:B:310:ARG:HB3	37:B:8949:HOH:O	2.09	0.51
11:I:101:LYS:O	11:I:105:GLU:HG3	2.11	0.51
13:K:65:ARG:O	13:K:66:ARG:HB2	2.11	0.51
16:N:143:ARG:HG2	16:N:172:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.40	0.51
22:T:23:VAL:O	22:T:93:THR:HG21	2.10	0.51
23:U:14:GLU:OE1	23:U:15:PRO:CD	2.59	0.51
25:W:18:GLN:O	25:W:22:GLU:HG3	2.11	0.51
25:W:107:LEU:O	25:W:112:LEU:HB2	2.11	0.51
1:0:110:C:H3'	37:0:5423:HOH:O	2.11	0.50
1:0:152:A:O2'	1:0:153:C:H5'	2.11	0.50
1:0:1266:U:H4'	27:Y:115:ARG:HH21	1.76	0.50
1:0:1439:C:O5'	1:0:1439:C:H6	1.94	0.50
1:0:2338:G:H4'	6:D:105:SER:O	2.11	0.50
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.92	0.50
6:D:89:PRO:C	6:D:91:ALA:H	2.14	0.50
6:D:146:LYS:CE	16:N:107:ASN:ND2	2.74	0.50
10:H:169:GLU:OE1	10:H:169:GLU:HA	2.11	0.50
14:L:149:ARG:NH2	37:L:8890:HOH:O	2.44	0.50
15:M:61:ILE:CG2	15:M:62:VAL:N	2.73	0.50
27:Y:235:GLU:N	27:Y:235:GLU:CD	2.64	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.89	0.50
1:0:1504:A:H5'	37:0:4218:HOH:O	2.11	0.50
1:0:2727:A:H2'	1:0:2728:C:H5'	1.93	0.50
2:9:1:U:O3'	2:9:3:A:H5'	2.11	0.50
3:A:58:VAL:O	3:A:65:ARG:HD2	2.12	0.50
4:B:88:GLU:HG3	4:B:88:GLU:O	2.11	0.50
5:C:132:ASP:O	5:C:161:ASP:HB2	2.11	0.50
5:C:159:ALA:O	5:C:160:LEU:HG	2.11	0.50
16:N:5:ARG:HG2	19:Q:18:PRO:HB3	1.92	0.50
26:X:7:GLU:HG2	26:X:8:ARG:N	2.26	0.50
27:Y:106:THR:HG22	27:Y:107:PRO:O	2.11	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
1:0:2248:C:H3'	37:0:5240:HOH:O	2.10	0.50
12:J:130:VAL:CG1	12:J:135:ILE:HG13	2.41	0.50
13:K:18:ILE:HG22	13:K:93:ASN:HB2	1.93	0.50
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.41	0.50
14:L:36:ASP:HB2	37:L:8839:HOH:O	2.09	0.50
14:L:57:VAL:O	14:L:57:VAL:HG12	2.11	0.50
22:T:55:PHE:O	22:T:56:ALA:C	2.48	0.50
25:W:108:ARG:HE	25:W:114:PRO:CG	2.24	0.50
26:X:73:ARG:O	26:X:85:VAL:HG13	2.11	0.50
27:Y:174:VAL:O	27:Y:177:LYS:HB2	2.12	0.50
27:Y:219:GLU:HG3	27:Y:220:GLU:H	1.76	0.50
1:0:1441:G:O2'	1:0:1442:A:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1450:C:O2'	1:0:1494:A:H5'	2.11	0.50
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.50
1:0:1655:G:H3'	37:0:6195:HOH:O	2.11	0.50
2:9:55:U:H4'	2:9:56:A:C8	2.46	0.50
4:B:195:ARG:N	4:B:198:GLU:OE1	2.43	0.50
5:C:7:ASP:C	5:C:9:ASP:H	2.15	0.50
7:E:11:VAL:HG12	7:E:12:ASP:H	1.76	0.50
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.11	0.50
1:0:1328:A:N7	1:0:1329:G:C5	2.80	0.50
1:0:1937:U:O2'	1:0:1938:G:H5'	2.12	0.50
13:K:23:ASN:HD21	13:K:107:THR:H	1.59	0.50
16:N:67:ALA:C	16:N:69:TYR:H	2.14	0.50
24:V:3:LEU:HD23	24:V:52:ALA:HB1	1.94	0.50
27:Y:219:GLU:CG	27:Y:220:GLU:N	2.74	0.50
1:0:1025:C:H5'	25:W:23:MET:O	2.12	0.50
1:0:1166:A:OP2	1:0:1174:A:H4'	2.12	0.50
1:0:1649:G:H1'	37:0:4882:HOH:O	2.11	0.50
1:0:1783:A:O2'	1:0:1784:U:H5'	2.11	0.50
1:0:2132:C:H1'	15:M:124:GLY:HA3	1.94	0.50
2:9:28:U:H5"	16:N:40:ASN:HD21	1.77	0.50
2:9:57:A:H5'	37:9:8717:HOH:O	2.11	0.50
2:9:61:C:H2'	2:9:62:A:H8	1.77	0.50
4:B:312:ARG:HG2	4:B:313:PRO:N	2.26	0.50
5:C:140:VAL:HG12	5:C:141:SER:N	2.27	0.50
6:D:21:VAL:HG23	6:D:80:ALA:HB1	1.94	0.50
6:D:144:ARG:CZ	37:D:3839:HOH:O	2.59	0.50
13:K:55:VAL:HG12	13:K:56:SER:H	1.75	0.50
14:L:68:GLU:HB2	37:L:8873:HOH:O	2.10	0.50
15:M:71:SER:O	15:M:73:ARG:NH1	2.44	0.50
24:V:19:GLU:O	24:V:22:ASP:HB2	2.12	0.50
1:0:1811:A:H2'	1:0:1812:G:H5'	1.94	0.50
37:0:9348:HOH:O	18:P:81:LYS:HG2	2.11	0.50
4:B:217:ARG:CG	4:B:257:THR:HG22	2.36	0.50
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.26	0.50
13:K:24:THR:HB	13:K:64:MET:HE1	1.94	0.50
26:X:75:ALA:O	26:X:83:ALA:HA	2.11	0.50
1:0:827:A:H2'	1:0:828:G:O4'	2.12	0.50
1:0:2377:U:H6	1:0:2377:U:O5'	1.94	0.50
1:0:2404:G:O5'	19:Q:68:GLY:HA3	2.12	0.50
5:C:165:ASP:O	5:C:168:ARG:HB3	2.10	0.50
6:D:94:ALA:HB3	6:D:97:GLN:NE2	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:16:ASP:O	7:E:17:HIS:HB2	2.11	0.50
8:F:91:VAL:CG1	8:F:92:GLY:H	2.23	0.50
14:L:145:LEU:HD23	14:L:145:LEU:O	2.11	0.50
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.11	0.50
25:W:8:ARG:HB3	37:W:1427:HOH:O	2.12	0.50
25:W:125:HIS:CD2	25:W:127:GLY:H	2.29	0.50
1:0:354:A:H2'	1:0:355:C:H6	1.76	0.50
1:0:1015:C:H2'	1:0:1016:U:C6	2.47	0.50
1:0:1276:U:H3'	17:O:19:ARG:NH1	2.26	0.50
1:0:1805:G:O2'	1:0:1806:G:H5'	2.12	0.50
1:0:2320:U:H4'	1:0:2321:A:O4'	2.12	0.50
6:D:39:ASP:HB2	37:D:5583:HOH:O	2.12	0.50
6:D:81:GLU:C	6:D:83:PHE:H	2.15	0.50
6:D:138:GLY:O	6:D:140:ARG:N	2.45	0.50
7:E:45:ASP:OD2	7:E:46:THR:HG23	2.12	0.50
13:K:49:LEU:HD21	13:K:74:VAL:C	2.32	0.50
22:T:16:LEU:O	22:T:19:ARG:HB2	2.12	0.50
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.92	0.50
1:0:383:A:H2'	1:0:384:G:O4'	2.12	0.49
1:0:969:G:H1	1:0:999:C:H42	1.60	0.49
1:0:1299:G:N7	14:L:6:ARG:NH1	2.60	0.49
1:0:1393:A:H2'	1:0:1394:C:C6	2.47	0.49
1:0:2115:U:H2'	1:0:2116:U:C6	2.47	0.49
1:0:2764:C:H2'	1:0:2765:C:H6	1.76	0.49
37:0:4720:HOH:O	15:M:14:ASN:HB3	2.12	0.49
5:C:20:ASP:O	5:C:23:GLU:HB2	2.12	0.49
8:F:38:LYS:HZ3	15:M:3:SER:HA	1.77	0.49
10:H:73:ASN:HB2	10:H:88:MET:CE	2.42	0.49
12:J:34:GLU:HA	12:J:34:GLU:OE1	2.11	0.49
20:R:44:VAL:O	20:R:48:GLU:HG3	2.11	0.49
1:0:130:C:O2'	1:0:131:A:N7	2.45	0.49
1:0:1139:U:H2'	1:0:1140:C:C6	2.47	0.49
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.12	0.49
1:0:1568:G:O2'	1:0:1569:U:H5'	2.12	0.49
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.49
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.12	0.49
2:9:43:G:H5'	37:9:8611:HOH:O	2.11	0.49
3:A:120:ARG:HA	3:A:159:VAL:HG21	1.93	0.49
3:A:194:MET:HE3	3:A:199:HIS:HB2	1.92	0.49
4:B:248:ARG:O	4:B:251:VAL:HG13	2.11	0.49
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:12:ASP:HA	37:E:1750:HOH:O	2.11	0.49
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.94	0.49
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.41	0.49
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.94	0.49
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.43	0.49
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.94	0.49
27:Y:172:THR:N	37:Y:8848:HOH:O	2.45	0.49
31:3:40:ARG:HD3	37:3:8856:HOH:O	2.12	0.49
1:0:470:U:O2'	29:1:16:HIS:HD2	1.94	0.49
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.76	0.49
14:L:144:ASP:O	14:L:147:GLU:HG3	2.13	0.49
15:M:28:GLN:HA	15:M:31:TRP:HB2	1.94	0.49
16:N:29:SER:OG	16:N:101:VAL:HG21	2.12	0.49
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.12	0.49
24:V:1:THR:HG23	24:V:2:VAL:N	2.18	0.49
28:Z:67:GLY:HA3	28:Z:73:THR:CG2	2.42	0.49
1:0:361:C:H2'	1:0:362:G:O4'	2.13	0.49
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:1525:G:N2	1:0:1526:A:H2'	2.27	0.49
1:0:1768:C:H2'	1:0:1769:C:O4'	2.12	0.49
1:0:2780:C:H2'	1:0:2781:U:C6	2.48	0.49
1:0:2840:A:H3'	37:0:7417:HOH:O	2.11	0.49
16:N:112:GLY:HA2	16:N:137:ALA:HB2	1.93	0.49
24:V:55:ARG:O	24:V:59:ILE:HG12	2.12	0.49
25:W:38:THR:CG2	25:W:39:ASP:N	2.75	0.49
25:W:65:VAL:CA	25:W:68:THR:HG22	2.42	0.49
26:X:81:GLY:O	26:X:82:GLU:HB3	2.12	0.49
1:0:506:G:H3'	37:0:3569:HOH:O	2.11	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.11	0.49
1:0:1167:G:H4'	11:I:130:LEU:HD22	1.95	0.49
1:0:2036:C:C1'	13:K:44:LEU:HG	2.42	0.49
7:E:81:GLU:HB3	37:E:4761:HOH:O	2.12	0.49
14:L:81:VAL:O	14:L:81:VAL:HG12	2.13	0.49
16:N:127:LEU:HB2	37:N:8853:HOH:O	2.12	0.49
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.76	0.49
25:W:129:LYS:HG2	37:W:1990:HOH:O	2.12	0.49
29:1:52:SER:HA	37:1:4248:HOH:O	2.12	0.49
1:0:545:G:H2'	1:0:546:C:O4'	2.12	0.49
1:0:1205:U:C2'	1:0:1206:U:H5'	2.40	0.49
1:0:1925:G:H5"	31:3:29:ARG:HH22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.76	0.49
1:0:2851:G:C2'	1:0:2852:A:H5'	2.42	0.49
37:0:6801:HOH:O	3:A:211:LYS:HG2	2.10	0.49
2:9:28:U:H5"	16:N:40:ASN:ND2	2.28	0.49
3:A:171:LYS:HB3	28:Z:18:TYR:HE2	1.78	0.49
4:B:138:GLY:O	4:B:139:ASP:O	2.29	0.49
6:D:39:ASP:O	6:D:43:GLU:HG3	2.13	0.49
7:E:154:ILE:HD11	7:E:157:LYS:HE2	1.94	0.49
8:F:52:GLU:HG3	8:F:77:VAL:O	2.11	0.49
11:I:128:THR:HG22	11:I:128:THR:O	2.12	0.49
15:M:164:THR:CG2	15:M:167:GLY:N	2.73	0.49
16:N:11:ARG:NH2	37:N:8817:HOH:O	2.45	0.49
20:R:117:HIS:HA	37:R:8826:HOH:O	2.11	0.49
24:V:39:ALA:N	24:V:40:PRO:HD2	2.22	0.49
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.94	0.49
1:0:363:C:H2'	1:0:364:U:C6	2.47	0.49
1:0:1066:U:H2'	1:0:1067:A:C8	2.47	0.49
1:0:1289:C:O2'	1:0:1290:G:H5'	2.13	0.49
1:0:1468:G:H5"	37:0:7227:HOH:O	2.11	0.49
1:0:1486:A:C4	30:2:2:LYS:HG3	2.47	0.49
1:0:1561:U:H2'	37:0:3944:HOH:O	2.11	0.49
1:0:1600:G:H4'	37:0:5444:HOH:O	2.11	0.49
1:0:1603:A:H5"	1:0:1605:G:H5'	1.93	0.49
1:0:1850:U:H2'	1:0:1851:G:C8	2.47	0.49
1:0:1972:U:H2'	1:0:1973:A:C5'	2.43	0.49
1:0:2072:G:H4'	37:0:6811:HOH:O	2.12	0.49
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.49
3:A:192:VAL:HB	37:A:8884:HOH:O	2.11	0.49
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.95	0.49
5:C:195:VAL:HA	5:C:213:ALA:O	2.13	0.49
20:R:100:ASP:C	20:R:102:GLN:H	2.14	0.49
30:2:36:ASN:C	30:2:38:LYS:H	2.15	0.49
1:0:303:C:H2'	1:0:304:G:O4'	2.13	0.49
1:0:525:G:H2'	1:0:526:U:O4'	2.12	0.49
1:0:894:A:C2	5:C:87:ARG:NH2	2.81	0.49
1:0:1661:A:H2'	1:0:1662:C:O4'	2.12	0.49
1:0:1825:U:O2'	1:0:1826:C:H5'	2.12	0.49
1:0:2577:A:H5'	37:0:7522:HOH:O	2.12	0.49
2:9:18:U:OP2	6:D:154:LYS:HE2	2.12	0.49
3:A:61:GLU:C	3:A:63:GLY:H	2.14	0.49
4:B:62:ARG:HA	4:B:65:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:230:GLY:N	37:C:8547:HOH:O	2.42	0.49
13:K:49:LEU:HA	13:K:73:VAL:HG12	1.93	0.49
18:P:121:ASP:O	18:P:125:LYS:HG3	2.13	0.49
24:V:4:HIS:HB3	37:V:6622:HOH:O	2.13	0.49
25:W:36:PRO:HD2	25:W:41:TYR:CE1	2.48	0.49
30:2:41:HIS:CD2	30:2:43:ARG:H	2.31	0.49
1:0:343:C:O2'	1:0:344:C:H5'	2.12	0.49
1:0:445:U:H2'	1:0:446:G:H8	1.78	0.49
1:0:1496:A:H5'	1:0:1572:A:H1'	1.95	0.49
1:0:2582:G:O3'	13:K:41:LYS:HA	2.13	0.49
37:0:4773:HOH:O	10:H:61:ARG:HG3	2.12	0.49
3:A:43:VAL:O	3:A:76:VAL:HG22	2.12	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
17:O:44:ASN:HA	17:O:65:LEU:O	2.13	0.49
24:V:27:LEU:CA	24:V:49:LEU:HD13	2.43	0.49
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.93	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.49
1:0:1513:C:O2'	1:0:1514:C:H5'	2.12	0.49
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.49
3:A:199:HIS:HD2	3:A:201:PHE:HB2	1.77	0.49
5:C:27:ARG:NH2	17:O:4:ASN:ND2	2.61	0.49
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.95	0.49
15:M:61:ILE:HD12	15:M:61:ILE:N	2.28	0.49
15:M:153:ASP:HB2	37:M:8910:HOH:O	2.13	0.49
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.48	0.49
20:R:129:ALA:O	20:R:130:MET:CB	2.61	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.49
25:W:46:ALA:O	25:W:49:ASN:HB2	2.13	0.49
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.48	0.49
1:0:321:A:O2'	1:0:322:G:H5'	2.12	0.48
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.48
1:0:661:G:C5	1:0:686:A:C2	3.01	0.48
1:0:1119:G:N2	1:0:1246:A:H2	2.08	0.48
2:9:73:A:H61	2:9:108:C:N4	2.08	0.48
3:A:57:ALA:HA	3:A:67:LEU:HD23	1.95	0.48
4:B:162:MET:HG3	4:B:310:ARG:NH1	2.28	0.48
5:C:132:ASP:O	5:C:133:ARG:HB2	2.12	0.48
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.37	0.48
11:I:129:SER:O	11:I:130:LEU:HD23	2.13	0.48
12:J:54:VAL:HG12	12:J:58:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.95	0.48
16:N:115:VAL:HG23	16:N:116:PHE:H	1.77	0.48
1:0:23:G:C6	1:0:24:G:N1	2.81	0.48
1:0:94:G:N2	37:0:4913:HOH:O	2.38	0.48
1:0:380:A:H2'	37:0:6998:HOH:O	2.13	0.48
1:0:485:A:N3	1:0:487:G:H5"	2.28	0.48
1:0:797:A:H5'	28:Z:10:ARG:N	2.27	0.48
3:A:86:ALA:HB1	3:A:92:ASN:ND2	2.29	0.48
3:A:191:GLY:HA2	3:A:194:MET:CE	2.42	0.48
4:B:23:THR:HG22	4:B:25:ARG:HE	1.78	0.48
5:C:5:ILE:HG23	37:C:8640:HOH:O	2.13	0.48
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.13	0.48
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.48	0.48
13:K:64:MET:HE1	13:K:105:ARG:HE	1.78	0.48
15:M:57:LYS:HG2	15:M:58:GLN:H	1.77	0.48
18:P:103:THR:HA	18:P:106:ARG:NH1	2.27	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.28	0.48
26:X:30:MET:HE1	26:X:55:ASN:HA	1.95	0.48
28:Z:33:MET:SD	28:Z:49:ARG:HD2	2.53	0.48
1:0:503:G:H2'	1:0:504:G:H8	1.78	0.48
1:0:539:G:H2'	1:0:540:A:C8	2.48	0.48
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.48
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.13	0.48
1:0:2505:G:O2'	1:0:2506:A:H5'	2.14	0.48
2:9:39:U:H3'	2:9:40:C:H5"	1.94	0.48
12:J:34:GLU:O	12:J:36:VAL:HG23	2.13	0.48
18:P:3:LEU:HA	18:P:6:GLN:OE1	2.13	0.48
21:S:57:THR:CG2	21:S:58:MET:N	2.77	0.48
25:W:29:VAL:O	25:W:30:ASN:HB2	2.12	0.48
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.26	0.48
1:0:1342:C:H2'	1:0:1343:C:H5'	1.96	0.48
1:0:1762:C:H2'	1:0:1763:C:C6	2.48	0.48
1:0:2561:C:OP1	7:E:153:ARG:NH2	2.47	0.48
2:9:73:A:N6	2:9:108:C:H42	2.09	0.48
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.95	0.48
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.56	0.48
16:N:37:ARG:NE	37:N:8830:HOH:O	2.46	0.48
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.78	0.48
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.95	0.48
26:X:86:GLU:O	26:X:87:ALA:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:215:A:P	14:L:52:LYS:HZ3	2.36	0.48
1:0:371:U:H2'	1:0:372:A:H8	1.79	0.48
1:0:807:A:H2'	1:0:808:A:C8	2.49	0.48
1:0:1155:G:H2'	1:0:1156:C:C6	2.48	0.48
1:0:1297:U:H1'	37:0:3185:HOH:O	2.13	0.48
1:0:1545:C:H2'	1:0:1546:G:O4'	2.14	0.48
4:B:23:THR:HB	4:B:25:ARG:HH21	1.79	0.48
7:E:21:THR:HG23	7:E:30:THR:OG1	2.13	0.48
11:I:68:PRO:CB	11:I:69:PRO:HD2	2.42	0.48
12:J:42:GLU:O	12:J:131:THR:HG23	2.13	0.48
