Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:51 PM GMT

PDB ID	:	1Q82
Title	:	Crystal Structure of CC-Puromycin bound to the A-site of the 50S ribosomal subunit
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	2.98 Å(reported)

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

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

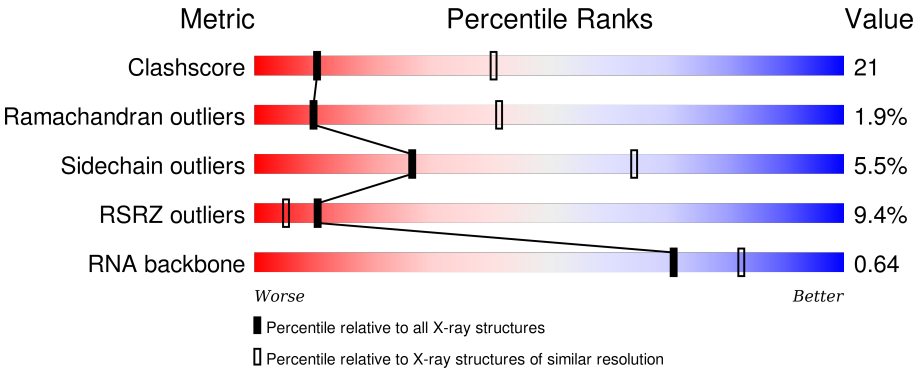
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)
RNA backbone	2183	1001 (3.36-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	2922	3% 50% 36% 7% • 6%
2	B	122	4% 51% 35% 10% •
3	5	2	50% 50% 50%
4	C	239	11% 54% 40% 5% •
5	D	337	2% 48% 46% 6%

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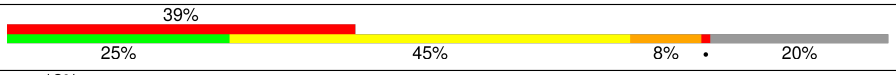
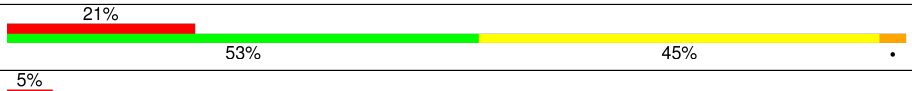
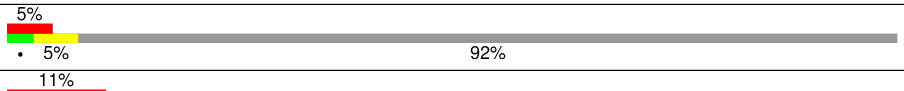
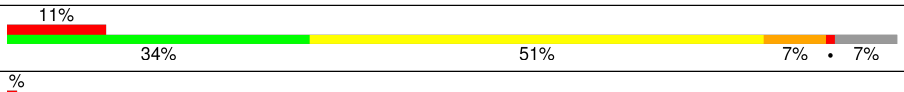
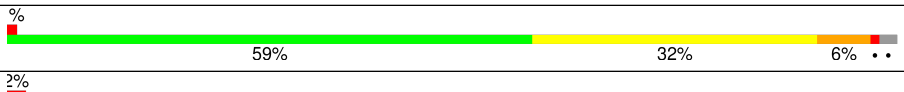
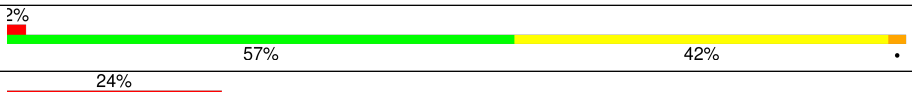
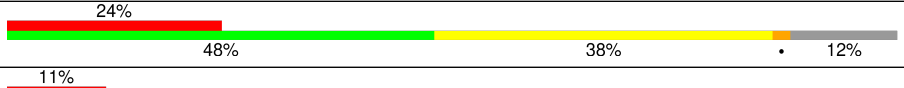
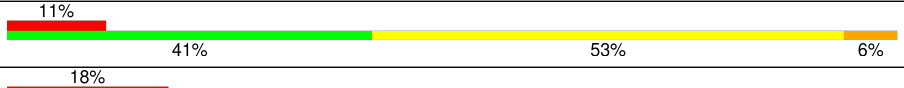
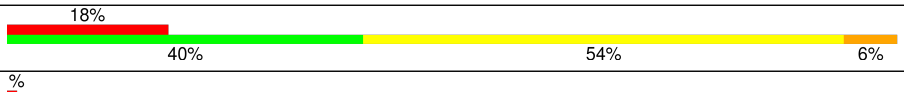
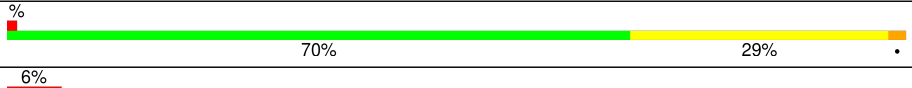
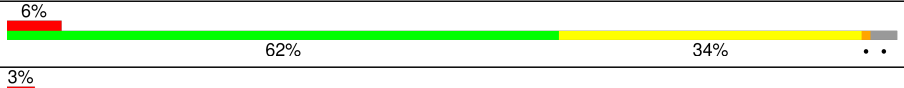
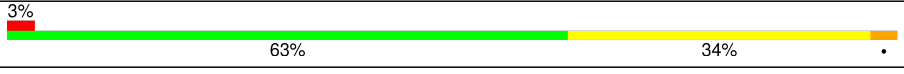
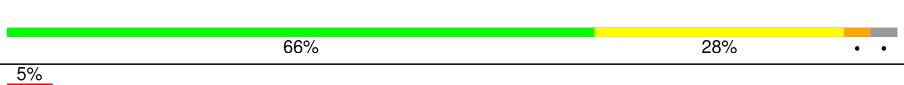
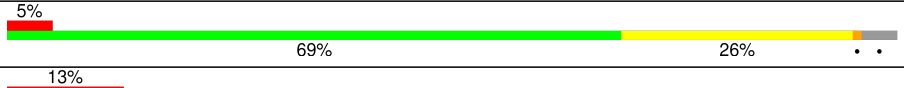
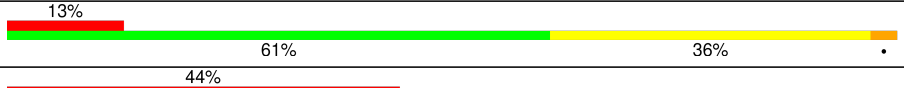
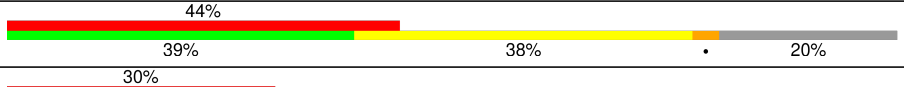
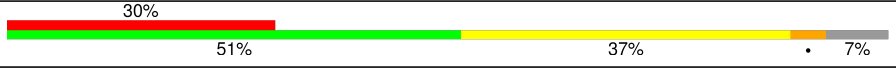
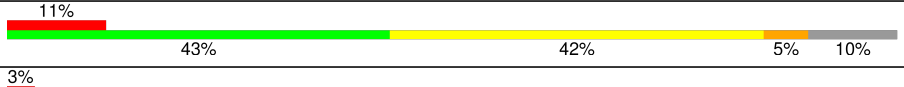
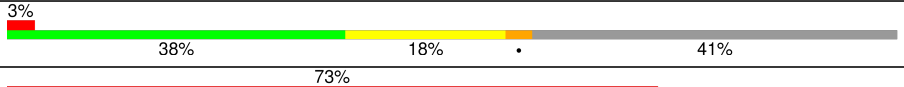
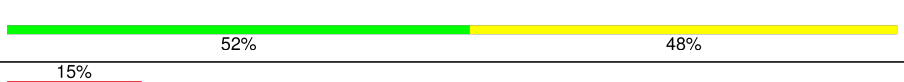
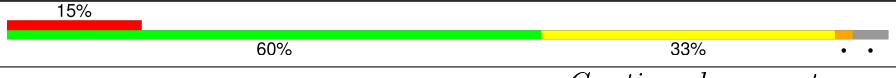
Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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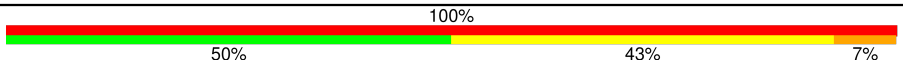
Mol	Chain	Length	Quality of chain
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	A	8011	-	-	X	-
32	MG	A	8053	-	-	-	X
32	MG	A	8060	-	-	-	X
32	MG	A	8064	-	-	-	X
32	MG	A	8112	-	-	-	X
33	K	A	8201	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8320	-	-	-	X
34	NA	A	8321	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8325	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8327	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8335	-	-	-	X
34	NA	A	8353	-	-	-	X
34	NA	A	8356	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8362	-	-	-	X
34	NA	A	8364	-	-	-	X
34	NA	A	8365	-	-	-	X
34	NA	A	8366	-	-	-	X
34	NA	A	8368	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8373	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8378	-	-	-	X
34	NA	A	8379	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	A	8505	-	-	-	X
35	CL	A	8515	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	D	8519	-	-	-	X
35	CL	M	8510	-	-	-	X
35	CL	N	8518	-	-	X	-
36	PPU	5	76	-	-	-	X
37	CD	4	8404	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98593 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	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