14:L:76:LEU:HB3	14:L:79:ASP:OD2	2.14	0.48
16:N:93:GLN:HG2	37:N:8853:HOH:O	2.14	0.48
17:O:79:VAL:HA	37:O:6810:HOH:O	2.13	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.48
25:W:144:GLU:O	25:W:144:GLU:HG3	2.14	0.48
29:1:5:THR:HB	29:1:6:PRO:CD	2.43	0.48
1:0:667:C:H2'	1:0:668:C:H6	1.77	0.48
1:0:1398:G:O2'	1:0:1399:A:H5'	2.13	0.48
2:9:91:C:H2'	2:9:92:G:O4'	2.14	0.48
4:B:139:ASP:CB	4:B:165:ARG:HE	2.26	0.48
5:C:109:LEU:HD12	5:C:109:LEU:O	2.13	0.48
8:F:115:VAL:O	8:F:118:LEU:N	2.47	0.48
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.94	0.48
16:N:152:GLU:C	16:N:154:LEU:N	2.63	0.48
25:W:76:ASP:O	25:W:77:ALA:C	2.52	0.48
1:0:682:A:H2'	1:0:683:G:O4'	2.13	0.48
1:0:1884:G:O6	3:A:190:ARG:HD2	2.13	0.48
1:0:1923:G:H4'	31:3:31:THR:O	2.13	0.48
1:0:2047:C:H5'	37:0:9623:HOH:O	2.12	0.48
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.49	0.48
5:C:233:THR:HG22	5:C:234:VAL:N	2.14	0.48
6:D:27:ILE:HG22	6:D:28:GLY:N	2.28	0.48
12:J:17:CYS:HA	12:J:119:THR:O	2.14	0.48
12:J:33:GLY:O	12:J:34:GLU:C	2.52	0.48
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.49	0.48
15:M:57:LYS:HZ2	15:M:144:ASP:HB2	1.78	0.48
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.14	0.48
20:R:61:GLN:CD	37:R:8831:HOH:O	2.51	0.48
24:V:50:ARG:HD3	37:V:2826:HOH:O	2.12	0.48
1:0:224:U:H1'	37:0:9698:HOH:O	2.14	0.48
1:0:581:G:H4'	1:0:1254:C:O2'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:624:U:H5”	37:0:9327:HOH:O	2.14	0.48
1:0:1189:A:O2’	1:0:1208:C:H2’	2.14	0.48
1:0:2389:U:H4’	19:Q:53:HIS:CD2	2.49	0.48
2:9:6:C:C5’	16:N:37:ARG:NH1	2.67	0.48
4:B:201:ASP:CB	4:B:312:ARG:HD2	2.38	0.48
16:N:34:LEU:HD13	16:N:47:LEU:CD2	2.44	0.48
1:0:656:G:OP2	17:O:37:ARG:HD2	2.14	0.48
1:0:1165:G:H4’	1:0:1166:A:OP2	2.14	0.48
1:0:1234:U:C4	4:B:244:PRO:HB3	2.48	0.48
1:0:2500:C:H1’	37:0:4465:HOH:O	2.14	0.48
3:A:65:ARG:C	3:A:66:ARG:HG3	2.33	0.48
4:B:14:GLY:HA2	4:B:15:PRO:C	2.34	0.48
5:C:26:VAL:HG21	5:C:123:LEU:CD1	2.44	0.48
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.49	0.48
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.53	0.48
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.96	0.48
27:Y:235:GLU:H	27:Y:235:GLU:CD	2.17	0.48
1:0:210:U:O2’	1:0:211:U:H5’	2.14	0.48
1:0:422:G:H2’	1:0:423:A:H8	1.79	0.48
1:0:835:U:H3’	37:0:9181:HOH:O	2.13	0.48
1:0:1184:C:O2’	1:0:1185:U:OP2	2.23	0.48
1:0:1205:U:C2’	1:0:1206:U:C5’	2.90	0.48
1:0:1656:A:H5’	37:0:4205:HOH:O	2.13	0.48
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.47	0.48
1:0:2629:C:N4	3:A:206:ARG:HH21	2.12	0.48
1:0:2672:C:O2’	1:0:2673:U:H5’	2.14	0.48
1:0:2906:A:H5’	1:0:2907:C:O4’	2.14	0.48
37:0:4785:HOH:O	5:C:219:ASN:HB2	2.14	0.48
2:9:57:A:C8	6:D:141:VAL:HG21	2.49	0.48
3:A:35:GLY:HA3	37:A:8887:HOH:O	2.13	0.48
4:B:63:GLU:HG3	4:B:63:GLU:O	2.14	0.48
4:B:211:THR:HA	4:B:255:GLY:O	2.14	0.48
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.13	0.48
8:F:105:ASP:O	8:F:109:GLU:HB2	2.13	0.48
11:I:127:CYS:C	11:I:129:SER:N	2.67	0.48
12:J:41:ALA:N	37:J:8866:HOH:O	2.46	0.48
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.49	0.48
15:M:54:TYR:CG	15:M:55:LYS:N	2.82	0.48
15:M:59:GLY:C	15:M:141:ILE:HD11	2.34	0.48
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.41	0.48
1:0:317:A:H4’	37:0:3570:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:553:G:H2'	1:0:554:G:H5'	1.96	0.47
1:0:710:G:H5'	17:O:25:VAL:CG1	2.43	0.47
1:0:1572:A:H2'	1:0:1573:A:C8	2.49	0.47
1:0:2256:G:H2'	1:0:2257:G:H5'	1.96	0.47
2:9:114:G:H2'	2:9:115:C:C6	2.49	0.47
4:B:96:PRO:HG3	37:B:8935:HOH:O	2.14	0.47
7:E:101:GLU:HB3	7:E:117:THR:HA	1.96	0.47
8:F:91:VAL:CG1	8:F:92:GLY:N	2.75	0.47
10:H:87:LYS:HB2	10:H:87:LYS:NZ	2.29	0.47
13:K:4:LEU:HD21	13:K:120:ARG:HD2	1.96	0.47
14:L:72:ASN:O	14:L:76:LEU:HG	2.13	0.47
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.45	0.47
18:P:83:LYS:NZ	37:P:201:HOH:O	2.47	0.47
18:P:126:ALA:C	18:P:128:GLY:H	2.17	0.47
19:Q:3:SER:HB3	37:Q:5998:HOH:O	2.13	0.47
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.36	0.47
1:0:1200:A:H3'	37:0:5546:HOH:O	2.14	0.47
1:0:1372:A:H3'	37:0:6959:HOH:O	2.13	0.47
1:0:2105:C:H2'	1:0:2106:C:C6	2.49	0.47
37:0:5264:HOH:O	9:G:65:THR:HG23	2.12	0.47
2:9:3:A:H2	2:9:21:G:N3	2.12	0.47
2:9:33:U:H2'	37:9:8651:HOH:O	2.12	0.47
4:B:238:ASN:ND2	4:B:240:GLY:N	2.47	0.47
5:C:150:THR:O	5:C:152:GLU:N	2.47	0.47
5:C:232:LEU:HA	37:C:8505:HOH:O	2.14	0.47
6:D:135:VAL:HG22	6:D:136:ARG:N	2.29	0.47
8:F:10:ALA:O	8:F:13:GLU:HB3	2.13	0.47
8:F:26:THR:HG21	8:F:102:GLY:C	2.34	0.47
11:I:95:LEU:CD2	11:I:99:GLN:HB3	2.34	0.47
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.49	0.47
18:P:138:GLU:C	18:P:140:TYR:H	2.17	0.47
25:W:38:THR:HG22	25:W:39:ASP:H	1.77	0.47
1:0:1086:A:C6	25:W:11:VAL:HG11	2.48	0.47
1:0:2050:G:H5"	20:R:80:TYR:O	2.14	0.47
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.47
1:0:2421:G:H3'	1:0:2422:U:C5'	2.39	0.47
5:C:246:ARG:NE	37:C:8633:HOH:O	2.46	0.47
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.27	0.47
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.15	0.47
22:T:47:THR:HB	22:T:100:ASP:HB3	1.95	0.47
25:W:38:THR:HG21	37:W:5390:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:102:LEU:HG	37:Y:8888:HOH:O	2.14	0.47
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.12	0.47
1:0:255:A:H2'	1:0:256:C:O4'	2.14	0.47
1:0:306:A:P	22:T:38:ARG:HH21	2.37	0.47
1:0:466:A:H2'	1:0:467:G:O4'	2.14	0.47
1:0:512:G:O3'	1:0:513:A:H8	1.96	0.47
1:0:711:G:C2	1:0:718:C:C2	3.02	0.47
1:0:1909:A:N1	1:0:2128:G:H1'	2.30	0.47
2:9:55:U:H4'	2:9:56:A:H8	1.80	0.47
3:A:217:ARG:CG	3:A:217:ARG:NH1	2.76	0.47
4:B:57:GLU:O	4:B:63:GLU:HB3	2.14	0.47
4:B:277:GLU:N	4:B:278:PRO:HD2	2.29	0.47
4:B:279:THR:HG22	4:B:280:VAL:N	2.29	0.47
7:E:137:ASP:O	7:E:141:VAL:HG23	2.15	0.47
10:H:139:ALA:HB3	37:H:232:HOH:O	2.15	0.47
11:I:98:ASP:C	11:I:100:VAL:H	2.17	0.47
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.49	0.47
14:L:68:GLU:O	14:L:69:ILE:C	2.53	0.47
17:O:47:ARG:HA	17:O:50:ARG:NH1	2.29	0.47
18:P:87:ARG:HA	37:P:188:HOH:O	2.13	0.47
25:W:69:ARG:NH2	25:W:119:HIS:HB2	2.28	0.47
26:X:88:GLU:OE1	26:X:88:GLU:O	2.32	0.47
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.17	0.47
1:0:656:G:H4'	37:C:8561:HOH:O	2.14	0.47
1:0:1167:G:H2'	1:0:1168:C:C6	2.49	0.47
1:0:1185:U:O2'	1:0:1186:C:H5'	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:C6	2.64	0.47
1:0:2598:U:O2	1:0:2600:A:H8	1.97	0.47
1:0:2717:C:O2'	1:0:2718:C:H5"	2.15	0.47
3:A:206:ARG:HH12	3:A:208:HIS:CE1	2.33	0.47
6:D:12:GLU:HB3	37:D:3359:HOH:O	2.14	0.47
11:I:102:GLN:HA	11:I:105:GLU:OE2	2.15	0.47
16:N:110:THR:HB	16:N:113:SER:OG	2.15	0.47
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.70	0.47
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.50	0.47
1:0:506:G:N2	1:0:509:A:H5'	2.26	0.47
1:0:675:U:H2'	1:0:676:C:H5'	1.96	0.47
1:0:1388:U:H2'	1:0:1389:G:O4'	2.14	0.47
1:0:2381:C:H2'	1:0:2382:A:H8	1.78	0.47
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.97	0.47
6:D:163:VAL:O	6:D:167:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:100:ASP:O	8:F:101:ALA:O	2.32	0.47
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.49	0.47
11:I:94:ASP:O	11:I:95:LEU:HG	2.14	0.47
13:K:87:ARG:NE	37:K:4854:HOH:O	2.48	0.47
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.45	0.47
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.96	0.47
16:N:179:LEU:C	16:N:181:ASP:H	2.18	0.47
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.45	0.47
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.48	0.47
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.30	0.47
1:0:113:A:OP2	1:0:114:A:H2'	2.15	0.47
1:0:212:A:O4'	1:0:214:U:C6	2.68	0.47
1:0:682:A:H5"	37:0:3492:HOH:O	2.15	0.47
1:0:695:C:O2'	1:0:696:C:H5'	2.14	0.47
1:0:1189:A:H1'	1:0:1209:C:H1'	1.97	0.47
1:0:1485:A:H4'	37:0:3088:HOH:O	2.14	0.47
1:0:1486:A:C5	30:2:2:LYS:HG3	2.49	0.47
1:0:1798:C:C4'	18:P:66:GLN:HG2	2.45	0.47
1:0:2656:G:C2'	1:0:2657:G:H5'	2.45	0.47
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.47
5:C:55:ARG:HB2	37:C:8510:HOH:O	2.14	0.47
5:C:104:ASP:O	5:C:108:GLN:HG3	2.14	0.47
10:H:41:LYS:HD3	10:H:46:TYR:CZ	2.50	0.47
11:I:69:PRO:HG2	11:I:72:GLU:HB2	1.97	0.47
12:J:107:ASN:ND2	12:J:107:ASN:C	2.67	0.47
16:N:115:VAL:HG23	16:N:116:PHE:N	2.30	0.47
20:R:39:THR:O	20:R:40:ALA:C	2.51	0.47
22:T:24:ARG:HG2	22:T:24:ARG:NH1	2.30	0.47
26:X:30:MET:CE	26:X:58:ALA:HB3	2.44	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
1:0:11:A:H5'	1:0:12:U:OP2	2.15	0.47
1:0:292:G:H2'	1:0:358:G:N2	2.29	0.47
1:0:2781:U:C2'	1:0:2782:G:H5'	2.44	0.47
37:0:9363:HOH:O	25:W:119:HIS:HE1	1.96	0.47
4:B:41:PHE:HA	4:B:79:MET:CE	2.45	0.47
4:B:62:ARG:NH2	4:B:66:GLU:O	2.47	0.47
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.44	0.47
6:D:44:ILE:O	6:D:44:ILE:HG23	2.15	0.47
10:H:48:VAL:HA	10:H:170:ARG:O	2.15	0.47
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.97	0.47
14:L:89:PHE:CD1	14:L:89:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.45	0.47
15:M:99:ARG:HG2	15:M:99:ARG:HH11	1.80	0.47
17:O:14:LEU:HA	17:O:102:ILE:HD11	1.96	0.47
18:P:18:LYS:O	18:P:21:VAL:HG22	2.15	0.47
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.95	0.47
21:S:52:VAL:CG2	21:S:66:VAL:HG13	2.44	0.47
25:W:13:MET:CE	25:W:17:ILE:HG22	2.44	0.47
1:0:183:A:O2'	1:0:184:G:H5'	2.15	0.47
1:0:1685:A:H4'	1:0:1686:C:OP2	2.15	0.47
1:0:1882:C:H2'	1:0:1883:U:C6	2.49	0.47
1:0:2003:U:H4'	1:0:2004:U:H5	1.79	0.47
1:0:2681:A:H4'	1:0:2682:C:C5'	2.45	0.47
1:0:2842:G:H5'	20:R:68:HIS:O	2.15	0.47
37:0:3490:HOH:O	7:E:143:GLN:HG2	2.15	0.47
4:B:27:ASN:HD22	4:B:27:ASN:N	2.11	0.47
4:B:75:GLU:C	4:B:77:PRO:HD3	2.35	0.47
4:B:258:GLY:H	4:B:260:HIS:CE1	2.33	0.47
7:E:107:PHE:CE1	7:E:152:THR:HB	2.50	0.47
14:L:143:THR:CG2	14:L:144:ASP:N	2.78	0.47
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.80	0.47
22:T:70:ALA:O	22:T:71:VAL:HG23	2.14	0.47
25:W:131:PRO:HG2	25:W:134:GLU:HB2	1.96	0.47
1:0:157:G:H3'	37:0:3755:HOH:O	2.15	0.47
1:0:710:G:O2'	1:0:711:G:H5'	2.14	0.47
1:0:1930:A:H2'	1:0:1931:A:C8	2.50	0.47
1:0:2503:A:H2	1:0:2517:A:N7	2.13	0.47
2:9:51:A:H5'	16:N:160:SER:HB3	1.96	0.47
4:B:53:LEU:HD11	4:B:327:VAL:HG22	1.97	0.47
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.45	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.97	0.47
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.44	0.47
18:P:67:LYS:O	18:P:68:LYS:C	2.53	0.47
23:U:13:ILE:HG12	23:U:32:CYS:CB	2.45	0.47
1:0:694:A:C2'	1:0:695:C:H5'	2.45	0.46
1:0:1186:C:H2'	1:0:1187:U:O4'	2.15	0.46
1:0:1477:C:C5'	1:0:1868:G:H5"	2.45	0.46
1:0:1735:C:H5'	4:B:235:ARG:HH21	1.79	0.46
1:0:1883:U:O2'	1:0:1884:G:H5'	2.15	0.46
1:0:2436:U:H5'	31:3:68:LYS:HE2	1.96	0.46
1:0:2570:G:H8	37:0:4714:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:56:ASP:HB3	4:B:322:ARG:HE	1.80	0.46
6:D:59:GLY:O	6:D:61:PHE:N	2.49	0.46
7:E:158:ASP:OD1	7:E:160:ARG:N	2.49	0.46
11:I:98:ASP:HA	11:I:101:LYS:HG3	1.97	0.46
17:O:26:TRP:N	37:O:3062:HOH:O	2.48	0.46
20:R:33:ARG:HH11	20:R:60:LYS:HG3	1.79	0.46
23:U:6:CYS:SG	23:U:8:TYR:HB3	2.55	0.46
26:X:43:VAL:CG1	26:X:44:ASP:H	2.25	0.46
30:2:41:HIS:HB3	30:2:44:ARG:HB2	1.97	0.46
1:0:742:G:O2'	1:0:743:G:H5'	2.15	0.46
1:0:1587:U:H2'	1:0:1588:G:O4'	2.14	0.46
1:0:2067:A:H2'	1:0:2068:G:O4'	2.15	0.46
1:0:2730:G:O2'	1:0:2731:G:H5'	2.16	0.46
1:0:2781:U:O2'	1:0:2782:G:H5'	2.15	0.46
3:A:223:ARG:O	3:A:223:ARG:HG2	2.14	0.46
4:B:214:PRO:HD2	37:B:8820:HOH:O	2.15	0.46
4:B:243:ASN:HA	4:B:244:PRO:C	2.35	0.46
6:D:167:GLU:C	6:D:169:THR:H	2.19	0.46
10:H:31:ILE:HA	10:H:66:GLU:OE1	2.15	0.46
10:H:49:GLN:O	10:H:169:GLU:HB2	2.15	0.46
10:H:98:LEU:O	10:H:124:VAL:HG22	2.15	0.46
21:S:45:TYR:CE2	21:S:81:ILE:HD13	2.47	0.46
25:W:26:ILE:O	25:W:26:ILE:CG1	2.63	0.46
28:Z:60:CYS:SG	28:Z:62:TYR:HB2	2.55	0.46
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.80	0.46
1:0:444:C:H1'	37:0:7106:HOH:O	2.14	0.46
1:0:776:A:OP1	29:1:28:HIS:HE1	1.98	0.46
1:0:825:U:H5"	1:0:826:U:OP1	2.16	0.46
1:0:843:A:C2	1:0:846:A:C8	3.03	0.46
1:0:1070:A:O5'	1:0:1070:A:H8	1.99	0.46
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.46
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.45	0.46
8:F:38:LYS:HZ1	15:M:3:SER:HA	1.79	0.46
10:H:50:ILE:HB	37:H:232:HOH:O	2.14	0.46
13:K:115:ARG:HG3	13:K:116:GLU:N	2.30	0.46
14:L:17:SER:C	14:L:19:LYS:N	2.68	0.46
14:L:55:GLN:HA	14:L:58:GLN:NE2	2.25	0.46
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.97	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.96	0.46
21:S:56:ASN:O	30:2:8:LYS:NZ	2.47	0.46
22:T:49:GLU:HG3	22:T:97:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.83	0.46
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.54	0.46
1:0:952:G:H4'	37:0:6512:HOH:O	2.16	0.46
37:0:3833:HOH:O	5:C:149:LYS:HE3	2.14	0.46
4:B:30:PRO:HG2	4:B:313:PRO:HD2	1.96	0.46
7:E:11:VAL:CG1	7:E:12:ASP:N	2.77	0.46
7:E:156:ASP:OD1	7:E:156:ASP:N	2.47	0.46
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.15	0.46
13:K:41:LYS:O	13:K:42:ASN:HB2	2.15	0.46
13:K:113:ILE:HD12	13:K:128:ALA:CB	2.45	0.46
16:N:58:LEU:HD12	16:N:58:LEU:H	1.80	0.46
19:Q:11:ARG:HD2	37:Q:5620:HOH:O	2.15	0.46
22:T:50:VAL:HG11	22:T:55:PHE:HB2	1.96	0.46
1:0:338:C:H4'	5:C:174:ILE:HD11	1.96	0.46
1:0:348:C:H2'	1:0:349:U:H6	1.80	0.46
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
1:0:2324:G:H4'	1:0:2418:G:O2'	2.15	0.46
3:A:9:ARG:O	3:A:11:ARG:N	2.49	0.46
3:A:171:LYS:HB3	28:Z:18:TYR:CE2	2.50	0.46
4:B:248:ARG:O	4:B:251:VAL:CG1	2.64	0.46
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.98	0.46
6:D:92:GLU:HB2	37:D:3862:HOH:O	2.16	0.46
7:E:9:GLU:HG3	7:E:10:ASP:N	2.29	0.46
14:L:35:ARG:HB2	14:L:43:HIS:CD2	2.51	0.46
24:V:12:THR:H	24:V:15:GLU:HB2	1.81	0.46
1:0:130:C:H5'	37:0:5015:HOH:O	2.15	0.46
1:0:1561:U:C5'	37:0:7201:HOH:O	2.61	0.46
1:0:2668:G:H2'	1:0:2669:U:C6	2.51	0.46
1:0:2911:C:H2'	1:0:2912:C:H6	1.81	0.46
2:9:8:G:O6	16:N:11:ARG:NH1	2.47	0.46
3:A:1:GLY:N	37:A:8900:HOH:O	2.48	0.46
4:B:205:VAL:N	37:B:8954:HOH:O	2.49	0.46
8:F:66:LEU:O	8:F:69:GLU:HG2	2.15	0.46
16:N:42:HIS:HA	16:N:75:THR:O	2.16	0.46
16:N:98:GLU:O	16:N:127:LEU:HD12	2.15	0.46
25:W:4:LEU:HD23	25:W:54:PHE:CB	2.41	0.46
28:Z:20:ARG:O	28:Z:21:VAL:C	2.54	0.46
1:0:35:U:H5'	5:C:47:GLY:O	2.16	0.46
1:0:612:U:H2'	1:0:613:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:727:G:H3'	1:0:728:C:H6	1.81	0.46
1:0:1197:G:N2	1:0:1202:A:H62	2.12	0.46
1:0:1268:C:H2'	1:0:1269:G:C8	2.50	0.46
1:0:1353:C:P	37:0:4479:HOH:O	2.74	0.46
1:0:2787:C:H2'	1:0:2788:A:O4'	2.14	0.46
1:0:2894:C:O2'	1:0:2895:C:H5'	2.15	0.46
12:J:131:THR:HB	12:J:134:GLU:OE1	2.15	0.46
19:Q:28:ARG:HD3	19:Q:92:ARG:NH1	2.30	0.46
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.31	0.46
25:W:6:GLN:HG2	25:W:29:VAL:HA	1.97	0.46
25:W:26:ILE:O	25:W:26:ILE:HG13	2.16	0.46
1:0:625:U:H5"	1:0:1044:C:N4	2.31	0.46
1:0:812:A:H1'	37:0:3756:HOH:O	2.16	0.46
1:0:858:U:H2'	1:0:859:C:C6	2.50	0.46
1:0:1072:G:P	27:Y:154:ARG:NH2	2.88	0.46
1:0:1175:G:H4'	37:0:6633:HOH:O	2.16	0.46
1:0:1829:A:H2'	1:0:1830:C:H5'	1.98	0.46
1:0:1878:G:O2'	1:0:1879:U:P	2.74	0.46
1:0:2878:U:H2'	1:0:2879:A:O4'	2.15	0.46
4:B:79:MET:O	4:B:80:ARG:HG3	2.15	0.46
6:D:10:PHE:CG	6:D:11:HIS:N	2.83	0.46
6:D:103:ASN:ND2	6:D:134:LEU:H	2.13	0.46
10:H:80:LEU:HD12	10:H:86:TYR:CD2	2.51	0.46
14:L:123:ASP:OD1	14:L:145:LEU:HB3	2.16	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.84	0.46
22:T:101:LEU:CD1	22:T:112:LEU:HD11	2.45	0.46
1:0:1245:C:O5'	1:0:1245:C:H6	1.98	0.46
1:0:1334:C:H2'	1:0:1335:C:C6	2.51	0.46
3:A:173:GLY:O	3:A:176:HIS:HB3	2.16	0.46
9:G:20:VAL:O	9:G:24:VAL:HG23	2.16	0.46
12:J:84:ARG:HB2	12:J:98:PHE:CE1	2.51	0.46
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.97	0.46
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.80	0.46
25:W:80:ASP:HB2	37:W:3312:HOH:O	2.16	0.46
1:0:29:C:O2'	1:0:30:U:H5'	2.16	0.46
1:0:247:A:H2'	37:0:3722:HOH:O	2.16	0.46
1:0:926:A:O2'	14:L:41:HIS:CD2	2.68	0.46
1:0:945:U:O2'	25:W:43:GLY:HA3	2.16	0.46
1:0:1855:G:O6	3:A:142:SER:HB3	2.16	0.46
1:0:2442:G:H2'	37:0:9007:HOH:O	2.15	0.46
37:0:3554:HOH:O	22:T:9:LYS:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:1:U:C4'	2:9:3:A:OP1	2.64	0.46
2:9:44:A:H1'	6:D:76:ARG:NH2	2.31	0.46
4:B:16:ARG:NH2	37:B:8854:HOH:O	2.32	0.46
4:B:115:VAL:HA	4:B:116:PRO:HD3	1.87	0.46
4:B:280:VAL:CG1	4:B:281:ASP:N	2.78	0.46
4:B:313:PRO:O	4:B:314:ALA:C	2.54	0.46
5:C:135:GLU:O	5:C:136:VAL:HB	2.15	0.46
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.98	0.46
12:J:126:ASN:O	12:J:129:PHE:HE2	1.99	0.46
14:L:26:HIS:HB2	37:L:8812:HOH:O	2.16	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.69	0.46
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.57	0.46
21:S:50:GLU:HG2	21:S:69:SER:HA	1.99	0.46
22:T:29:ALA:N	37:T:5241:HOH:O	2.48	0.46
1:0:97:G:N1	22:T:107:LYS:HG3	2.31	0.45
1:0:558:C:C2'	1:0:559:U:H5"	2.45	0.45
1:0:611:U:H2'	1:0:612:U:C6	2.51	0.45
1:0:652:G:H5"	37:0:9812:HOH:O	2.16	0.45
1:0:1461:U:H2'	1:0:1462:C:C6	2.51	0.45
1:0:1553:C:H2'	1:0:1554:C:H6	1.81	0.45
1:0:2032:U:H2'	1:0:2033:G:C5'	2.46	0.45
1:0:2241:C:H2'	1:0:2242:U:C6	2.51	0.45
1:0:2314:G:H2'	1:0:2315:C:H5'	1.97	0.45
1:0:2526:C:C2'	1:0:2527:U:H5'	2.46	0.45
5:C:21:VAL:HG23	5:C:22:PHE:HD1	1.79	0.45
5:C:149:LYS:HB2	5:C:152:GLU:HG3	1.98	0.45
6:D:95:THR:OG1	6:D:174:VAL:HA	2.16	0.45
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.98	0.45
8:F:58:GLU:HA	8:F:61:MET:CE	2.45	0.45
16:N:73:ALA:N	37:N:8863:HOH:O	2.46	0.45
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.16	0.45
24:V:58:THR:O	24:V:62:GLU:HG3	2.16	0.45
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.56	0.45
1:0:317:A:OP1	22:T:52:ARG:O	2.34	0.45
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.45
1:0:1159:G:P	37:0:4097:HOH:O	2.74	0.45
37:0:9753:HOH:O	26:X:23:HIS:HD2	1.98	0.45
4:B:148:PRO:HD2	37:B:8881:HOH:O	2.16	0.45
5:C:16:VAL:CG1	5:C:17:ASP:H	2.27	0.45
6:D:25:MET:CE	6:D:37:ALA:HB1	2.40	0.45
10:H:91:ARG:H	10:H:91:ARG:HG2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:108:HIS:H	11:I:109:PRO:HD2	1.81	0.45
11:I:125:GLY:HA3	37:I:3512:HOH:O	2.15	0.45
16:N:5:ARG:HB2	37:N:8854:HOH:O	2.15	0.45
19:Q:72:LYS:HG2	19:Q:85:ILE:HD13	1.98	0.45
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.79	0.45
31:3:18:GLN:HG3	37:3:8861:HOH:O	2.16	0.45
1:0:290:C:H2'	1:0:291:C:O4'	2.15	0.45
1:0:920:C:H5'	1:0:921:G:C4	2.51	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.51	0.45
1:0:2053:G:H4'	20:R:136:TRP:CD2	2.51	0.45
1:0:2326:C:H4'	1:0:2412:G:H4'	1.98	0.45
3:A:235:ARG:HD3	37:A:8833:HOH:O	2.15	0.45
4:B:5:ARG:HD2	4:B:8:LYS:HZ1	1.80	0.45
6:D:40:ILE:HG23	37:D:5583:HOH:O	2.15	0.45
6:D:64:ARG:O	6:D:67:ASP:OD1	2.34	0.45
11:I:95:LEU:HD22	11:I:99:GLN:CB	2.35	0.45
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.81	0.45
18:P:109:ARG:NH1	18:P:119:TYR:CE2	2.84	0.45
22:T:50:VAL:HG11	37:T:6384:HOH:O	2.16	0.45
24:V:11:MET:HE1	24:V:15:GLU:O	2.16	0.45
25:W:76:ASP:O	25:W:77:ALA:O	2.35	0.45
30:2:20:ARG:CG	30:2:20:ARG:NH1	2.72	0.45
1:0:1515:A:H2'	1:0:1516:U:C6	2.51	0.45
1:0:1940:C:H4'	37:0:7117:HOH:O	2.14	0.45
1:0:2246:U:N3	1:0:2256:G:C2	2.85	0.45
5:C:16:VAL:CG1	5:C:17:ASP:N	2.80	0.45
7:E:14:GLU:HG2	7:E:15:GLN:N	2.31	0.45
8:F:58:GLU:OE2	15:M:20:LEU:HD13	2.17	0.45
8:F:63:ILE:HB	8:F:64:PRO:CD	2.42	0.45
19:Q:25:PRO:HB2	37:Q:4350:HOH:O	2.17	0.45
21:S:6:LYS:HB2	21:S:27:ALA:O	2.14	0.45
22:T:9:LYS:NZ	22:T:13:ARG:NH1	2.64	0.45
27:Y:97:LEU:CD2	27:Y:235:GLU:HG3	2.46	0.45
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.17	0.45
1:0:23:G:H1'	1:0:520:A:N6	2.32	0.45
1:0:80:A:H5"	22:T:41:ARG:CZ	2.47	0.45
1:0:903:U:O4	14:L:18:HIS:HB2	2.17	0.45
1:0:1163:G:H5'	11:I:110:ASP:O	2.17	0.45
1:0:1855:G:H4'	1:0:1856:C:O5'	2.16	0.45
1:0:2437:A:H2'	1:0:2438:G:C8	2.51	0.45
1:0:2541:U:H5'	1:0:2611:G:O6	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2543:G:H2'	1:0:2544:G:O4'	2.16	0.45
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.99	0.45
10:H:149:VAL:HG21	37:H:232:HOH:O	2.16	0.45
13:K:110:LYS:O	13:K:111:GLY:O	2.34	0.45
16:N:175:LEU:HD12	16:N:175:LEU:HA	1.81	0.45
21:S:25:GLN:HG2	21:S:65:VAL:HG22	1.98	0.45
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.51	0.45
1:0:395:A:H5"	37:0:3721:HOH:O	2.17	0.45
1:0:1067:A:H5'	37:0:4151:HOH:O	2.15	0.45
1:0:1127:C:C5	1:0:1128:U:C4	3.05	0.45
1:0:1894:C:C2	1:0:1939:U:C4	3.04	0.45
1:0:2084:C:H2'	1:0:2085:A:H8	1.82	0.45
1:0:2506:A:O2'	1:0:2507:G:C8	2.56	0.45
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.80	0.45
3:A:30:ARG:HE	3:A:30:ARG:HB3	1.55	0.45
3:A:32:VAL:O	3:A:33:GLU:C	2.54	0.45
4:B:148:PRO:HB2	4:B:156:LYS:O	2.16	0.45
6:D:10:PHE:HA	37:D:7345:HOH:O	2.17	0.45
8:F:4:VAL:HA	8:F:76:PHE:CE1	2.51	0.45
10:H:65:LEU:H	10:H:65:LEU:HD22	1.82	0.45
11:I:86:GLU:O	11:I:89:GLU:HB2	2.16	0.45
11:I:87:PRO:HD3	37:I:6825:HOH:O	2.16	0.45
15:M:74:LYS:HE2	37:M:8928:HOH:O	2.16	0.45
22:T:41:ARG:O	22:T:42:VAL:C	2.55	0.45
25:W:21:LEU:HD21	25:W:48:VAL:HG13	1.96	0.45
1:0:1173:A:H2	37:0:6065:HOH:O	2.00	0.45
1:0:2897:C:O2'	1:0:2898:G:H5'	2.17	0.45
4:B:162:MET:CE	4:B:310:ARG:HD3	2.47	0.45
5:C:88:SER:O	5:C:91:PRO:HD3	2.17	0.45
6:D:49:PRO:HA	6:D:73:VAL:HG22	1.99	0.45
10:H:48:VAL:HG21	10:H:143:VAL:HA	1.99	0.45
10:H:122:LYS:HB2	10:H:122:LYS:HE3	1.81	0.45
13:K:23:ASN:HD21	13:K:107:THR:HB	1.81	0.45
17:O:66:GLY:HA3	17:O:84:THR:HG22	1.97	0.45
18:P:67:LYS:O	18:P:70:ALA:N	2.50	0.45
25:W:132:VAL:HG23	25:W:138:LEU:O	2.17	0.45
27:Y:163:THR:HB	37:Y:8908:HOH:O	2.16	0.45
1:0:338:C:H4'	5:C:174:ILE:HD12	1.99	0.45
1:0:344:C:H2'	1:0:345:G:O4'	2.17	0.45
1:0:1181:A:H2'	1:0:1182:C:C5'	2.43	0.45
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1517:C:H2'	1:0:1518:A:C8	2.51	0.45
1:0:1539:U:O2'	1:0:1540:G:H5'	2.17	0.45
1:0:1735:C:H5'	4:B:235:ARG:NH2	2.32	0.45
1:0:2239:C:H6	37:0:6451:HOH:O	1.99	0.45
37:0:3035:HOH:O	14:L:22:ARG:HG2	2.16	0.45
37:0:3324:HOH:O	21:S:13:LYS:HE2	2.16	0.45
2:9:39:U:HO2'	2:9:42:C:H5	1.65	0.45
11:I:72:GLU:C	11:I:74:ILE:N	2.69	0.45
12:J:99:GLU:HA	37:J:8876:HOH:O	2.15	0.45
25:W:5:VAL:HG11	25:W:153:MET:CE	2.47	0.45
1:0:10:U:O4	1:0:532:A:OP2	2.33	0.45
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.45
1:0:745:G:H5"	1:0:746:A:OP1	2.16	0.45
1:0:1942:A:O3'	3:A:213:LYS:HE2	2.16	0.45
1:0:2488:A:H2	37:0:7044:HOH:O	2.00	0.45
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.98	0.45
1:0:2787:C:H5	37:0:4434:HOH:O	1.99	0.45
37:0:9331:HOH:O	20:R:139:PRO:HD3	2.15	0.45
2:9:95:C:O2'	2:9:96:C:H5'	2.17	0.45
3:A:145:MET:HG2	37:A:8828:HOH:O	2.15	0.45
4:B:141:ARG:HB3	4:B:164:THR:O	2.16	0.45
5:C:139:VAL:CG1	37:C:8657:HOH:O	2.63	0.45
5:C:180:SER:N	37:C:8579:HOH:O	2.47	0.45
6:D:128:LEU:O	6:D:128:LEU:HD23	2.17	0.45
11:I:124:VAL:O	11:I:124:VAL:HG12	2.17	0.45
13:K:75:ARG:HH21	13:K:94:ALA:HB2	1.82	0.45
13:K:132:VAL:HG21	23:U:22:VAL:HG11	1.98	0.45
16:N:115:VAL:O	16:N:118:ILE:HB	2.16	0.45
16:N:139:TRP:CZ2	16:N:176:ARG:NH1	2.85	0.45
17:O:32:ARG:HG2	17:O:32:ARG:NH1	2.32	0.45
17:O:107:GLU:O	17:O:108:GLY:C	2.55	0.45
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.47	0.45
21:S:16:ASN:O	21:S:20:PHE:N	2.50	0.45
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.17	0.45
1:0:586:C:H5"	37:0:7055:HOH:O	2.17	0.45
1:0:612:U:H2'	1:0:613:C:H6	1.81	0.45
1:0:645:U:OP2	14:L:4:LYS:HE2	2.17	0.45
1:0:746:A:H5'	37:0:5310:HOH:O	2.17	0.45
1:0:941:G:C5	1:0:942:U:C4	3.05	0.45
1:0:1071:G:H4'	27:Y:154:ARG:NH2	2.32	0.45
1:0:1072:G:P	27:Y:154:ARG:HH22	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1643:C:O2'	1:0:1644:C:H5'	2.16	0.45
1:0:1682:A:H5"	37:0:9263:HOH:O	2.17	0.45
1:0:1942:A:H3'	37:0:7117:HOH:O	2.17	0.45
1:0:2057:U:O5'	1:0:2057:U:H6	1.99	0.45
1:0:2318:C:H1'	37:0:3939:HOH:O	2.17	0.45
1:0:2651:C:H2'	1:0:2652:U:O4'	2.17	0.45
3:A:32:VAL:O	3:A:34:ASP:N	2.49	0.45
3:A:36:ASP:HB2	3:A:84:VAL:H	1.81	0.45
6:D:164:ALA:O	6:D:165:PHE:C	2.56	0.45
16:N:67:ALA:O	16:N:69:TYR:N	2.50	0.45
19:Q:93:ARG:HG3	19:Q:93:ARG:HH11	1.81	0.45
20:R:125:ARG:NH1	20:R:125:ARG:HB3	2.32	0.45
22:T:9:LYS:HE3	22:T:13:ARG:NH1	2.31	0.45
23:U:52:THR:CG2	23:U:54:THR:HB	2.47	0.45
28:Z:38:ALA:N	37:Z:8725:HOH:O	2.50	0.45
1:0:241:A:C2	1:0:378:A:H4'	2.51	0.44
1:0:1755:A:H2'	1:0:1756:G:O4'	2.17	0.44
37:0:7197:HOH:O	22:T:9:LYS:HD2	2.16	0.44
2:9:110:G:C2'	2:9:111:U:H5'	2.47	0.44
5:C:20:ASP:O	5:C:23:GLU:N	2.47	0.44
5:C:126:ASP:C	5:C:128:GLY:N	2.69	0.44
5:C:194:PHE:HA	5:C:234:VAL:HG13	1.98	0.44
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.99	0.44
6:D:81:GLU:C	6:D:83:PHE:N	2.70	0.44
16:N:184:ILE:HG23	16:N:184:ILE:O	2.18	0.44
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.60	0.44
30:2:41:HIS:H	30:2:45:ASN:ND2	2.09	0.44
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.44
1:0:506:G:N2	1:0:508:A:H3'	2.32	0.44
1:0:1020:A:H1'	37:Q:6976:HOH:O	2.16	0.44
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.50	0.44
1:0:1154:A:H2'	1:0:1155:G:C8	2.52	0.44
1:0:1496:A:N6	37:0:6898:HOH:O	2.49	0.44
1:0:2453:G:H3'	37:0:5707:HOH:O	2.16	0.44
1:0:2633:A:H2'	1:0:2634:G:H5'	1.99	0.44
1:0:2720:C:O2	13:K:87:ARG:NH2	2.49	0.44
1:0:2831:C:C2'	1:0:2832:C:H5'	2.48	0.44
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.81	0.44
4:B:304:PRO:CG	4:B:307:ARG:NH1	2.80	0.44
6:D:28:GLY:O	6:D:29:HIS:HB3	2.17	0.44
7:E:101:GLU:HG3	7:E:101:GLU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:41:LYS:HD3	10:H:46:TYR:CE1	2.52	0.44
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.48	0.44
16:N:114:LYS:O	16:N:117:ALA:HB3	2.17	0.44
23:U:17:THR:HG22	23:U:18:GLY:H	1.81	0.44
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.48	0.44
31:3:15:ASN:HB2	37:3:8846:HOH:O	2.17	0.44
1:0:222:A:H2'	1:0:223:G:O4'	2.17	0.44
1:0:485:A:HO2'	1:0:487:G:H8	1.65	0.44
1:0:1044:C:H5"	37:0:8844:HOH:O	2.17	0.44
1:0:1822:A:O2'	1:0:1823:G:H5'	2.17	0.44
1:0:2831:C:H2'	1:0:2832:C:C5'	2.46	0.44
1:0:2850:C:H5'	1:0:2850:C:C6	2.44	0.44
2:9:3:A:N6	2:9:22:G:H1'	2.33	0.44
3:A:94:LEU:CG	3:A:99:ILE:HD11	2.40	0.44
4:B:38:VAL:HA	4:B:166:VAL:HG22	2.00	0.44
4:B:240:GLY:HA3	37:B:8829:HOH:O	2.17	0.44
7:E:32:ARG:O	7:E:33:LEU:HD23	2.17	0.44
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.32	0.44
17:O:7:LEU:HD22	37:O:5650:HOH:O	2.16	0.44
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.47	0.44
22:T:48:VAL:HG12	22:T:96:VAL:HG22	2.00	0.44
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.47	0.44
1:0:1872:C:H5	3:A:20:SER:HB3	1.82	0.44
1:0:1947:G:N2	1:0:1966:U:C2	2.85	0.44
1:0:2265:U:H2'	1:0:2266:A:H8	1.81	0.44
1:0:2508:C:H2'	37:0:6533:HOH:O	2.17	0.44
37:0:3634:HOH:O	15:M:48:LYS:NZ	2.44	0.44
5:C:214:THR:HG23	5:C:216:SER:H	1.82	0.44
6:D:164:ALA:O	6:D:167:GLU:N	2.50	0.44
7:E:170:ARG:NH2	37:E:4761:HOH:O	2.49	0.44
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.17	0.44
11:I:84:SER:N	37:I:7210:HOH:O	2.50	0.44
11:I:127:CYS:N	37:I:5371:HOH:O	2.45	0.44
17:O:10:LEU:HD13	17:O:99:GLU:HG3	1.98	0.44
23:U:25:ASP:OD2	23:U:27:ALA:HB2	2.17	0.44
24:V:12:THR:O	24:V:15:GLU:N	2.48	0.44
25:W:96:LEU:O	25:W:99:ALA:N	2.51	0.44
25:W:132:VAL:HG21	25:W:141:HIS:CD2	2.52	0.44
27:Y:122:ARG:NH2	37:Y:8835:HOH:O	2.50	0.44
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.44
1:0:1174:A:H5'	37:0:4217:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1314:U:H5”	1:0:1316:G:O4’	2.17	0.44
1:0:1845:A:O3’	3:A:187:PRO:HB2	2.16	0.44
2:9:13:A:OP1	2:9:113:C:H5’	2.16	0.44
3:A:51:ARG:NH2	37:A:8843:HOH:O	2.49	0.44
5:C:27:ARG:HH11	5:C:27:ARG:HG3	1.82	0.44
5:C:133:ARG:HD2	37:C:8615:HOH:O	2.17	0.44
6:D:60:GLU:O	6:D:61:PHE:C	2.55	0.44
10:H:4:LYS:HB3	10:H:5:PRO:CD	2.48	0.44
10:H:79:GLU:O	10:H:80:LEU:HD23	2.17	0.44
10:H:131:GLN:O	10:H:134:GLU:HG3	2.18	0.44
12:J:47:THR:O	12:J:53:ILE:HD11	2.18	0.44
12:J:131:THR:HG22	12:J:133:GLY:N	2.33	0.44
14:L:101:ASP:OD1	14:L:101:ASP:N	2.51	0.44
14:L:145:LEU:O	14:L:148:GLU:HG3	2.18	0.44
15:M:49:ALA:HB1	15:M:54:TYR:HB2	1.99	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.83	0.44
22:T:48:VAL:HG22	22:T:98:VAL:HA	1.99	0.44
22:T:73:HIS:HD2	22:T:88:PRO:HG3	1.82	0.44
26:X:26:ALA:HB2	26:X:63:ARG:HA	1.99	0.44
30:2:26:MET:O	30:2:31:ARG:N	2.43	0.44
1:0:820:G:H5’	1:0:821:U:H5’	1.98	0.44
1:0:1149:U:C5	1:0:1215:A:C5	3.06	0.44
1:0:1450:C:C4’	1:0:1451:C:OP2	2.61	0.44
1:0:1471:A:H2’	1:0:1472:C:C6	2.53	0.44
1:0:1484:G:H2’	37:0:8922:HOH:O	2.17	0.44
1:0:1506:U:H5’	1:0:1506:U:C6	2.50	0.44
1:0:1864:C:C5	15:M:75:ARG:HD2	2.53	0.44
1:0:2379:G:H4’	1:0:2380:A:H5”	1.98	0.44
1:0:2860:G:H1’	37:0:6361:HOH:O	2.18	0.44
2:9:80:A:C2	2:9:103:A:C4	3.06	0.44
10:H:36:MET:HB3	10:H:73:ASN:ND2	2.32	0.44
10:H:91:ARG:HD3	10:H:135:GLN:HB2	1.99	0.44
11:I:71:ALA:O	11:I:75:LYS:HG3	2.16	0.44
16:N:144:GLY:O	16:N:147:ILE:CG2	2.65	0.44
18:P:109:ARG:C	18:P:111:GLU:H	2.20	0.44
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.21	0.44
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.37	0.44
24:V:33:VAL:CG1	24:V:38:GLY:HA3	2.44	0.44
25:W:48:VAL:CG1	25:W:48:VAL:O	2.66	0.44
26:X:43:VAL:CG1	26:X:44:ASP:N	2.79	0.44
1:0:777:U:O2’	29:1:11:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:793:A:C5'	18:P:83:LYS:HG2	2.48	0.44
1:0:1001:U:H1'	37:H:219:HOH:O	2.17	0.44
1:0:2281:C:H2'	1:0:2282:U:H5'	2.00	0.44
1:0:2764:C:H2'	1:0:2765:C:C6	2.53	0.44
2:9:31:C:H2'	2:9:32:G:O4'	2.18	0.44
3:A:35:GLY:O	3:A:36:ASP:CB	2.53	0.44
4:B:189:ALA:O	4:B:192:ASP:HB2	2.18	0.44
6:D:10:PHE:CD2	6:D:11:HIS:N	2.85	0.44
6:D:94:ALA:HA	6:D:174:VAL:O	2.17	0.44
6:D:104:PHE:N	6:D:104:PHE:CD2	2.86	0.44
8:F:1:PRO:HB2	37:F:5897:HOH:O	2.18	0.44
11:I:127:CYS:O	11:I:130:LEU:N	2.50	0.44
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.37	0.44
16:N:67:ALA:C	16:N:69:TYR:N	2.69	0.44
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.88	0.44
25:W:142:ASP:HB2	37:W:2729:HOH:O	2.18	0.44
28:Z:28:GLU:O	28:Z:31:SER:N	2.51	0.44
1:0:249:G:H2'	1:0:250:C:C6	2.53	0.44
1:0:533:U:H3'	37:0:3547:HOH:O	2.16	0.44
1:0:945:U:H2'	1:0:946:C:H6	1.81	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.18	0.44
1:0:1086:A:N6	25:W:11:VAL:HG11	2.33	0.44
1:0:1743:G:O4'	13:K:78:LYS:HD3	2.17	0.44
1:0:2107:U:O2'	1:0:2108:A:H5'	2.18	0.44
1:0:2438:G:H5'	37:0:5953:HOH:O	2.18	0.44
3:A:206:ARG:NH1	3:A:208:HIS:NE2	2.66	0.44
5:C:115:LEU:HD13	5:C:115:LEU:HA	1.85	0.44
7:E:23:GLU:HG2	7:E:28:SER:CB	2.47	0.44
16:N:144:GLY:O	16:N:147:ILE:HG22	2.18	0.44
18:P:82:GLY:HA2	37:P:174:HOH:O	2.17	0.44
22:T:16:LEU:HA	22:T:19:ARG:HG3	2.00	0.44
22:T:20:HIS:O	22:T:23:VAL:HG23	2.18	0.44
22:T:37:GLN:HB3	37:T:6711:HOH:O	2.16	0.44
23:U:35:LYS:HB2	37:U:774:HOH:O	2.17	0.44
1:0:363:C:H2'	1:0:364:U:H6	1.82	0.44
1:0:812:A:H2'	1:0:813:C:O4'	2.18	0.44
1:0:1160:G:O2'	1:0:1190:G:H1'	2.17	0.44
1:0:1462:C:O2'	1:0:1463:U:H5'	2.18	0.44
1:0:1782:G:O2'	1:0:1783:A:H5'	2.18	0.44
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.44
1:0:2064:U:H5'	1:0:2652:U:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2846:C:H4'	4:B:156:LYS:HB3	2.00	0.44
4:B:215:VAL:O	4:B:219:GLY:HA2	2.18	0.44
4:B:224:LYS:HD3	4:B:224:LYS:HA	1.79	0.44
7:E:84:MET:HE1	7:E:133:VAL:CG2	2.48	0.44
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.99	0.44
1:0:74:G:H2'	1:0:75:U:C6	2.52	0.43
1:0:321:A:C2'	1:0:322:G:H5'	2.48	0.43
1:0:969:G:H2'	1:0:970:U:C6	2.52	0.43
1:0:1555:G:O2'	1:0:1556:G:H5'	2.18	0.43
1:0:1723:G:H2'	37:0:9433:HOH:O	2.18	0.43
1:0:2281:C:C2'	1:0:2282:U:H5'	2.48	0.43
37:0:9600:HOH:O	13:K:39:GLY:HA3	2.18	0.43
2:9:49:G:O2'	2:9:50:G:H5'	2.17	0.43
14:L:35:ARG:O	14:L:40:PHE:HA	2.18	0.43
15:M:158:ARG:HB2	15:M:163:LEU:HB2	1.99	0.43
16:N:37:ARG:NH2	16:N:105:GLY:CA	2.81	0.43
16:N:93:GLN:HG3	16:N:125:ALA:O	2.18	0.43
1:0:169:A:H1'	31:3:48:ASN:ND2	2.33	0.43
1:0:371:U:H2'	1:0:372:A:C8	2.52	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.52	0.43
1:0:958:G:O2'	1:0:959:C:H5'	2.18	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.18	0.43
1:0:1414:A:H2'	1:0:1415:G:O4'	2.19	0.43
1:0:1556:G:O2'	1:0:1557:G:H5'	2.17	0.43
1:0:1644:C:H2'	1:0:1645:U:H6	1.84	0.43
1:0:1659:A:H2'	1:0:1660:G:O4'	2.17	0.43
3:A:93:THR:HG23	3:A:154:ALA:O	2.18	0.43
5:C:13:ASP:OD1	5:C:13:ASP:O	2.36	0.43
5:C:21:VAL:HG23	5:C:22:PHE:N	2.34	0.43
5:C:84:VAL:O	5:C:85:LYS:CB	2.66	0.43
7:E:120:GLY:C	7:E:122:THR:H	2.21	0.43
8:F:32:GLY:N	37:F:3111:HOH:O	2.51	0.43
10:H:73:ASN:HB2	10:H:88:MET:HE1	1.98	0.43
13:K:11:GLY:O	13:K:12:LEU:HD23	2.18	0.43
13:K:115:ARG:CG	13:K:116:GLU:N	2.81	0.43
16:N:115:VAL:HG23	37:N:8856:HOH:O	2.18	0.43
16:N:179:LEU:HA	16:N:184:ILE:CD1	2.48	0.43
17:O:35:LYS:HB3	17:O:36:PRO:HD2	1.99	0.43
17:O:39:THR:O	17:O:115:ARG:NH2	2.51	0.43
20:R:22:GLN:HG2	20:R:140:GLN:HE21	1.83	0.43
21:S:52:VAL:HG22	21:S:66:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:55:PHE:CD1	22:T:55:PHE:N	2.86	0.43
23:U:17:THR:CG2	23:U:18:GLY:H	2.30	0.43
23:U:34:SER:HA	23:U:37:GLU:OE1	2.17	0.43
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.53	0.43
1:0:92:G:O2'	1:0:93:C:H5'	2.18	0.43
1:0:1181:A:C2	1:0:1192:A:C8	3.06	0.43
1:0:1426:C:H4'	1:0:1427:A:C8	2.52	0.43
1:0:2820:A:H2'	1:0:2821:C:O4'	2.18	0.43
3:A:82:VAL:HG13	3:A:93:THR:HB	2.00	0.43
3:A:132:ASP:OD1	3:A:133:ARG:N	2.48	0.43
10:H:4:LYS:N	37:H:221:HOH:O	2.52	0.43
11:I:127:CYS:O	11:I:129:SER:N	2.51	0.43
12:J:70:PHE:N	37:J:8869:HOH:O	2.51	0.43
14:L:17:SER:O	14:L:19:LYS:N	2.51	0.43
14:L:112:GLY:O	14:L:132:LYS:NZ	2.36	0.43
18:P:138:GLU:O	18:P:140:TYR:N	2.51	0.43
20:R:19:ARG:HA	20:R:142:ASP:OD1	2.17	0.43
20:R:91:LEU:CD2	20:R:143:VAL:HG22	2.49	0.43
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.53	0.43
31:3:22:VAL:HG11	31:3:67:LEU:HD13	1.99	0.43
1:0:31:C:H2'	37:0:7457:HOH:O	2.17	0.43
1:0:259:G:H21	15:M:58:GLN:NE2	2.15	0.43
1:0:541:C:O2'	1:0:542:A:H5"	2.17	0.43
1:0:2121:G:H3'	37:0:6357:HOH:O	2.19	0.43
1:0:2432:C:H1'	37:0:6075:HOH:O	2.17	0.43
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.43
37:0:9572:HOH:O	14:L:41:HIS:HE1	2.01	0.43
2:9:73:A:H2'	2:9:74:G:C8	2.54	0.43
3:A:48:ASP:HB3	37:A:8898:HOH:O	2.16	0.43
3:A:194:MET:HE2	3:A:199:HIS:CB	2.49	0.43
8:F:119:ARG:HD3	8:F:119:ARG:C	2.37	0.43
15:M:87:GLY:O	15:M:91:ILE:HD11	2.19	0.43
17:O:15:LYS:O	17:O:16:SER:C	2.56	0.43
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.45	0.43
22:T:103:LEU:C	22:T:105:ASP:H	2.21	0.43
25:W:60:GLU:O	25:W:63:GLU:HB2	2.18	0.43
30:2:41:HIS:N	30:2:45:ASN:HD22	2.09	0.43
1:0:368:C:H2'	1:0:369:G:H5'	2.00	0.43
1:0:818:A:O2'	28:Z:13:ARG:HD3	2.19	0.43
1:0:1181:A:C2'	1:0:1182:C:H5'	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1182:C:O5'	1:0:1182:C:H6	2.01	0.43
1:0:1557:G:O2'	1:0:1558:C:H5'	2.18	0.43
1:0:1688:G:H2'	1:0:1692:C:H42	1.83	0.43
1:0:1798:C:H4'	18:P:66:GLN:HG2	1.99	0.43
1:0:2266:A:H2'	1:0:2267:G:C8	2.53	0.43
1:0:2434:A:H2'	1:0:2435:U:O4'	2.18	0.43
4:B:77:PRO:HG2	4:B:151:VAL:HG22	2.00	0.43
4:B:79:MET:HG2	4:B:146:THR:HG22	2.01	0.43
4:B:280:VAL:HG13	4:B:334:SER:HA	2.00	0.43
5:C:98:ARG:NH1	37:C:8559:HOH:O	2.51	0.43
6:D:104:PHE:N	6:D:104:PHE:HD2	2.17	0.43
6:D:136:ARG:O	6:D:138:GLY:N	2.50	0.43
7:E:103:VAL:HG21	7:E:115:ARG:NH2	2.33	0.43
10:H:27:PRO:HD3	10:H:123:ILE:HG22	1.98	0.43
12:J:11:ILE:HD11	12:J:109:TYR:CD2	2.54	0.43
15:M:133:LEU:O	15:M:134:ILE:HD13	2.18	0.43
22:T:62:VAL:N	37:T:3851:HOH:O	2.51	0.43
22:T:85:GLU:HG2	22:T:86:GLU:H	1.83	0.43
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.49	0.43
27:Y:125:LYS:HB2	27:Y:126:PRO:HD2	2.00	0.43
1:0:88:G:H5'	1:0:88:G:C8	2.43	0.43
1:0:185:G:H4'	1:0:186:A:H4'	2.01	0.43
1:0:263:U:O4'	8:F:59:ILE:HD13	2.17	0.43
1:0:275:G:C2	1:0:376:C:N3	2.87	0.43
1:0:638:C:H2'	1:0:639:A:H8	1.83	0.43
1:0:1091:U:O2'	1:0:1092:A:H5'	2.19	0.43
1:0:1145:G:H1	1:0:1218:U:H3	1.66	0.43
1:0:1157:C:H2'	1:0:1158:G:H8	1.82	0.43
1:0:2311:A:H5'	10:H:120:PHE:CD1	2.53	0.43
1:0:2834:G:OP1	26:X:39:LYS:HE2	2.18	0.43
2:9:63:C:O2'	2:9:64:C:H5'	2.19	0.43
3:A:164:ARG:HE	3:A:164:ARG:HB3	1.60	0.43
11:I:107:LYS:CD	11:I:110:ASP:HB2	2.36	0.43
12:J:127:ILE:O	12:J:127:ILE:HG12	2.19	0.43
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.00	0.43
19:Q:93:ARG:HG3	19:Q:93:ARG:NH1	2.34	0.43
22:T:48:VAL:HG11	22:T:96:VAL:HG22	2.01	0.43
22:T:65:VAL:HG22	22:T:72:ILE:HG22	2.01	0.43
23:U:48:ASN:ND2	37:U:3104:HOH:O	2.50	0.43
25:W:90:TYR:CD1	25:W:90:TYR:N	2.86	0.43
25:W:125:HIS:HE1	37:W:3071:HOH:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:12:ILE:O	26:X:69:LYS:HA	2.17	0.43
30:2:41:HIS:O	30:2:45:ASN:HB2	2.18	0.43
1:0:100:C:H2'	1:0:101:C:H6	1.84	0.43
1:0:153:C:P	37:0:6629:HOH:O	2.76	0.43
1:0:250:C:O5'	1:0:250:C:H6	2.01	0.43
1:0:350:G:O2'	1:0:351:A:H5'	2.18	0.43
1:0:1544:U:H2'	1:0:1545:C:H6	1.84	0.43
1:0:1588:G:C6	1:0:1589:G:N1	2.86	0.43
1:0:1840:A:H4'	1:0:1841:C:O5'	2.18	0.43
1:0:1942:A:O2'	1:0:1943:C:H5'	2.19	0.43
1:0:2381:C:H2'	1:0:2382:A:C8	2.53	0.43
37:0:6069:HOH:O	27:Y:158:LYS:HD3	2.17	0.43
3:A:60:PHE:HD1	3:A:64:ASP:O	2.02	0.43
3:A:165:THR:O	3:A:165:THR:HG22	2.19	0.43
3:A:215:ILE:HG13	3:A:216:SER:N	2.32	0.43
4:B:62:ARG:CA	4:B:65:MET:HE3	2.47	0.43
5:C:168:ARG:NH2	5:C:190:ALA:O	2.51	0.43
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.83	0.43
10:H:36:MET:SD	10:H:88:MET:HE2	2.59	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.43
15:M:55:LYS:O	15:M:57:LYS:N	2.52	0.43
15:M:61:ILE:HG22	15:M:62:VAL:N	2.33	0.43
16:N:34:LEU:HD13	16:N:47:LEU:HD23	1.99	0.43
16:N:171:HIS:CE1	37:N:8863:HOH:O	2.71	0.43
18:P:10:ALA:HA	18:P:13:VAL:HG12	2.01	0.43
18:P:94:TRP:CH2	18:P:98:ILE:HG13	2.54	0.43
19:Q:28:ARG:CD	19:Q:92:ARG:NH1	2.81	0.43
20:R:39:THR:HB	20:R:42:GLU:CD	2.39	0.43
1:0:795:G:H1'	1:0:817:G:N2	2.33	0.43
1:0:835:U:OP1	4:B:230:GLN:NE2	2.48	0.43
1:0:911:G:H5'	1:0:932:U:OP1	2.19	0.43
1:0:1014:A:H2'	1:0:1015:C:H5'	1.99	0.43
1:0:1808:C:O2'	1:0:1809:G:H5'	2.19	0.43
1:0:1811:A:C2	1:0:2752:C:H1'	2.54	0.43
1:0:2830:U:H4'	37:0:9892:HOH:O	2.19	0.43
37:0:3038:HOH:O	11:I:87:PRO:HG2	2.19	0.43
3:A:232:ARG:NH2	3:A:236:GLY:O	2.51	0.43
4:B:76:THR:N	4:B:77:PRO:HD3	2.34	0.43
5:C:188:ARG:HD2	37:C:8677:HOH:O	2.19	0.43
6:D:94:ALA:HB3	6:D:97:GLN:HG3	1.99	0.43
8:F:45:ALA:HA	37:F:3461:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.49	0.43
23:U:36:CYS:O	23:U:37:GLU:C	2.56	0.43
27:Y:110:SER:O	27:Y:111:ASP:C	2.56	0.43
27:Y:149:GLN:NE2	37:Y:8910:HOH:O	2.50	0.43
1:0:622:G:P	27:Y:148:GLY:HA3	2.58	0.43
1:0:644:G:H5'	1:0:644:G:N3	2.34	0.43
1:0:902:G:N7	14:L:18:HIS:CD2	2.79	0.43
1:0:951:A:C2'	1:0:952:G:H5'	2.49	0.43
1:0:1163:G:N2	37:0:5830:HOH:O	2.51	0.43
1:0:1350:U:H1'	37:0:9473:HOH:O	2.19	0.43
1:0:1379:A:H1'	37:0:9503:HOH:O	2.19	0.43
2:9:51:A:C5	16:N:41:LYS:HE2	2.54	0.43
2:9:61:C:H2'	2:9:62:A:C8	2.53	0.43
3:A:55:VAL:CG1	3:A:67:LEU:HB3	2.48	0.43
5:C:5:ILE:CG2	5:C:6:TYR:N	2.82	0.43
5:C:35:VAL:HG21	5:C:227:GLY:HA2	2.00	0.43
13:K:10:GLN:NE2	13:K:10:GLN:N	2.42	0.43
15:M:33:ASN:HB2	37:M:8866:HOH:O	2.19	0.43
1:0:166:A:N7	14:L:25:GLY:HA2	2.34	0.43
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.43
1:0:1827:G:H2'	1:0:1828:G:C8	2.54	0.43
1:0:1828:G:H5'	37:0:3780:HOH:O	2.18	0.43
1:0:2870:C:O2'	1:0:2871:G:H5'	2.18	0.43
37:0:4471:HOH:O	15:M:4:ALA:HB3	2.19	0.43
2:9:22:G:H5'	37:9:8723:HOH:O	2.19	0.43
2:9:56:A:O2'	6:D:14:ARG:HD3	2.19	0.43
4:B:182:VAL:O	4:B:184:ASP:N	2.52	0.43
8:F:37:THR:O	8:F:41:GLU:HG3	2.18	0.43
8:F:67:ALA:C	8:F:69:GLU:H	2.22	0.43
14:L:147:GLU:C	37:L:8856:HOH:O	2.57	0.43
17:O:14:LEU:CG	17:O:102:ILE:HD11	2.49	0.43
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.53	0.43
22:T:63:ILE:HD11	22:T:75:GLU:OE1	2.19	0.43
25:W:1:MET:N	25:W:103:GLU:OE2	2.52	0.43
25:W:108:ARG:C	25:W:110:GLN:N	2.72	0.43
26:X:8:ARG:NH1	37:X:2479:HOH:O	2.52	0.43
27:Y:189:ASN:HD22	27:Y:191:ASP:N	2.17	0.43
1:0:240:C:O2	1:0:240:C:H2'	2.19	0.42
1:0:275:G:N2	1:0:376:C:C2	2.87	0.42
1:0:319:A:H4'	1:0:338:C:C4	2.53	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:795:G:N3	1:0:817:G:C2	2.87	0.42
1:0:1759:A:N3	1:0:1818:C:H2'	2.34	0.42
1:0:1876:C:C4	3:A:123:GLY:HA3	2.54	0.42
1:0:2385:G:H2'	1:0:2386:U:C6	2.54	0.42
1:0:2518:C:H2'	1:0:2519:C:O4'	2.19	0.42
1:0:2669:U:H2'	1:0:2670:G:C8	2.53	0.42
1:0:2673:U:C2'	1:0:2674:G:H5'	2.48	0.42
1:0:2781:U:H2'	1:0:2782:G:H5'	2.01	0.42
3:A:74:VAL:O	28:Z:65:THR:HG23	2.19	0.42
3:A:191:GLY:O	3:A:194:MET:HG3	2.19	0.42
4:B:55:ASN:CB	4:B:63:GLU:HA	2.40	0.42
4:B:277:GLU:N	4:B:278:PRO:CD	2.81	0.42
5:C:51:TYR:CE2	29:1:53:LYS:HB3	2.54	0.42
6:D:89:PRO:O	6:D:91:ALA:N	2.52	0.42
6:D:91:ALA:HB1	37:D:5198:HOH:O	2.18	0.42
6:D:138:GLY:O	6:D:141:VAL:HG23	2.19	0.42
6:D:153:THR:C	6:D:155:HIS:H	2.22	0.42
20:R:125:ARG:O	20:R:126:LYS:CB	2.62	0.42
21:S:39:ASP:O	21:S:40:ALA:C	2.57	0.42
22:T:48:VAL:CG1	22:T:49:GLU:N	2.81	0.42
26:X:27:ASP:OD2	26:X:27:ASP:N	2.48	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
1:0:488:U:H2'	37:0:3801:HOH:O	2.19	0.42
1:0:695:C:H2'	1:0:696:C:H6	1.84	0.42
1:0:1353:C:H6	37:0:4479:HOH:O	2.01	0.42
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.42
1:0:2064:U:H5'	1:0:2652:U:O3'	2.19	0.42
1:0:2506:A:O2'	1:0:2507:G:O5'	2.38	0.42
1:0:2607:U:H4'	37:0:9249:HOH:O	2.18	0.42
1:0:2687:G:O2'	1:0:2688:U:H5'	2.18	0.42
37:0:4423:HOH:O	3:A:6:GLY:HA3	2.19	0.42
2:9:28:U:H2'	2:9:29:C:C6	2.54	0.42
4:B:57:GLU:OE1	4:B:60:SER:HB2	2.19	0.42
5:C:15:GLU:O	5:C:15:GLU:HG3	2.19	0.42
6:D:35:ALA:N	37:D:5576:HOH:O	2.52	0.42
6:D:169:THR:O	6:D:169:THR:HG22	2.19	0.42
8:F:48:VAL:HG23	8:F:74:PHE:HB2	2.00	0.42
10:H:68:SER:O	10:H:69:ARG:C	2.57	0.42
13:K:98:VAL:HG12	13:K:99:ASP:N	2.34	0.42
15:M:43:PRO:HD2	37:M:8919:HOH:O	2.19	0.42
16:N:119:GLN:HG2	16:N:123:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:16:VAL:HG12	18:P:17:GLY:H	1.83	0.42
19:Q:40:HIS:CE1	19:Q:94:GLN:HA	2.54	0.42
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.53	0.42
21:S:77:VAL:O	21:S:80:ARG:HG2	2.20	0.42
22:T:28:SER:HB2	37:T:4606:HOH:O	2.19	0.42
26:X:25:ARG:HD3	26:X:64:ALA:O	2.19	0.42
28:Z:28:GLU:O	28:Z:29:ILE:C	2.58	0.42
1:0:39:G:N2	1:0:444:C:C2	2.87	0.42
1:0:480:C:H4'	37:0:7494:HOH:O	2.18	0.42
1:0:823:U:H2'	1:0:824:G:O4'	2.19	0.42
1:0:1055:G:OP2	10:H:99:ARG:NH1	2.52	0.42
1:0:1215:A:O3'	1:0:1216:G:C4'	2.67	0.42
1:0:1496:A:H2'	1:0:1497:G:C8	2.54	0.42
1:0:1933:G:O2'	1:0:1934:A:H5'	2.18	0.42
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.55	0.42
4:B:122:ASP:O	4:B:123:ALA:C	2.57	0.42
4:B:241:PRO:HD2	37:B:8956:HOH:O	2.19	0.42
5:C:19:PRO:HD2	5:C:240:LEU:HD21	2.02	0.42
5:C:27:ARG:NH1	5:C:29:ASP:OD2	2.52	0.42
7:E:93:MET:HG2	7:E:94:GLN:H	1.84	0.42
10:H:12:ILE:HD12	10:H:57:THR:CG2	2.46	0.42
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.49	0.42
12:J:88:PRO:HA	35:J:8802:CL:CL	2.57	0.42
13:K:34:VAL:HG22	13:K:47:ALA:HB2	2.01	0.42
15:M:69:LYS:HG3	15:M:126:GLN:HA	2.00	0.42
15:M:139:PRO:HA	15:M:142:GLN:HB2	2.01	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.81	0.42
25:W:110:GLN:HE21	25:W:110:GLN:CA	2.27	0.42
26:X:12:ILE:HB	26:X:70:ILE:CG2	2.49	0.42
1:0:345:G:N2	1:0:346:U:H1'	2.34	0.42
1:0:445:U:H2'	1:0:446:G:C8	2.53	0.42
1:0:659:A:N1	17:O:42:GLU:OE2	2.52	0.42
1:0:2011:A:H5'	1:0:2013:G:H1'	2.01	0.42
1:0:2248:C:C2	1:0:2254:G:C2	3.07	0.42
5:C:19:PRO:HD2	5:C:240:LEU:CD2	2.49	0.42
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.42
7:E:101:GLU:CB	7:E:117:THR:HA	2.50	0.42
14:L:98:GLU:C	14:L:99:GLU:HG3	2.39	0.42
27:Y:144:ARG:CZ	37:Y:8921:HOH:O	2.66	0.42
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.92	0.42
1:0:733:U:H5"	37:0:9658:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1221:G:C8	37:0:5773:HOH:O	2.57	0.42
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.53	0.42
1:0:1878:G:C1'	37:0:5905:HOH:O	2.65	0.42
1:0:1916:C:H2'	1:0:1917:G:O4'	2.20	0.42
1:0:2408:A:H4'	31:3:15:ASN:O	2.20	0.42
1:0:2673:U:H2'	1:0:2674:G:H5'	2.01	0.42
2:9:110:G:H2'	2:9:111:U:H5'	2.01	0.42
5:C:144:PHE:HE1	5:C:153:VAL:HG13	1.84	0.42
5:C:246:ARG:CZ	37:C:8633:HOH:O	2.67	0.42
6:D:170:TYR:CD1	6:D:170:TYR:N	2.87	0.42
8:F:77:VAL:HG21	8:F:83:LEU:HD13	2.01	0.42
9:G:12:ILE:HG22	9:G:12:ILE:O	2.19	0.42
10:H:34:HIS:HD2	10:H:90:LEU:O	2.03	0.42
13:K:63:GLU:HG2	37:K:6344:HOH:O	2.19	0.42
14:L:73:VAL:HG23	14:L:74:THR:N	2.35	0.42
16:N:23:ARG:NH1	37:N:8842:HOH:O	2.52	0.42
16:N:116:PHE:O	16:N:119:GLN:HB3	2.19	0.42
16:N:132:ASN:N	37:N:8851:HOH:O	2.52	0.42
17:O:14:LEU:HA	17:O:102:ILE:CD1	2.49	0.42
22:T:30:ASP:O	22:T:33:GLU:HB3	2.20	0.42
22:T:103:LEU:O	22:T:105:ASP:N	2.53	0.42
24:V:42:ASN:N	24:V:43:PRO:HD3	2.34	0.42
27:Y:98:GLN:HA	37:Y:8839:HOH:O	2.19	0.42
1:0:282:C:H1'	1:0:368:C:H41	1.79	0.42
1:0:567:U:H5"	37:0:6184:HOH:O	2.20	0.42
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.03	0.42
1:0:1166:A:H1'	1:0:1192:A:C2	2.55	0.42
1:0:1213:C:C2'	1:0:1214:G:H5'	2.50	0.42
1:0:1396:C:H1'	18:P:1:THR:O	2.20	0.42
1:0:1473:U:C1'	29:1:42:SER:HB3	2.50	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.42
1:0:2453:G:H4'	14:L:50:GLY:C	2.39	0.42
1:0:2909:G:H2'	1:0:2910:A:H8	1.84	0.42
37:0:5502:HOH:O	7:E:57:LYS:HE2	2.19	0.42
37:0:9010:HOH:O	5:C:107:ARG:NH1	2.53	0.42
2:9:4:G:H1'	37:9:8716:HOH:O	2.20	0.42
2:9:47:A:C2	2:9:48:C:C2	3.08	0.42
2:9:56:A:H1'	6:D:14:ARG:HG2	2.02	0.42
2:9:72:C:O2'	2:9:73:A:H5'	2.20	0.42
3:A:180:LYS:HB2	37:A:8916:HOH:O	2.20	0.42
4:B:79:MET:C	4:B:80:ARG:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:40:ALA:O	5:C:43:LYS:HB2	2.20	0.42
5:C:214:THR:CG2	5:C:216:SER:H	2.32	0.42
10:H:92:LYS:HA	10:H:92:LYS:HD3	1.88	0.42
11:I:115:ASP:C	11:I:117:THR:N	2.69	0.42
15:M:66:SER:HB3	15:M:128:TRP:NE1	2.34	0.42
15:M:146:ASP:O	15:M:147:LEU:HG	2.18	0.42
22:T:103:LEU:HD22	22:T:112:LEU:CD1	2.49	0.42
30:2:48:ASP:O	30:2:49:GLU:CB	2.66	0.42
1:0:328:U:O4'	5:C:202:THR:HG22	2.20	0.42
1:0:417:G:P	37:0:7190:HOH:O	2.77	0.42
1:0:1235:G:N2	37:0:4680:HOH:O	2.51	0.42
1:0:2132:C:H2'	37:0:7327:HOH:O	2.20	0.42
1:0:2689:A:H2'	1:0:2690:U:H5'	2.02	0.42
1:0:2694:A:C4'	7:E:91:PHE:HE1	2.31	0.42
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.19	0.42
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.84	0.42
4:B:71:VAL:HG11	4:B:296:LEU:HB3	2.02	0.42
4:B:178:ALA:O	4:B:179:LEU:C	2.57	0.42
6:D:23:VAL:HG22	6:D:73:VAL:HB	2.02	0.42
6:D:166:ILE:H	6:D:166:ILE:HG13	1.68	0.42
7:E:100:ASP:HB2	37:E:2789:HOH:O	2.18	0.42
13:K:23:ASN:HA	37:K:7075:HOH:O	2.19	0.42
15:M:18:GLY:O	15:M:21:ALA:HB3	2.19	0.42
15:M:24:GLN:O	15:M:28:GLN:HG3	2.19	0.42
16:N:176:ARG:O	16:N:180:LEU:HD13	2.19	0.42
18:P:58:SER:HB3	37:P:184:HOH:O	2.20	0.42
20:R:66:VAL:HG13	20:R:79:ARG:HE	1.85	0.42
20:R:141:VAL:HG12	20:R:142:ASP:N	2.34	0.42
24:V:1:THR:C	24:V:3:LEU:H	2.23	0.42
1:0:414:C:H5'	37:0:5897:HOH:O	2.20	0.42
1:0:1335:C:OP2	27:Y:207:SER:CB	2.67	0.42
1:0:1684:A:H1'	30:2:43:ARG:NH2	2.28	0.42
1:0:2000:G:O2'	1:0:2001:G:H5'	2.20	0.42
1:0:2002:C:C2'	1:0:2003:U:H5'	2.49	0.42
37:0:5206:HOH:O	3:A:164:ARG:CZ	2.67	0.42
37:0:6661:HOH:O	3:A:165:THR:HG23	2.18	0.42
3:A:36:ASP:O	3:A:37:VAL:C	2.58	0.42
6:D:11:HIS:CG	6:D:12:GLU:N	2.88	0.42
10:H:86:TYR:CD1	10:H:86:TYR:C	2.93	0.42
14:L:82:ALA:O	14:L:83:GLU:C	2.58	0.42
14:L:105:TYR:N	37:L:8868:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:47:ASP:CG	15:M:48:LYS:H	2.22	0.42
22:T:71:VAL:HG13	22:T:91:LEU:H	1.85	0.42
25:W:108:ARG:C	25:W:110:GLN:H	2.23	0.42
26:X:45:GLU:HG3	37:X:6178:HOH:O	2.19	0.42
31:3:87:ARG:HG2	37:3:8869:HOH:O	2.19	0.42
1:0:52:A:H2'	1:0:53:C:O4'	2.20	0.42
1:0:57:C:H2'	1:0:58:C:O4'	2.20	0.42
1:0:281:U:H2'	1:0:282:C:O4'	2.19	0.42
1:0:319:A:H4'	1:0:338:C:C5	2.54	0.42
1:0:366:U:H2'	1:0:367:G:O4'	2.20	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.20	0.42
1:0:432:G:N2	1:0:433:C:C2	2.87	0.42
1:0:598:C:H2'	1:0:599:G:H8	1.82	0.42
1:0:1008:C:OP1	10:H:19:ARG:NH2	2.51	0.42
1:0:1276:U:H3'	17:O:19:ARG:HH11	1.85	0.42
1:0:1311:G:C2	1:0:1312:G:C8	3.08	0.42
1:0:1449:G:H2'	1:0:1493:A:C2	2.55	0.42
1:0:2134:G:N2	1:0:2242:U:C2	2.88	0.42
4:B:88:GLU:HB3	4:B:97:LEU:HG	2.01	0.42
4:B:279:THR:CG2	4:B:280:VAL:N	2.83	0.42
8:F:11:ASP:HA	8:F:14:ASP:OD2	2.19	0.42
8:F:60:VAL:O	8:F:62:HIS:N	2.53	0.42
10:H:57:THR:N	10:H:132:ALA:HB2	2.34	0.42
11:I:91:PHE:CD2	11:I:131:GLY:HA2	2.55	0.42
12:J:42:GLU:HG2	12:J:43:ARG:HG3	2.01	0.42
12:J:121:LEU:HD21	12:J:129:PHE:CD2	2.55	0.42
13:K:41:LYS:HE3	37:K:7871:HOH:O	2.18	0.42
13:K:72:VAL:O	13:K:95:ALA:HA	2.19	0.42
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.86	0.42
14:L:67:ARG:O	14:L:71:GLU:HG3	2.20	0.42
15:M:139:PRO:O	15:M:143:ASN:ND2	2.53	0.42
27:Y:103:THR:O	27:Y:103:THR:HG22	2.20	0.42
27:Y:234:VAL:CG1	27:Y:235:GLU:N	2.82	0.42
1:0:383:A:H4'	37:0:5126:HOH:O	2.19	0.42
1:0:613:C:H2'	1:0:614:U:H6	1.85	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.55	0.42
1:0:1758:U:H2'	1:0:1759:A:O4'	2.20	0.42
1:0:1846:U:O2'	3:A:172:ALA:HB2	2.19	0.42
1:0:1860:U:H2'	1:0:1861:C:O4'	2.19	0.42
1:0:2764:C:O2'	1:0:2765:C:H5'	2.20	0.42
1:0:2825:C:H4'	1:0:2826:G:O5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:ARG:HH11	3:A:208:HIS:CD2	2.38	0.42
4:B:7:ARG:CZ	4:B:7:ARG:HB2	2.50	0.42
4:B:24:PRO:C	4:B:25:ARG:HD3	2.39	0.42
5:C:93:LYS:HB3	5:C:95:GLU:OE1	2.20	0.42
12:J:51:GLU:O	12:J:55:GLU:HG3	2.19	0.42
16:N:43:VAL:O	16:N:43:VAL:HG12	2.20	0.42
16:N:62:HIS:O	16:N:65:ASP:OD1	2.38	0.42
18:P:138:GLU:C	18:P:140:TYR:N	2.73	0.42
21:S:7:HIS:HB2	21:S:8:PRO:CD	2.50	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.97	0.42
26:X:22:ASN:O	26:X:25:ARG:HG3	2.20	0.42
1:0:790:A:H2'	1:0:791:A:O4'	2.20	0.41
1:0:858:U:H2'	1:0:859:C:H6	1.85	0.41
1:0:1044:C:C5'	37:0:8844:HOH:O	2.67	0.41
1:0:1504:A:O2'	1:0:1506:U:OP2	2.31	0.41
1:0:1601:G:H1'	37:0:9701:HOH:O	2.18	0.41
1:0:1703:G:N2	18:P:57:ASN:HD21	2.18	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
1:0:2248:C:H2'	1:0:2249:G:H8	1.85	0.41
1:0:2392:C:O5'	1:0:2392:C:H6	2.03	0.41
1:0:2511:A:H2'	1:0:2512:U:O4'	2.19	0.41
1:0:2896:A:P	26:X:15:ARG:NH1	2.93	0.41
2:9:3:A:C8	2:9:3:A:O5'	2.74	0.41
2:9:9:C:H2'	2:9:10:C:H5'	2.02	0.41
6:D:35:ALA:C	6:D:37:ALA:H	2.22	0.41
8:F:49:PHE:N	8:F:49:PHE:CD1	2.87	0.41
8:F:99:THR:HG23	8:F:99:THR:O	2.20	0.41
9:G:24:VAL:HA	9:G:27:ILE:HD12	2.02	0.41
17:O:32:ARG:HG2	17:O:32:ARG:HH11	1.85	0.41
17:O:77:ALA:HB1	17:O:98:LEU:HD12	2.02	0.41
17:O:96:VAL:HG12	17:O:97:SER:N	2.35	0.41
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.20	0.41
23:U:6:CYS:C	23:U:8:TYR:N	2.74	0.41
1:0:253:U:H1'	1:0:256:C:H41	1.86	0.41
1:0:372:A:H2'	1:0:373:G:H8	1.86	0.41
1:0:794:U:H3	1:0:819:A:N6	2.11	0.41
1:0:844:A:H2'	37:0:9368:HOH:O	2.19	0.41
1:0:847:C:H5	37:0:9056:HOH:O	2.02	0.41
1:0:1194:A:O5'	1:0:1194:A:H8	2.02	0.41
1:0:1503:U:H2'	1:0:1504:A:O4'	2.20	0.41
1:0:1771:U:H4'	1:0:1772:C:OP2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2096:A:N3	1:0:2096:A:H3'	2.35	0.41
1:0:2135:A:O2'	1:0:2136:G:H5'	2.19	0.41
1:0:2365:G:H4'	19:Q:45:PRO:O	2.20	0.41
1:0:2420:G:H2'	1:0:2421:G:C8	2.55	0.41
1:0:2506:A:H1'	37:0:3545:HOH:O	2.20	0.41
1:0:2729:C:H2'	1:0:2730:G:H8	1.85	0.41
37:0:3151:HOH:O	19:Q:16:ASN:HB2	2.19	0.41
2:9:41:C:O4'	6:D:50:VAL:HG22	2.21	0.41
2:9:73:A:N1	2:9:108:C:N3	2.68	0.41
5:C:141:SER:C	5:C:143:ASP:H	2.23	0.41
5:C:150:THR:C	5:C:152:GLU:N	2.74	0.41
6:D:140:ARG:HH11	6:D:140:ARG:HG3	1.84	0.41
7:E:2:ARG:HA	7:E:49:ILE:O	2.20	0.41
10:H:46:TYR:HE2	10:H:85:ASP:O	2.03	0.41
12:J:21:ARG:HH11	12:J:21:ARG:HG2	1.85	0.41
14:L:117:GLU:HG3	14:L:117:GLU:O	2.21	0.41
16:N:67:ALA:HA	16:N:71:TRP:CB	2.48	0.41
16:N:70:GLY:O	16:N:71:TRP:C	2.57	0.41
16:N:178:THR:O	16:N:181:ASP:HB3	2.20	0.41
20:R:6:VAL:HG21	20:R:113:HIS:CD2	2.54	0.41
20:R:125:ARG:NH1	20:R:134:SER:HB2	2.33	0.41
22:T:49:GLU:CG	22:T:97:ARG:HB3	2.50	0.41
25:W:36:PRO:HD2	25:W:41:TYR:CD1	2.55	0.41
25:W:140:LYS:C	25:W:141:HIS:HD2	2.23	0.41
28:Z:17:ARG:HB2	28:Z:18:TYR:CE1	2.54	0.41
1:0:329:A:OP2	5:C:206:ASN:HB2	2.19	0.41
1:0:447:A:O2'	1:0:448:G:H5'	2.20	0.41
1:0:474:C:O3'	5:C:73:LEU:CD2	2.68	0.41
1:0:566:A:H2'	1:0:567:U:O4'	2.20	0.41
1:0:890:C:O2'	29:1:50:TRP:O	2.35	0.41
1:0:1353:C:N3	14:L:5:LYS:NZ	2.68	0.41
1:0:1439:C:H4'	20:R:132:ARG:NH1	2.34	0.41
1:0:1548:U:O2'	1:0:1549:C:H5'	2.20	0.41
1:0:1576:G:H2'	1:0:1577:U:O4'	2.21	0.41
1:0:1773:G:H2'	1:0:1774:G:H5'	2.02	0.41
1:0:1773:G:C2'	1:0:1774:G:H5'	2.50	0.41
1:0:1856:C:H5'	1:0:1858:A:O4'	2.21	0.41
1:0:2039:A:H4'	1:0:2760:C:O2'	2.21	0.41
1:0:2079:G:H2'	1:0:2080:G:O4'	2.20	0.41
1:0:2416:G:H2'	1:0:2417:C:C6	2.55	0.41
1:0:2766:A:O2'	1:0:2767:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:27:C:N3	37:9:8644:HOH:O	2.37	0.41
3:A:54:PRO:HG2	3:A:160:ALA:HB3	2.02	0.41
3:A:94:LEU:N	3:A:94:LEU:CD2	2.81	0.41
3:A:206:ARG:NH1	3:A:208:HIS:CD2	2.88	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.90	0.41
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.21	0.41
5:C:2:GLN:HB3	37:C:8537:HOH:O	2.20	0.41
6:D:128:LEU:N	37:D:6007:HOH:O	2.52	0.41
10:H:37:GLY:HA3	10:H:87:LYS:HA	2.01	0.41
17:O:47:ARG:HA	17:O:50:ARG:HH12	1.85	0.41
22:T:9:LYS:HE3	22:T:13:ARG:HD2	2.01	0.41
25:W:68:THR:HG23	25:W:69:ARG:N	2.36	0.41
25:W:93:ILE:HB	37:W:4301:HOH:O	2.19	0.41
26:X:21:PRO:HG2	26:X:24:LYS:HD3	2.01	0.41
30:2:21:VAL:O	30:2:22:PRO:C	2.58	0.41
1:0:178:U:H2'	1:0:179:C:H6	1.84	0.41
1:0:182:G:O3'	15:M:157:ASP:OD2	2.38	0.41
1:0:201:G:N2	35:0:8805:CL:CL	2.91	0.41
1:0:318:U:O2'	1:0:319:A:OP1	2.35	0.41
1:0:1194:A:O2'	1:0:1195:G:H5'	2.21	0.41
1:0:1246:A:H5'	1:0:1246:A:H8	1.85	0.41
1:0:1266:U:O2'	1:0:1267:C:H5'	2.20	0.41
1:0:1711:A:C2'	1:0:1712:A:H5'	2.50	0.41
1:0:2090:G:H2'	1:0:2091:G:C8	2.55	0.41
1:0:2613:G:O2'	1:0:2614:C:H5'	2.20	0.41
37:0:5207:HOH:O	14:L:34:GLY:HA2	2.19	0.41
2:9:19:G:O2'	2:9:20:G:H5'	2.21	0.41
6:D:19:GLU:HG3	37:D:6165:HOH:O	2.20	0.41
6:D:81:GLU:O	6:D:83:PHE:N	2.53	0.41
10:H:50:ILE:HD12	10:H:149:VAL:HG11	2.03	0.41
12:J:24:SER:HA	12:J:86:MET:SD	2.61	0.41
13:K:76:GLN:HA	13:K:93:ASN:HA	2.01	0.41
15:M:31:TRP:C	15:M:33:ASN:H	2.24	0.41
15:M:134:ILE:O	15:M:136:PRO:CD	2.67	0.41
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.84	0.41
18:P:135:ALA:O	18:P:139:ARG:HG3	2.20	0.41
21:S:7:HIS:HD2	21:S:27:ALA:HB3	1.83	0.41
31:3:43:ASN:ND2	37:3:8806:HOH:O	2.54	0.41
1:0:569:A:H5"	1:0:587:A:N1	2.35	0.41
1:0:622:G:O2'	1:0:623:U:H5'	2.19	0.41
1:0:721:A:H5"	17:O:51:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:963:C:O5'	1:0:963:C:H6	2.03	0.41
1:0:1051:C:H2'	1:0:1052:G:O4'	2.21	0.41
1:0:1746:A:O4'	1:0:1747:A:C2	2.73	0.41
37:0:6465:HOH:O	22:T:38:ARG:NH1	2.54	0.41
3:A:48:ASP:HA	3:A:49:PRO:HD3	1.93	0.41
4:B:36:PRO:CG	4:B:169:GLY:H	2.27	0.41
5:C:94:THR:HG22	37:C:8684:HOH:O	2.21	0.41
7:E:84:MET:HA	7:E:167:TYR:O	2.20	0.41
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.36	0.41
17:O:78:ALA:C	17:O:98:LEU:HD13	2.41	0.41
20:R:59:PHE:HZ	20:R:81:PRO:HG3	1.85	0.41
20:R:89:LEU:HD23	20:R:89:LEU:HA	1.85	0.41
25:W:52:VAL:CG2	25:W:53:ALA:N	2.82	0.41
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.56	0.41
26:X:25:ARG:HB3	26:X:66:THR:HG22	2.03	0.41
26:X:43:VAL:HG22	26:X:76:ARG:HH12	1.84	0.41
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.50	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:251:C:C2	1:0:259:G:C2	3.09	0.41
1:0:1634:G:H2'	1:0:1635:U:C6	2.54	0.41
1:0:1667:A:H2'	1:0:1668:U:C6	2.55	0.41
1:0:2839:C:H2'	1:0:2840:A:H5"	2.02	0.41
1:0:2911:C:H2'	1:0:2912:C:C6	2.56	0.41
37:9:8645:HOH:O	16:N:41:LYS:HD2	2.20	0.41
5:C:5:ILE:HD11	5:C:16:VAL:HG23	2.03	0.41
5:C:233:THR:CG2	5:C:234:VAL:N	2.80	0.41
16:N:74:PRO:HG2	16:N:159:TYR:CZ	2.56	0.41
16:N:113:SER:N	37:N:8848:HOH:O	2.53	0.41
16:N:155:GLU:HG2	16:N:156:GLU:HG3	2.03	0.41
24:V:51:LYS:O	24:V:54:ALA:HB3	2.21	0.41
25:W:73:LEU:HD12	25:W:113:SER:HA	2.03	0.41
31:3:8:ASN:O	31:3:9:THR:HB	2.20	0.41
1:0:151:A:C2	1:0:442:A:C8	3.09	0.41
1:0:183:A:H1'	15:M:161:ARG:NH1	2.36	0.41
1:0:302:A:H5"	37:0:7219:HOH:O	2.21	0.41
1:0:338:C:H5"	37:0:5626:HOH:O	2.20	0.41
1:0:431:G:O2'	1:0:432:G:H5'	2.21	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.56	0.41
1:0:1552:G:C6	1:0:1553:C:C4	3.08	0.41
1:0:1761:U:H4'	18:P:82:GLY:O	2.20	0.41
1:0:1789:G:H2'	1:0:1790:C:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
1:0:2898:G:H4'	4:B:288:GLY:HA2	2.02	0.41
37:0:9502:HOH:O	15:M:182:LYS:HE3	2.20	0.41
2:9:4:G:O2'	16:N:44:ARG:NH2	2.54	0.41
2:9:106:U:O2'	2:9:107:C:H5'	2.21	0.41
3:A:9:ARG:O	3:A:10:GLY:C	2.59	0.41
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.50	0.41
7:E:68:HIS:O	7:E:72:MET:HG3	2.21	0.41
8:F:46:GLU:N	37:F:3461:HOH:O	2.53	0.41
10:H:123:ILE:N	10:H:123:ILE:CD1	2.84	0.41
11:I:72:GLU:C	11:I:74:ILE:H	2.24	0.41
12:J:142:ASN:O	12:J:144:THR:HG23	2.21	0.41
16:N:37:ARG:HD3	16:N:37:ARG:HA	1.94	0.41
16:N:90:LEU:HD23	16:N:125:ALA:HB1	2.03	0.41
17:O:33:LEU:HA	17:O:40:HIS:NE2	2.36	0.41
17:O:77:ALA:HA	17:O:96:VAL:O	2.21	0.41
25:W:24:LEU:O	25:W:26:ILE:HG23	2.21	0.41
31:3:7:PHE:CD1	31:3:7:PHE:C	2.93	0.41
1:0:12:U:H2'	1:0:13:G:H5'	2.01	0.41
1:0:68:U:O2'	1:0:69:A:H5"	2.21	0.41
1:0:218:C:C5	1:0:220:C:C4	3.08	0.41
1:0:244:C:OP1	8:F:42:ARG:NH2	2.51	0.41
1:0:290:C:O2'	1:0:291:C:H5'	2.19	0.41
1:0:356:C:H3'	1:0:357:A:H2'	2.02	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
1:0:1079:A:H4'	1:0:2078:U:H5'	2.03	0.41
1:0:1838:U:O2'	1:0:2644:C:H5'	2.21	0.41
1:0:1904:A:H2'	1:0:1905:U:O4'	2.21	0.41
1:0:2296:C:H2'	1:0:2297:U:H6	1.86	0.41
1:0:2506:A:N6	1:0:2511:A:O2'	2.52	0.41
1:0:2598:U:O2	1:0:2600:A:C8	2.73	0.41
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.41
3:A:87:GLU:HB2	37:A:8918:HOH:O	2.20	0.41
3:A:211:LYS:CB	37:A:8914:HOH:O	2.64	0.41
6:D:15:GLU:O	6:D:16:PRO:O	2.39	0.41
6:D:35:ALA:HB3	37:D:6716:HOH:O	2.20	0.41
7:E:38:ILE:HA	7:E:51:SER:HB2	2.02	0.41
10:H:32:ALA:N	10:H:66:GLU:OE1	2.44	0.41
13:K:28:GLU:HG2	13:K:58:THR:HB	2.03	0.41
16:N:35:VAL:HB	16:N:46:GLN:HB2	2.03	0.41
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:97:ARG:HD2	37:P:162:HOH:O	2.21	0.41
22:T:89:ARG:C	22:T:89:ARG:HD2	2.41	0.41
24:V:39:ALA:H	24:V:40:PRO:CD	2.25	0.41
25:W:62:LEU:HD23	25:W:97:ALA:HB1	2.02	0.41
25:W:131:PRO:O	25:W:136:GLY:N	2.48	0.41
26:X:18:ARG:NH1	37:X:2351:HOH:O	2.53	0.41
1:0:154:C:C2	1:0:155:C:C5	3.09	0.41
1:0:196:G:H1'	1:0:198:A:N7	2.35	0.41
1:0:249:G:H1'	1:0:265:U:O2	2.21	0.41
1:0:764:C:OP1	5:C:87:ARG:NH1	2.54	0.41
1:0:772:G:H2'	1:0:773:A:O4'	2.20	0.41
1:0:1064:U:H2'	1:0:1065:G:C8	2.56	0.41
1:0:1120:U:H2'	1:0:1121:G:H5'	2.02	0.41
1:0:1191:A:H3'	1:0:1192:A:H5"	2.02	0.41
1:0:1473:U:O4'	29:1:42:SER:HB3	2.20	0.41
1:0:1553:C:H2'	1:0:1554:C:C6	2.56	0.41
1:0:1767:A:O2'	1:0:1768:C:H5'	2.21	0.41
1:0:1794:G:P	18:P:133:SER:HB2	2.60	0.41
1:0:2028:U:H2'	1:0:2029:C:H6	1.86	0.41
1:0:2032:U:H1'	37:0:6047:HOH:O	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.86	0.41
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.56	0.41
1:0:2731:G:H2'	1:0:2732:U:O4'	2.20	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.56	0.41
37:0:9389:HOH:O	15:M:186:SER:HB3	2.21	0.41
2:9:38:A:H2	2:9:43:G:H5"	1.85	0.41
2:9:39:U:H3'	37:9:8707:HOH:O	2.20	0.41
3:A:36:ASP:CG	3:A:85:SER:H	2.25	0.41
4:B:33:ASP:O	4:B:34:GLY:O	2.38	0.41
4:B:162:MET:HG3	4:B:310:ARG:NE	2.35	0.41
5:C:57:PRO:HD2	5:C:73:LEU:HD22	2.01	0.41
6:D:25:MET:HE1	6:D:37:ALA:O	2.20	0.41
6:D:95:THR:O	6:D:97:GLN:N	2.54	0.41
10:H:140:TYR:CD1	10:H:140:TYR:N	2.89	0.41
11:I:114:TYR:CD1	11:I:114:TYR:N	2.88	0.41
11:I:126:THR:C	37:I:7439:HOH:O	2.59	0.41
12:J:130:VAL:HG11	12:J:135:ILE:CG1	2.51	0.41
14:L:89:PHE:O	14:L:119:THR:N	2.50	0.41
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.02	0.41
15:M:46:LEU:HD22	15:M:50:ARG:CD	2.51	0.41
16:N:76:GLY:N	37:N:8840:HOH:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:25:VAL:HG23	17:O:26:TRP:N	2.36	0.41
18:P:13:VAL:HG11	18:P:40:VAL:HG12	2.02	0.41
18:P:63:ARG:HA	18:P:66:GLN:HB2	2.02	0.41
19:Q:77:ASP:N	19:Q:80:LYS:O	2.53	0.41
22:T:61:GLU:N	37:T:4772:HOH:O	2.53	0.41
22:T:103:LEU:N	22:T:103:LEU:HD23	2.35	0.41
25:W:3:ALA:O	25:W:54:PHE:HA	2.21	0.41
29:1:25:LYS:NZ	37:1:3076:HOH:O	2.52	0.41
30:2:13:LYS:O	30:2:17:GLN:HG3	2.20	0.41
1:0:135:G:OP1	15:M:39:ARG:NH1	2.53	0.41
1:0:696:C:H4'	37:0:7047:HOH:O	2.21	0.41
1:0:735:C:N4	31:3:15:ASN:HD21	2.19	0.41
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.41
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.41
1:0:2134:G:C6	1:0:2258:A:C8	3.09	0.41
1:0:2909:G:H2'	1:0:2910:A:C8	2.56	0.41
37:0:9900:HOH:O	27:Y:212:ARG:HB3	2.20	0.41
3:A:66:ARG:HG2	37:A:8907:HOH:O	2.21	0.41
3:A:77:GLY:O	3:A:78:ASP:C	2.60	0.41
3:A:199:HIS:CD2	3:A:201:PHE:HB2	2.56	0.41
5:C:21:VAL:C	5:C:23:GLU:N	2.73	0.41
5:C:57:PRO:HG2	5:C:73:LEU:HD13	2.03	0.41
5:C:157:LEU:HD22	5:C:162:VAL:CG1	2.51	0.41
5:C:169:ALA:HB3	5:C:208:ALA:O	2.21	0.41
5:C:236:THR:HG23	5:C:238:SER:H	1.86	0.41
6:D:17:ARG:HG3	6:D:18:ILE:N	2.35	0.41
6:D:67:ASP:O	6:D:69:ILE:HG13	2.20	0.41
6:D:75:LEU:HD22	6:D:79:MET:HB3	2.02	0.41
12:J:77:GLY:O	12:J:78:ILE:C	2.59	0.41
14:L:89:PHE:N	14:L:117:GLU:O	2.54	0.41
16:N:47:LEU:HD22	16:N:47:LEU:HA	1.79	0.41
19:Q:86:VAL:HG22	19:Q:87:THR:N	2.35	0.41
21:S:23:LYS:HE2	37:S:8522:HOH:O	2.21	0.41
24:V:12:THR:HG23	24:V:14:ALA:N	2.31	0.41
25:W:56:GLU:O	25:W:143:THR:HG23	2.20	0.41
25:W:108:ARG:O	25:W:110:GLN:N	2.54	0.41
28:Z:47:VAL:HA	28:Z:56:GLN:O	2.20	0.41
1:0:204:A:C2'	1:0:205:U:H5'	2.51	0.40
1:0:268:U:H1'	37:0:3602:HOH:O	2.20	0.40
1:0:706:G:N2	1:0:707:C:H41	2.18	0.40
1:0:727:G:H3'	1:0:728:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1097:A:H5”	25:W:125:HIS:CE1	2.56	0.40
1:0:2071:C:H5’	37:0:9338:HOH:O	2.21	0.40
1:0:2296:C:H2’	1:0:2297:U:C6	2.57	0.40
1:0:2600:A:H2’	1:0:2601:A:O4’	2.21	0.40
1:0:2649:A:H5’	1:0:2649:A:H8	1.86	0.40
1:0:2708:G:N2	13:K:1:MET:O	2.54	0.40
2:9:34:A:H1’	16:N:153:GLN:HE22	1.85	0.40
2:9:49:G:OP1	16:N:78:MET:HG2	2.21	0.40
4:B:109:LEU:CD1	4:B:113:LEU:HD12	2.50	0.40
4:B:321:PRO:HA	37:B:8958:HOH:O	2.19	0.40
5:C:93:LYS:HA	37:C:8555:HOH:O	2.21	0.40
6:D:85:GLN:O	6:D:86:THR:HG23	2.21	0.40
8:F:4:VAL:HA	8:F:76:PHE:CZ	2.56	0.40
10:H:49:GLN:NE2	10:H:140:TYR:CE2	2.83	0.40
12:J:6:PHE:O	12:J:8:ALA:N	2.45	0.40
13:K:69:LEU:HD12	13:K:97:ILE:HD13	2.03	0.40
16:N:94:GLU:HG3	16:N:186:LEU:HD12	2.03	0.40
17:O:113:VAL:O	17:O:114:ILE:HD13	2.21	0.40
20:R:100:ASP:C	20:R:102:GLN:N	2.74	0.40
25:W:118:LEU:HD23	25:W:118:LEU:N	2.36	0.40
25:W:146:ILE:O	25:W:150:LEU:HG	2.21	0.40
1:0:939:A:C2	1:0:1027:G:N3	2.90	0.40
1:0:1494:A:C4	1:0:1495:C:C5	3.09	0.40
1:0:2779:G:H21	7:E:143:GLN:NE2	2.18	0.40
2:9:37:C:H4’	16:N:111:PRO:HD2	2.02	0.40
5:C:124:VAL:HA	5:C:230:GLY:O	2.20	0.40
6:D:28:GLY:CA	6:D:69:ILE:HG23	2.43	0.40
6:D:105:SER:HB2	6:D:131:THR:HG23	2.03	0.40
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.20	0.40
16:N:31:LYS:HB2	16:N:101:VAL:HG23	2.04	0.40
19:Q:86:VAL:CG2	19:Q:87:THR:N	2.84	0.40
22:T:52:ARG:C	22:T:56:ALA:HB2	2.42	0.40
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.37	0.40
26:X:41:PHE:CZ	26:X:74:ALA:HB3	2.56	0.40
29:1:53:LYS:HA	29:1:53:LYS:HD3	1.93	0.40
1:0:66:G:H2’	37:0:9911:HOH:O	2.20	0.40
1:0:69:A:C2’	1:0:70:A:OP2	2.70	0.40
1:0:201:G:N2	1:0:202:U:C2	2.90	0.40
1:0:294:C:H2’	1:0:295:C:O4’	2.22	0.40
1:0:394:G:H1	15:M:181:GLU:CD	2.24	0.40
1:0:695:C:H2’	1:0:696:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1370:G:H5"	37:R:8838:HOH:O	2.21	0.40
1:0:1456:C:H2'	1:0:1457:U:C6	2.56	0.40
1:0:1771:U:O2	28:Z:19:GLY:HA2	2.21	0.40
1:0:1845:A:P	3:A:190:ARG:HH11	2.45	0.40
1:0:2493:C:H2'	1:0:2493:C:O2	2.22	0.40
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	2.02	0.40
5:C:1:MET:HG2	5:C:2:GLN:HE21	1.86	0.40
5:C:175:LYS:HD3	5:C:184:ARG:O	2.21	0.40
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.49	0.40
7:E:162:PHE:CD1	7:E:162:PHE:N	2.89	0.40
9:G:64:ASN:O	9:G:68:GLU:HG3	2.20	0.40
9:G:69:ARG:NH1	37:G:3513:HOH:O	2.54	0.40
10:H:46:TYR:HA	10:H:47:PRO:HD3	1.77	0.40
15:M:19:GLN:N	37:M:8864:HOH:O	2.54	0.40
16:N:62:HIS:O	16:N:64:SER:N	2.55	0.40
17:O:53:GLN:NE2	17:O:112:ARG:HH21	2.19	0.40
18:P:103:THR:HB	37:P:180:HOH:O	2.21	0.40
20:R:119:VAL:O	20:R:119:VAL:HG12	2.21	0.40
25:W:96:LEU:O	25:W:97:ALA:C	2.59	0.40
27:Y:143:TRP:C	37:Y:8921:HOH:O	2.59	0.40
1:0:145:A:N3	15:M:111:ASN:HB3	2.37	0.40
1:0:1127:C:H2'	1:0:1128:U:H5'	2.03	0.40
1:0:1839:A:H5'	1:0:2643:G:H4'	2.02	0.40
1:0:1851:G:O2'	1:0:1852:A:H5'	2.20	0.40
1:0:2419:U:H5"	1:0:2420:G:H5'	2.03	0.40
1:0:2479:A:H5"	37:0:4453:HOH:O	2.21	0.40
1:0:2768:A:H3'	37:0:4229:HOH:O	2.21	0.40
3:A:150:PRO:HD3	37:A:8886:HOH:O	2.21	0.40
4:B:42:ALA:HB1	4:B:308:LEU:HD11	2.04	0.40
4:B:79:MET:HB2	4:B:188:HIS:CE1	2.57	0.40
4:B:127:GLN:HG3	37:B:8943:HOH:O	2.21	0.40
4:B:153:SER:HB2	4:B:287:TYR:CZ	2.57	0.40
6:D:80:ALA:O	6:D:84:LEU:HG	2.20	0.40
11:I:85:GLY:C	11:I:86:GLU:HG3	2.41	0.40
12:J:143:LYS:HA	12:J:145:TRP:CZ3	2.56	0.40
13:K:120:ARG:HB3	13:K:121:PHE:CE1	2.55	0.40
15:M:5:TYR:O	15:M:7:TYR:N	2.55	0.40
18:P:124:ASP:HA	37:P:167:HOH:O	2.20	0.40
20:R:63:ASN:OD1	20:R:63:ASN:N	2.54	0.40
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.35	0.40
27:Y:177:LYS:HG3	27:Y:183:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:22:CYS:HA	37:1:2086:HOH:O	2.20	0.40
1:0:47:G:N3	1:0:114:A:C2	2.90	0.40
1:0:95:A:H5"	1:0:97:G:O4'	2.21	0.40
1:0:645:U:OP2	14:L:4:LYS:CE	2.69	0.40
1:0:694:A:H2'	1:0:695:C:C5'	2.51	0.40
1:0:1012:A:O5'	1:0:1012:A:H8	2.05	0.40
1:0:1483:C:O2'	1:0:1484:G:H5'	2.21	0.40
1:0:1641:A:C2'	1:0:1642:A:H5'	2.51	0.40
1:0:2375:A:H2'	1:0:2376:C:C6	2.57	0.40
1:0:2419:U:H5"	1:0:2420:G:C5'	2.51	0.40
1:0:2450:C:H6	1:0:2450:C:O5'	2.04	0.40
1:0:2769:C:H2'	1:0:2770:G:C5'	2.51	0.40
1:0:2880:A:C2'	1:0:2881:C:H5'	2.48	0.40
3:A:186:TRP:CG	3:A:187:PRO:HA	2.57	0.40
6:D:162:ALA:C	6:D:164:ALA:N	2.73	0.40
8:F:49:PHE:O	8:F:95:ALA:HB1	2.21	0.40
11:I:72:GLU:O	11:I:74:ILE:N	2.54	0.40
16:N:22:GLN:HA	16:N:25:ARG:CZ	2.52	0.40
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.40	0.40
24:V:27:LEU:O	24:V:30:ALA:HB3	2.21	0.40
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	2.04	0.40
30:2:20:ARG:HG3	30:2:20:ARG:NH1	2.11	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	235/240 (98%)	191 (81%)	31 (13%)	13 (6%)	2 5
4	B	335/338 (99%)	291 (87%)	35 (10%)	9 (3%)	5 17
5	C	244/246 (99%)	201 (82%)	32 (13%)	11 (4%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	D	134/177 (76%)	85 (63%)	31 (23%)	18 (13%)	0 0
7	E	170/178 (96%)	150 (88%)	15 (9%)	5 (3%)	4 15
8	F	117/120 (98%)	93 (80%)	17 (14%)	7 (6%)	1 4
9	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
10	H	156/177 (88%)	134 (86%)	17 (11%)	5 (3%)	4 13
11	I	68/162 (42%)	49 (72%)	14 (21%)	5 (7%)	1 2
12	J	140/145 (97%)	121 (86%)	14 (10%)	5 (4%)	3 11
13	K	130/132 (98%)	111 (85%)	17 (13%)	2 (2%)	10 33
14	L	141/165 (86%)	114 (81%)	25 (18%)	2 (1%)	11 34
15	M	192/195 (98%)	169 (88%)	20 (10%)	3 (2%)	9 31
16	N	184/187 (98%)	149 (81%)	23 (12%)	12 (6%)	1 3
17	O	113/116 (97%)	102 (90%)	8 (7%)	3 (3%)	5 17
18	P	141/149 (95%)	125 (89%)	12 (8%)	4 (3%)	5 17
19	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6 22
20	R	145/152 (95%)	122 (84%)	18 (12%)	5 (3%)	3 13
21	S	79/85 (93%)	69 (87%)	9 (11%)	1 (1%)	12 36
22	T	117/120 (98%)	92 (79%)	19 (16%)	6 (5%)	2 6
23	U	51/66 (77%)	43 (84%)	7 (14%)	1 (2%)	7 24
24	V	63/71 (89%)	50 (79%)	9 (14%)	4 (6%)	1 3
25	W	152/154 (99%)	136 (90%)	14 (9%)	2 (1%)	12 36
26	X	80/92 (87%)	69 (86%)	8 (10%)	3 (4%)	3 10
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	56 (79%)	10 (14%)	5 (7%)	1 3
29	1	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
30	2	47/50 (94%)	44 (94%)	1 (2%)	2 (4%)	2 8
31	3	90/92 (98%)	84 (93%)	6 (7%)	0	100 100
All	All	3707/4434 (84%)	3148 (85%)	424 (11%)	135 (4%)	3 11

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
4	B	34	GLY

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Mol	Chain	Res	Type
4	B	139	ASP
4	B	206	THR
5	C	8	LEU
6	D	16	PRO
6	D	56	ARG
6	D	139	TYR
6	D	165	PHE
6	D	173	GLU
8	F	101	ALA
14	L	105	TYR
16	N	154	LEU
16	N	164	ASP
16	N	184	ILE
18	P	116	SER
20	R	121	GLU
20	R	135	ALA
22	T	100	ASP
24	V	43	PRO
25	W	77	ALA
26	X	70	ILE
26	X	87	ALA
28	Z	20	ARG
28	Z	81	ARG
3	A	10	GLY
3	A	33	GLU
3	A	37	VAL
3	A	38	ILE
3	A	87	GLU
3	A	119	ALA
4	B	184	ASP
5	C	13	ASP
5	C	15	GLU
5	C	58	ALA
5	C	151	GLN
5	C	234	VAL
6	D	60	GLU
6	D	61	PHE
6	D	90	LEU
6	D	99	ASP
6	D	137	PRO
6	D	171	ASP
7	E	110	GLU

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Mol	Chain	Res	Type
8	F	44	SER
8	F	61	MET
8	F	68	ASP
10	H	143	VAL
12	J	34	GLU
12	J	89	HIS
13	K	111	GLY
15	M	6	SER
16	N	113	SER
16	N	134	ASP
16	N	183	ASP
17	O	20	SER
17	O	21	SER
20	R	20	GLU
22	T	104	GLU
28	Z	21	VAL
30	2	37	HIS
3	A	122	SER
4	B	183	GLU
5	C	178	GLN
5	C	244	ALA
6	D	96	SER
8	F	64	PRO
11	I	113	SER
11	I	128	THR
12	J	5	GLU
12	J	65	ASN
16	N	63	SER
16	N	65	ASP
16	N	133	ASP
18	P	139	ARG
20	R	126	LYS
23	U	7	ASP
30	2	22	PRO
3	A	101	GLU
4	B	107	SER
5	C	85	LYS
5	C	232	LEU
6	D	82	GLU
6	D	86	THR
7	E	121	ASP
10	H	19	ARG

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Mol	Chain	Res	Type
10	H	70	LEU
10	H	115	GLY
13	K	24	THR
16	N	68	GLU
17	O	108	GLY
18	P	68	LYS
20	R	130	MET
26	X	82	GLU
28	Z	28	GLU
3	A	35	GLY
3	A	236	GLY
4	B	2	GLN
6	D	44	ILE
7	E	17	HIS
7	E	98	GLU
10	H	82	GLU
12	J	7	ASP
16	N	165	ALA
19	Q	89	ALA
24	V	39	ALA
25	W	49	ASN
28	Z	67	GLY
5	C	142	ASP
6	D	45	THR
6	D	164	ALA
11	I	100	VAL
15	M	146	ASP
15	M	147	LEU
16	N	139	TRP
18	P	117	SER
24	V	20	LEU
3	A	102	GLY
11	I	109	PRO
24	V	2	VAL
3	A	192	VAL
7	E	136	PRO
8	F	43	GLY
11	I	92	VAL
14	L	69	ILE
21	S	47	VAL
22	T	53	GLY
4	B	181	ILE

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Mol	Chain	Res	Type
6	D	27	ILE
4	B	82	VAL
8	F	59	ILE
22	T	42	VAL
22	T	62	VAL
22	T	90	PRO
19	Q	18	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	
3	A	179/182 (98%)	171 (96%)	8 (4%)	27	60
4	B	282/283 (100%)	258 (92%)	24 (8%)	10	31
5	C	193/193 (100%)	182 (94%)	11 (6%)	20	50
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
7	E	152/156 (97%)	147 (97%)	5 (3%)	38	72
8	F	93/94 (99%)	90 (97%)	3 (3%)	39	73
9	G	27/283 (10%)	26 (96%)	1 (4%)	34	68
10	H	134/145 (92%)	125 (93%)	9 (7%)	16	43
11	I	58/130 (45%)	55 (95%)	3 (5%)	23	55
12	J	118/121 (98%)	111 (94%)	7 (6%)	19	49
13	K	106/106 (100%)	104 (98%)	2 (2%)	57	85
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
15	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
16	N	149/150 (99%)	143 (96%)	6 (4%)	31	65
17	O	93/94 (99%)	88 (95%)	5 (5%)	22	53
18	P	113/117 (97%)	107 (95%)	6 (5%)	22	54
19	Q	79/80 (99%)	77 (98%)	2 (2%)	47	80
20	R	114/120 (95%)	109 (96%)	5 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	S	71/74 (96%)	66 (93%)	5 (7%)	15 40
22	T	105/106 (99%)	99 (94%)	6 (6%)	20 50
23	U	44/52 (85%)	41 (93%)	3 (7%)	16 42
24	V	51/57 (90%)	48 (94%)	3 (6%)	19 49
25	W	130/130 (100%)	125 (96%)	5 (4%)	33 67
26	X	66/74 (89%)	60 (91%)	6 (9%)	9 27
27	Y	120/196 (61%)	114 (95%)	6 (5%)	24 56
28	Z	60/68 (88%)	58 (97%)	2 (3%)	38 72
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	45/46 (98%)	42 (93%)	3 (7%)	16 43
31	3	79/79 (100%)	75 (95%)	4 (5%)	24 55
All	All	3095/3617 (86%)	2935 (95%)	160 (5%)	23 55

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	8	ARG
3	A	33	GLU
3	A	36	ASP
3	A	69	LEU
3	A	94	LEU
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	53	LEU
4	B	68	THR
4	B	97	LEU
4	B	103	ASP
4	B	110	ASP
4	B	140	LEU
4	B	149	ASP
4	B	162	MET
4	B	175	LEU
4	B	190	MET

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Mol	Chain	Res	Type
4	B	192	ASP
4	B	234	ARG
4	B	245	SER
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	265	LEU
4	B	274	GLU
4	B	277	GLU
4	B	307	ARG
5	C	2	GLN
5	C	42	ARG
5	C	76	ARG
5	C	78	ARG
5	C	87	ARG
5	C	91	PRO
5	C	115	LEU
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	236	THR
6	D	24	HIS
6	D	61	PHE
6	D	86	THR
6	D	104	PHE
6	D	133	ASN
6	D	136	ARG
6	D	139	TYR
6	D	153	THR
7	E	7	ILE
7	E	100	ASP
7	E	126	ILE
7	E	156	ASP
7	E	164	ASP
8	F	46	GLU
8	F	65	GLU
8	F	78	GLU
9	G	64	ASN
10	H	21	GLU
10	H	44	ASP
10	H	61	ARG
10	H	62	HIS

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Mol	Chain	Res	Type
10	H	71	SER
10	H	87	LYS
10	H	114	ASP
10	H	157	TYR
10	H	170	ARG
11	I	81	GLU
11	I	108	HIS
11	I	114	TYR
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	79	PHE
12	J	92	GLN
12	J	99	GLU
12	J	107	ASN
13	K	7	ASP
13	K	10	GLN
14	L	18	HIS
14	L	30	ARG
14	L	35	ARG
14	L	99	GLU
14	L	144	ASP
15	M	23	LEU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	116	ASN
15	M	130	GLU
15	M	186	SER
16	N	26	LEU
16	N	47	LEU
16	N	53	ASN
16	N	93	GLN
16	N	139	TRP
16	N	164	ASP
17	O	32	ARG
17	O	34	GLU
17	O	38	ARG
17	O	81	PHE
17	O	100	GLN
18	P	52	LYS
18	P	66	GLN

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Mol	Chain	Res	Type
18	P	91	LYS
18	P	94	TRP
18	P	98	ILE
18	P	110	ASP
19	Q	57	ASP
19	Q	95	GLU
20	R	39	THR
20	R	82	GLU
20	R	109	MET
20	R	142	ASP
20	R	143	VAL
21	S	7	HIS
21	S	30	ASP
21	S	71	ASP
21	S	72	ASP
21	S	80	ARG
22	T	5	ASP
22	T	23	VAL
22	T	39	ASN
22	T	96	VAL
22	T	112	LEU
22	T	115	GLU
23	U	11	THR
23	U	48	ASN
23	U	53	ASP
24	V	13	PRO
24	V	43	PRO
24	V	65	ASP
25	W	1	MET
25	W	26	ILE
25	W	144	GLU
25	W	146	ILE
25	W	154	ARG
26	X	27	ASP
26	X	49	ARG
26	X	72	VAL
26	X	80	GLU
26	X	82	GLU
26	X	88	GLU
27	Y	154	ARG
27	Y	163	THR
27	Y	187	VAL

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Mol	Chain	Res	Type
27	Y	189	ASN
27	Y	191	ASP
27	Y	201	GLU
28	Z	36	ASP
28	Z	41	ASN
30	2	16	ASN
30	2	18	ASN
30	2	20	ARG
31	3	11	CYS
31	3	70	ARG
31	3	87	ARG
31	3	89	GLU

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

Mol	Chain	Res	Type
3	A	29	HIS
3	A	47	HIS
3	A	125	ASN
3	A	127	GLN
3	A	199	HIS
4	B	2	GLN
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	47	GLN
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN

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Mol	Chain	Res	Type
10	H	62	HIS
10	H	73	ASN
10	H	148	HIS
11	I	88	GLN
12	J	52	GLN
12	J	92	GLN
12	J	107	ASN
13	K	10	GLN
14	L	7	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
14	L	58	GLN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN
15	M	190	ASN
16	N	40	ASN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
18	P	50	GLN
18	P	57	ASN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
19	Q	59	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	140	GLN
21	S	51	GLN
22	T	11	GLN
22	T	39	ASN
22	T	43	ASN
22	T	64	ASN
22	T	73	HIS
23	U	39	ASN

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Mol	Chain	Res	Type
24	V	60	GLN
25	W	28	HIS
25	W	59	GLN
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2744/2922 (93%)	247 (9%)	26 (0%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2865/3044 (94%)	264 (9%)	27 (0%)

All (264) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A

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Mol	Chain	Res	Type
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	236	A
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	319	A
1	0	331	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	473	A
1	0	486	A
1	0	487	G
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

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Mol	Chain	Res	Type
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	674	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	841	A
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G

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Mol	Chain	Res	Type
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	1120	U
1	0	1127	C
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	G
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	1457	U
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	1528	A
1	0	1562	C

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Mol	Chain	Res	Type
1	0	1580	A
1	0	1592	G
1	0	1617	C
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	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	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U

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Mol	Chain	Res	Type
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	2133	U
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2346	C
1	0	2354	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2469	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	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

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Mol	Chain	Res	Type
1	0	2613	G
1	0	2638	G
1	0	2648	U
1	0	2649	A
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	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2836	G
1	0	2840	A
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	7	G
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	34	A
2	9	40	C
2	9	41	C
2	9	43	G
2	9	52	A
2	9	57	A

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Mol	Chain	Res	Type
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	318	U
1	0	644	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1120	U
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2791	U
2	9	65	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UR3	0	2619	1	19,22,23	0.35	0	26,32,35	0.64	1 (3%)
1	OMG	0	2588	1	18,26,27	1.07	2 (11%)	19,38,41	0.75	1 (5%)
1	OMU	0	2587	1	19,22,23	0.34	0	26,31,34	0.42	0
1	1MA	0	628	1	16,25,26	1.38	3 (18%)	18,37,40	1.13	2 (11%)
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	22,30,33	1.16	3 (13%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.13	1.43	1.36
1	0	628	1MA	C2-N3	3.66	1.33	1.29
1	0	2621	PSU	C6-C5	3.06	1.38	1.35
1	0	2588	OMG	C5-C6	-2.88	1.41	1.47
1	0	628	1MA	C6-N6	2.61	1.34	1.27
1	0	2588	OMG	C8-N7	-2.40	1.30	1.35
1	0	628	1MA	C8-N7	-2.19	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	628	1MA	N1-C2-N3	2.86	129.36	126.02
1	0	2621	PSU	C6-C5-C4	2.79	120.15	118.20
1	0	2621	PSU	O2-C2-N1	2.71	125.78	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-N1-C2	-2.59	120.04	122.68
1	0	628	1MA	C5-C6-N1	2.50	117.62	113.90
1	0	2619	UR3	C4-N3-C2	2.37	126.80	124.56
1	0	2588	OMG	O6-C6-C5	2.15	128.57	124.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	2749/2922 (94%)	-0.26	14 (0%) 91 88	29, 55, 100, 157	0
2	9	122/122 (100%)	-0.22	3 (2%) 57 47	44, 68, 95, 159	0
3	A	237/240 (98%)	0.12	8 (3%) 45 35	34, 62, 95, 116	0
4	B	337/338 (99%)	-0.06	5 (1%) 73 68	32, 64, 90, 97	0
5	C	246/246 (100%)	-0.21	1 (0%) 92 91	29, 58, 81, 90	0
6	D	140/177 (79%)	1.27	39 (27%) 0 0	62, 107, 129, 138	0
7	E	172/178 (96%)	0.58	13 (7%) 13 7	52, 75, 97, 101	0
8	F	119/120 (99%)	0.64	13 (10%) 5 3	65, 84, 105, 117	0
9	G	29/348 (8%)	1.78	10 (34%) 0 0	76, 98, 106, 107	0
10	H	160/177 (90%)	-0.02	1 (0%) 89 86	40, 61, 96, 107	0
11	I	70/162 (43%)	2.71	43 (61%) 0 0	112, 126, 144, 147	0
12	J	142/145 (97%)	-0.21	1 (0%) 87 84	43, 58, 82, 95	0
13	K	132/132 (100%)	-0.05	0 100 100	40, 61, 84, 89	0
14	L	145/165 (87%)	0.28	11 (7%) 13 7	29, 75, 115, 126	0
15	M	194/195 (99%)	-0.24	0 100 100	40, 55, 69, 79	0
16	N	186/187 (99%)	0.25	10 (5%) 25 17	46, 71, 115, 125	0
17	O	115/116 (99%)	-0.05	0 100 100	47, 65, 81, 83	0
18	P	143/149 (95%)	0.20	1 (0%) 87 84	44, 66, 80, 86	0
19	Q	95/96 (98%)	-0.12	0 100 100	39, 51, 64, 79	0
20	R	147/152 (96%)	0.24	10 (6%) 17 10	41, 56, 114, 128	0
21	S	81/85 (95%)	0.21	3 (3%) 41 31	52, 72, 88, 95	0
22	T	119/120 (99%)	0.51	6 (5%) 28 19	51, 69, 94, 111	0
23	U	53/66 (80%)	0.13	3 (5%) 23 15	51, 64, 79, 85	0
24	V	65/71 (91%)	0.99	13 (20%) 1 0	63, 85, 118, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.20	0 100 100	41, 56, 76, 85	0
26	X	82/92 (89%)	0.38	8 (9%) 7 4	49, 66, 87, 101	0
27	Y	142/241 (58%)	0.04	5 (3%) 44 34	31, 53, 79, 95	0
28	Z	73/83 (87%)	-0.11	0 100 100	53, 69, 86, 102	0
29	1	56/57 (98%)	-0.42	0 100 100	35, 43, 49, 58	0
30	2	49/50 (98%)	0.20	3 (6%) 21 13	40, 66, 94, 104	0
31	3	92/92 (100%)	0.07	1 (1%) 80 75	42, 63, 76, 91	0
All	All	6646/7478 (88%)	-0.00	225 (3%) 45 35	29, 61, 106, 159	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	9.6
20	R	131	GLY	7.2
22	T	119	ALA	6.8
6	D	69	ILE	6.4
20	R	134	SER	6.1
11	I	104	ALA	6.0
11	I	97	VAL	5.9
11	I	92	VAL	5.9
9	G	27	ILE	5.7
20	R	129	ALA	5.7
20	R	130	MET	5.7
2	9	1	U	5.5
6	D	64	ARG	5.4
11	I	83	GLY	5.3
11	I	112	LEU	5.1
6	D	63	ILE	5.0
11	I	80	PHE	4.9
11	I	71	ALA	4.9
11	I	74	ILE	4.9
24	V	8	ILE	4.8
9	G	23	ILE	4.7
6	D	56	ARG	4.7
24	V	43	PRO	4.7
11	I	113	SER	4.6
24	V	40	PRO	4.5
6	D	66	GLY	4.5
20	R	132	ARG	4.5
6	D	65	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
11	I	91	PHE	4.4
11	I	128	THR	4.3
20	R	128	ARG	4.2
6	D	57	THR	4.2
6	D	10	PHE	4.1
22	T	112	LEU	4.1
11	I	93	ALA	4.1
6	D	88	LEU	4.0
11	I	72	GLU	4.0
11	I	98	ASP	4.0
6	D	27	ILE	4.0
11	I	108	HIS	4.0
11	I	78	ALA	3.9
20	R	127	PRO	3.9
6	D	61	PHE	3.9
11	I	86	GLU	3.8
6	D	58	VAL	3.8
14	L	60	GLU	3.8
6	D	18	ILE	3.7
11	I	109	PRO	3.7
20	R	135	ALA	3.7
7	E	45	ASP	3.6
31	3	92	GLU	3.6
22	T	117	ASP	3.6
6	D	85	GLN	3.5
11	I	76	ASP	3.5
7	E	44	GLY	3.4
8	F	17	LEU	3.4
11	I	111	LEU	3.4
16	N	166	ALA	3.4
22	T	118	SER	3.4
14	L	105	TYR	3.4
14	L	106	VAL	3.4
11	I	123	VAL	3.3
11	I	82	THR	3.3
3	A	35	GLY	3.3
2	9	23	U	3.3
11	I	132	VAL	3.3
16	N	159	TYR	3.3
11	I	67	VAL	3.3
11	I	106	GLN	3.3
11	I	116	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
14	L	80	ASP	3.3
11	I	118	ASN	3.2
18	P	1	THR	3.2
27	Y	97	LEU	3.2
8	F	19	ALA	3.1
3	A	237	GLY	3.1
8	F	16	ALA	3.1
11	I	68	PRO	3.1
9	G	21	ASP	3.1
27	Y	95	THR	3.1
8	F	106	ALA	3.0
6	D	62	ASP	3.0
6	D	44	ILE	3.0
11	I	70	THR	3.0
1	0	284	C	3.0
24	V	39	ALA	3.0
9	G	24	VAL	3.0
11	I	114	TYR	3.0
23	U	51	TRP	3.0
1	0	1199	A	3.0
3	A	82	VAL	3.0
1	0	1198	U	2.9
20	R	126	LYS	2.9
6	D	25	MET	2.9
8	F	6	PHE	2.9
1	0	282	C	2.9
6	D	23	VAL	2.9
6	D	41	LEU	2.9
6	D	170	TYR	2.9
16	N	158	LEU	2.9
6	D	90	LEU	2.9
8	F	47	LEU	2.8
30	2	49	GLU	2.8
11	I	100	VAL	2.8
6	D	43	GLU	2.8
9	G	71	LEU	2.8
11	I	88	GLN	2.8
20	R	125	ARG	2.8
1	0	2237	G	2.8
11	I	121	LYS	2.7
1	0	970	U	2.7
11	I	117	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	1172	G	2.7
21	S	81	ILE	2.7
14	L	123	ASP	2.7
3	A	38	ILE	2.7
3	A	36	ASP	2.7
6	D	134	LEU	2.7
11	I	81	GLU	2.7
16	N	149	GLU	2.6
22	T	116	ASP	2.6
24	V	3	LEU	2.6
6	D	166	ILE	2.6
7	E	11	VAL	2.6
6	D	28	GLY	2.6
4	B	104	GLU	2.6
10	H	76	LEU	2.6
6	D	106	PHE	2.6
11	I	90	ASP	2.6
26	X	88	GLU	2.6
8	F	75	ILE	2.6
30	2	35	ARG	2.6
14	L	140	VAL	2.6
8	F	107	ASP	2.6
1	0	1951	G	2.6
7	E	43	ASP	2.6
11	I	134	ILE	2.5
7	E	10	ASP	2.5
24	V	38	GLY	2.5
24	V	37	GLY	2.5
30	2	39	ARG	2.5
7	E	95	VAL	2.5
6	D	68	PRO	2.5
11	I	79	GLY	2.5
8	F	98	VAL	2.5
11	I	110	ASP	2.4
6	D	17	ARG	2.4
1	0	735	C	2.4
6	D	70	GLY	2.4
16	N	183	ASP	2.4
9	G	28	GLU	2.4
24	V	49	LEU	2.4
9	G	65	THR	2.4
26	X	41	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
24	V	9	ARG	2.4
27	Y	235	GLU	2.4
26	X	72	VAL	2.4
11	I	105	GLU	2.3
2	9	24	U	2.3
6	D	67	ASP	2.3
6	D	128	LEU	2.3
7	E	131	LEU	2.3
6	D	104	PHE	2.3
3	A	37	VAL	2.3
4	B	115	VAL	2.3
26	X	10	VAL	2.2
11	I	73	LEU	2.2
14	L	120	LEU	2.2
16	N	186	LEU	2.2
4	B	105	PHE	2.2
6	D	51	ARG	2.2
7	E	100	ASP	2.2
1	0	960	G	2.2
26	X	85	VAL	2.2
1	0	2004	U	2.2
21	S	68	LEU	2.2
26	X	74	ALA	2.2
14	L	81	VAL	2.2
24	V	59	ILE	2.2
8	F	108	VAL	2.2
1	0	1950	G	2.2
22	T	63	ILE	2.2
24	V	63	GLU	2.2
16	N	172	PHE	2.2
7	E	47	VAL	2.2
5	C	244	ALA	2.1
11	I	99	GLN	2.1
16	N	150	TYR	2.1
3	A	96	LEU	2.1
14	L	90	ARG	2.1
14	L	59	GLU	2.1
6	D	47	GLN	2.1
8	F	119	ARG	2.1
6	D	29	HIS	2.1
24	V	41	GLU	2.1
27	Y	96	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
11	I	84	SER	2.1
7	E	108	LEU	2.1
23	U	52	THR	2.1
27	Y	108	ASP	2.1
7	E	93	MET	2.1
9	G	26	MET	2.1
7	E	170	ARG	2.1
1	0	10	U	2.1
4	B	128	ILE	2.1
6	D	55	LYS	2.1
9	G	67	LEU	2.1
4	B	119	HIS	2.0
8	F	20	LEU	2.0
12	J	105	LEU	2.0
9	G	15	TRP	2.0
16	N	175	LEU	2.0
3	A	64	ASP	2.0
1	0	1177	A	2.0
23	U	54	THR	2.0
7	E	42	VAL	2.0
6	D	83	PHE	2.0
8	F	49	PHE	2.0
26	X	8	ARG	2.0
6	D	40	ILE	2.0
6	D	86	THR	2.0
16	N	75	THR	2.0
21	S	48	THR	2.0
14	L	89	PHE	2.0
26	X	76	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
1	OMU	0	2587	21/22	0.98	0.14	39,42,43,46	0
1	OMG	0	2588	24/25	0.98	0.14	40,42,44,44	0
1	UR3	0	2619	21/22	0.98	0.14	40,42,43,46	0
1	PSU	0	2621	20/21	0.98	0.14	40,41,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	1MA	0	628	23/24	0.99	0.16	32,37,39,39	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8568	1/1	0.49	0.46	84,84,84,84	0
34	NA	0	8513	1/1	0.60	0.18	72,72,72,72	0
34	NA	R	8586	1/1	0.61	0.50	81,81,81,81	0
34	NA	0	8526	1/1	0.64	0.83	78,78,78,78	0
32	MG	0	8031	1/1	0.70	0.19	34,34,34,34	0
35	CL	0	8815	1/1	0.70	0.76	112,112,112,112	0
34	NA	0	8556	1/1	0.71	0.69	58,58,58,58	0
34	NA	0	8552	1/1	0.73	0.65	62,62,62,62	0
34	NA	0	8571	1/1	0.75	0.28	61,61,61,61	0
32	MG	0	8104	1/1	0.78	0.29	61,61,61,61	0
34	NA	0	8563	1/1	0.79	0.46	51,51,51,51	0
32	MG	0	8050	1/1	0.80	0.11	97,97,97,97	0
34	NA	0	8507	1/1	0.82	0.46	61,61,61,61	0
32	MG	9	8095	1/1	0.82	0.09	54,54,54,54	0
34	NA	0	8564	1/1	0.83	0.17	40,40,40,40	0
32	MG	0	8038	1/1	0.84	0.21	38,38,38,38	0
34	NA	L	8580	1/1	0.85	0.72	72,72,72,72	0
34	NA	0	8572	1/1	0.85	0.31	69,69,69,69	0
34	NA	9	8551	1/1	0.85	0.19	46,46,46,46	0
34	NA	0	8567	1/1	0.86	0.17	70,70,70,70	0
34	NA	0	8530	1/1	0.86	0.30	72,72,72,72	0
34	NA	0	8582	1/1	0.86	0.25	78,78,78,78	0
34	NA	0	8585	1/1	0.86	0.53	60,60,60,60	0
34	NA	0	8541	1/1	0.87	0.24	53,53,53,53	0
34	NA	0	8524	1/1	0.87	0.26	68,68,68,68	0
32	MG	0	8041	1/1	0.87	0.22	59,59,59,59	0
34	NA	R	8537	1/1	0.87	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8097	1/1	0.87	0.19	51,51,51,51	0
34	NA	0	8538	1/1	0.87	0.09	61,61,61,61	0
35	CL	0	8816	1/1	0.87	0.47	79,79,79,79	0
34	NA	0	8522	1/1	0.88	0.19	68,68,68,68	0
34	NA	0	8532	1/1	0.88	0.36	47,47,47,47	0
32	MG	0	8043	1/1	0.88	0.12	62,62,62,62	0
32	MG	0	8099	1/1	0.88	0.14	62,62,62,62	0
34	NA	0	8528	1/1	0.88	0.74	61,61,61,61	0
35	CL	N	8807	1/1	0.88	0.33	74,74,74,74	0
34	NA	0	8506	1/1	0.89	0.71	51,51,51,51	0
32	MG	0	8107	1/1	0.89	0.19	65,65,65,65	0
35	CL	0	8805	1/1	0.89	0.23	77,77,77,77	0
34	NA	9	8583	1/1	0.89	0.64	71,71,71,71	0
34	NA	C	8504	1/1	0.89	0.34	48,48,48,48	0
35	CL	0	8817	1/1	0.89	0.17	74,74,74,74	0
34	NA	0	8508	1/1	0.89	0.23	73,73,73,73	0
35	CL	R	8806	1/1	0.89	0.18	63,63,63,63	0
32	MG	0	8114	1/1	0.90	0.16	47,47,47,47	0
32	MG	0	8049	1/1	0.90	0.31	70,70,70,70	0
32	MG	0	8040	1/1	0.90	0.12	57,57,57,57	0
34	NA	0	8566	1/1	0.91	0.33	68,68,68,68	0
32	MG	0	8082	1/1	0.91	0.10	76,76,76,76	0
32	MG	0	8115	1/1	0.91	0.14	70,70,70,70	0
34	NA	0	8569	1/1	0.91	0.59	66,66,66,66	0
32	MG	0	8085	1/1	0.91	0.13	62,62,62,62	0
35	CL	B	8819	1/1	0.91	0.40	74,74,74,74	0
32	MG	T	8073	1/1	0.91	0.21	68,68,68,68	0
34	NA	0	8581	1/1	0.91	0.14	52,52,52,52	0
34	NA	0	8579	1/1	0.92	0.27	62,62,62,62	0
32	MG	0	8103	1/1	0.92	0.16	67,67,67,67	0
35	CL	0	8822	1/1	0.92	0.20	79,79,79,79	0
34	NA	S	8512	1/1	0.92	0.14	48,48,48,48	0
32	MG	2	8076	1/1	0.92	0.17	69,69,69,69	0
32	MG	0	8092	1/1	0.92	0.24	80,80,80,80	0
35	CL	Y	8820	1/1	0.92	0.14	55,55,55,55	0
35	CL	3	8804	1/1	0.92	0.29	74,74,74,74	0
34	NA	0	8540	1/1	0.93	0.24	40,40,40,40	0
34	NA	0	8529	1/1	0.93	0.15	79,79,79,79	0
34	NA	0	8550	1/1	0.93	0.26	56,56,56,56	0
34	NA	0	8511	1/1	0.93	0.13	43,43,43,43	0
32	MG	0	8062	1/1	0.93	0.13	65,65,65,65	0
34	NA	0	8570	1/1	0.93	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CL	J	8802	1/1	0.93	0.12	75,75,75,75	0
34	NA	0	8559	1/1	0.93	0.41	66,66,66,66	0
34	NA	0	8560	1/1	0.93	0.65	61,61,61,61	0
34	NA	0	8574	1/1	0.93	0.79	63,63,63,63	0
34	NA	0	8510	1/1	0.93	0.24	40,40,40,40	0
36	CD	3	8704	1/1	0.93	0.08	72,72,72,72	0
32	MG	0	8112	1/1	0.94	0.18	64,64,64,64	0
35	CL	0	8814	1/1	0.94	0.17	71,71,71,71	0
34	NA	0	8584	1/1	0.94	0.17	70,70,70,70	0
34	NA	0	8561	1/1	0.94	0.34	50,50,50,50	0
34	NA	0	8533	1/1	0.94	0.14	49,49,49,49	0
34	NA	0	8535	1/1	0.94	0.20	73,73,73,73	0
35	CL	A	8809	1/1	0.94	0.23	82,82,82,82	0
34	NA	0	8573	1/1	0.94	0.64	73,73,73,73	0
32	MG	0	8070	1/1	0.94	0.12	54,54,54,54	0
35	CL	L	8810	1/1	0.94	0.13	73,73,73,73	0
34	NA	M	8547	1/1	0.94	0.22	45,45,45,45	0
34	NA	0	8578	1/1	0.94	0.58	77,77,77,77	0
34	NA	0	8557	1/1	0.94	0.11	65,65,65,65	0
32	MG	0	8111	1/1	0.94	0.07	48,48,48,48	0
35	CL	0	8803	1/1	0.94	0.20	80,80,80,80	0
32	MG	0	8024	1/1	0.95	0.14	45,45,45,45	0
32	MG	0	8042	1/1	0.95	0.11	55,55,55,55	0
32	MG	0	8089	1/1	0.95	0.08	69,69,69,69	0
34	NA	0	8514	1/1	0.95	0.09	39,39,39,39	0
34	NA	0	8515	1/1	0.95	0.26	65,65,65,65	0
34	NA	0	8521	1/1	0.95	0.38	73,73,73,73	0
34	NA	0	8549	1/1	0.95	0.16	54,54,54,54	0
32	MG	K	8069	1/1	0.95	0.09	62,62,62,62	0
35	CL	J	8801	1/1	0.95	0.10	67,67,67,67	0
32	MG	0	8015	1/1	0.95	0.06	41,41,41,41	0
32	MG	0	8109	1/1	0.95	0.05	33,33,33,33	0
34	NA	Q	8548	1/1	0.95	0.17	49,49,49,49	0
35	CL	O	8808	1/1	0.95	0.40	99,99,99,99	0
32	MG	0	8093	1/1	0.95	0.20	50,50,50,50	0
32	MG	0	8044	1/1	0.95	0.16	51,51,51,51	0
34	NA	0	8576	1/1	0.95	0.18	51,51,51,51	0
32	MG	0	8113	1/1	0.95	0.12	49,49,49,49	0
32	MG	0	8088	1/1	0.96	0.10	34,34,34,34	0
34	NA	A	8545	1/1	0.96	0.10	46,46,46,46	0
34	NA	0	8516	1/1	0.96	0.23	61,61,61,61	0
34	NA	0	8517	1/1	0.96	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8014	1/1	0.96	0.10	20,20,20,20	0
34	NA	0	8562	1/1	0.96	0.31	81,81,81,81	0
32	MG	0	8091	1/1	0.96	0.13	53,53,53,53	0
34	NA	0	8523	1/1	0.96	0.10	37,37,37,37	0
32	MG	0	8051	1/1	0.96	0.15	67,67,67,67	0
34	NA	T	8543	1/1	0.96	0.14	43,43,43,43	0
32	MG	0	8052	1/1	0.96	0.06	44,44,44,44	0
32	MG	0	8059	1/1	0.96	0.10	44,44,44,44	0
32	MG	Y	8108	1/1	0.96	0.15	48,48,48,48	0
32	MG	0	8003	1/1	0.96	0.10	47,47,47,47	0
33	K	0	8401	1/1	0.96	0.41	91,91,91,91	0
33	K	0	8402	1/1	0.96	0.13	69,69,69,69	0
34	NA	0	8505	1/1	0.96	0.17	49,49,49,49	0
34	NA	0	8536	1/1	0.96	0.09	52,52,52,52	0
34	NA	0	8575	1/1	0.96	0.25	58,58,58,58	0
32	MG	0	8100	1/1	0.96	0.13	66,66,66,66	0
34	NA	0	8577	1/1	0.96	0.20	72,72,72,72	0
32	MG	0	8063	1/1	0.96	0.23	73,73,73,73	0
32	MG	0	8068	1/1	0.96	0.05	70,70,70,70	0
32	MG	0	8004	1/1	0.96	0.07	43,43,43,43	0
35	CL	Q	8811	1/1	0.96	0.16	72,72,72,72	0
32	MG	0	8048	1/1	0.96	0.09	62,62,62,62	0
32	MG	0	8027	1/1	0.96	0.09	63,63,63,63	0
34	NA	0	8554	1/1	0.96	0.15	38,38,38,38	0
32	MG	0	8087	1/1	0.96	0.10	81,81,81,81	0
32	MG	0	8094	1/1	0.97	0.04	67,67,67,67	0
32	MG	0	8096	1/1	0.97	0.11	53,53,53,53	0
32	MG	0	8116	1/1	0.97	0.08	39,39,39,39	0
32	MG	0	8074	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8081	1/1	0.97	0.14	74,74,74,74	0
34	NA	0	8558	1/1	0.97	0.70	107,107,107,107	0
34	NA	0	8518	1/1	0.97	0.18	32,32,32,32	0
34	NA	0	8519	1/1	0.97	0.07	34,34,34,34	0
32	MG	0	8007	1/1	0.97	0.09	29,29,29,29	0
32	MG	0	8101	1/1	0.97	0.09	70,70,70,70	0
32	MG	0	8102	1/1	0.97	0.19	71,71,71,71	0
32	MG	3	8078	1/1	0.97	0.07	43,43,43,43	0
34	NA	0	8525	1/1	0.97	0.10	50,50,50,50	0
35	CL	0	8812	1/1	0.97	0.14	65,65,65,65	0
35	CL	0	8813	1/1	0.97	0.10	67,67,67,67	0
32	MG	0	8053	1/1	0.97	0.15	47,47,47,47	0
34	NA	0	8527	1/1	0.97	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8046	1/1	0.97	0.06	55,55,55,55	0
34	NA	0	8501	1/1	0.97	0.11	29,29,29,29	0
34	NA	0	8502	1/1	0.97	0.23	49,49,49,49	0
34	NA	0	8503	1/1	0.97	0.20	70,70,70,70	0
32	MG	0	8105	1/1	0.97	0.08	63,63,63,63	0
34	NA	0	8534	1/1	0.97	0.11	55,55,55,55	0
32	MG	0	8025	1/1	0.97	0.12	58,58,58,58	0
35	CL	J	8821	1/1	0.97	0.10	54,54,54,54	0
32	MG	0	8008	1/1	0.97	0.08	35,35,35,35	0
32	MG	0	8064	1/1	0.97	0.19	43,43,43,43	0
34	NA	0	8539	1/1	0.97	0.10	26,26,26,26	0
34	NA	0	8509	1/1	0.97	0.12	37,37,37,37	0
32	MG	0	8016	1/1	0.97	0.13	48,48,48,48	0
34	NA	0	8542	1/1	0.97	0.20	51,51,51,51	0
34	NA	0	8544	1/1	0.97	0.07	33,33,33,33	0
32	MG	0	8033	1/1	0.97	0.13	37,37,37,37	0
32	MG	0	8011	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8057	1/1	0.98	0.20	67,67,67,67	0
32	MG	0	8013	1/1	0.98	0.16	54,54,54,54	0
32	MG	0	8028	1/1	0.98	0.06	48,48,48,48	0
32	MG	A	8066	1/1	0.98	0.06	88,88,88,88	0
32	MG	0	8029	1/1	0.98	0.12	55,55,55,55	0
32	MG	0	8018	1/1	0.98	0.11	50,50,50,50	0
32	MG	0	8045	1/1	0.98	0.10	59,59,59,59	0
34	NA	0	8520	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8032	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8047	1/1	0.98	0.09	59,59,59,59	0
32	MG	0	8075	1/1	0.98	0.09	54,54,54,54	0
32	MG	0	8077	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8022	1/1	0.98	0.06	42,42,42,42	0
32	MG	0	8035	1/1	0.98	0.03	58,58,58,58	0
32	MG	0	8083	1/1	0.98	0.04	52,52,52,52	0
32	MG	0	8084	1/1	0.98	0.07	54,54,54,54	0
32	MG	0	8036	1/1	0.98	0.08	44,44,44,44	0
35	CL	M	8818	1/1	0.98	0.19	60,60,60,60	0
32	MG	0	8110	1/1	0.98	0.04	59,59,59,59	0
34	NA	0	8531	1/1	0.98	0.17	55,55,55,55	0
34	NA	J	8546	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8086	1/1	0.98	0.07	46,46,46,46	0
34	NA	0	8565	1/1	0.98	0.29	49,49,49,49	0
32	MG	0	8037	1/1	0.98	0.08	51,51,51,51	0
36	CD	O	8705	1/1	0.98	0.08	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8010	1/1	0.98	0.10	45,45,45,45	0
32	MG	0	8012	1/1	0.99	0.10	33,33,33,33	0
32	MG	0	8023	1/1	0.99	0.07	42,42,42,42	0
32	MG	0	8079	1/1	0.99	0.11	43,43,43,43	0
32	MG	0	8080	1/1	0.99	0.09	47,47,47,47	0
32	MG	0	8001	1/1	0.99	0.09	33,33,33,33	0
32	MG	0	8106	1/1	0.99	0.09	38,38,38,38	0
32	MG	0	8002	1/1	0.99	0.06	35,35,35,35	0
32	MG	0	8026	1/1	0.99	0.09	28,28,28,28	0
32	MG	0	8054	1/1	0.99	0.10	43,43,43,43	0
32	MG	0	8056	1/1	0.99	0.11	49,49,49,49	0
32	MG	0	8009	1/1	0.99	0.04	36,36,36,36	0
32	MG	0	8005	1/1	0.99	0.09	45,45,45,45	0
32	MG	0	8060	1/1	0.99	0.13	50,50,50,50	0
32	MG	0	8061	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8090	1/1	0.99	0.10	59,59,59,59	0
32	MG	0	8017	1/1	0.99	0.04	33,33,33,33	0
32	MG	A	8065	1/1	0.99	0.08	43,43,43,43	0
34	NA	0	8553	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8030	1/1	0.99	0.13	34,34,34,34	0
34	NA	0	8555	1/1	0.99	0.23	67,67,67,67	0
32	MG	B	8055	1/1	0.99	0.07	46,46,46,46	0
32	MG	0	8006	1/1	0.99	0.06	37,37,37,37	0
32	MG	0	8019	1/1	0.99	0.03	39,39,39,39	0
32	MG	0	8021	1/1	0.99	0.10	31,31,31,31	0
32	MG	0	8071	1/1	0.99	0.08	80,80,80,80	0
32	MG	0	8098	1/1	0.99	0.11	30,30,30,30	0
32	MG	0	8072	1/1	0.99	0.11	61,61,61,61	0
36	CD	U	8701	1/1	0.99	0.10	76,76,76,76	0
36	CD	Z	8703	1/1	0.99	0.11	71,71,71,71	0
32	MG	0	8034	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8058	1/1	1.00	0.09	46,46,46,46	0
32	MG	0	8067	1/1	1.00	0.07	54,54,54,54	0
32	MG	0	8039	1/1	1.00	0.07	44,44,44,44	0
36	CD	1	8702	1/1	1.00	0.07	68,68,68,68	0
32	MG	0	8020	1/1	1.00	0.06	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.