- Molecule 3 is a RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	2	40	18	6	14	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	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	U	119	Total	C	N	O	0	0	0
			949	568	180	201			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	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	W	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	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	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	1	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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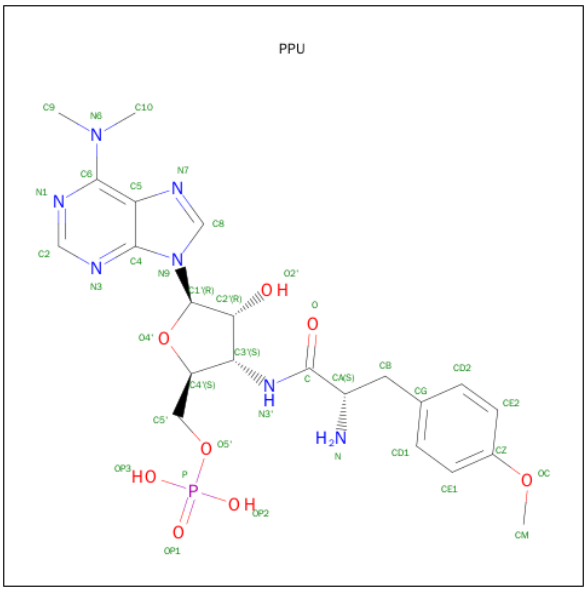
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	U	1	Total Na 1 1	0	0
34	4	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	2	Total Na 2 2	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	Z	2	Total Cl 2 2	0	0
35	A	7	Total Cl 7 7	0	0
35	4	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	R	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total C N O P 37 22 7 7 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	P	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	4	1	Total Cd 1 1	0	0
37	V	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	5860	Total O 5860 5860	0	0
38	B	146	Total O 146 146	0	0
38	5	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	C	140	Total O 140 140	0	0
38	D	146	Total O 146 146	0	0
38	E	176	Total O 176 176	0	0
38	F	52	Total O 52 52	0	0
38	G	45	Total O 45 45	0	0
38	H	32	Total O 32 32	0	0
38	I	22	Total O 22 22	0	0
38	J	78	Total O 78 78	0	0
38	K	54	Total O 54 54	0	0
38	L	64	Total O 64 64	0	0
38	M	86	Total O 86 86	0	0
38	N	138	Total O 138 138	0	0
38	O	64	Total O 64 64	0	0
38	P	44	Total O 44 44	0	0
38	Q	70	Total O 70 70	0	0
38	R	57	Total O 57 57	0	0
38	S	83	Total O 83 83	0	0
38	T	36	Total O 36 36	0	0
38	U	38	Total O 38 38	0	0
38	V	22	Total O 22 22	0	0
38	W	16	Total O 16 16	0	0

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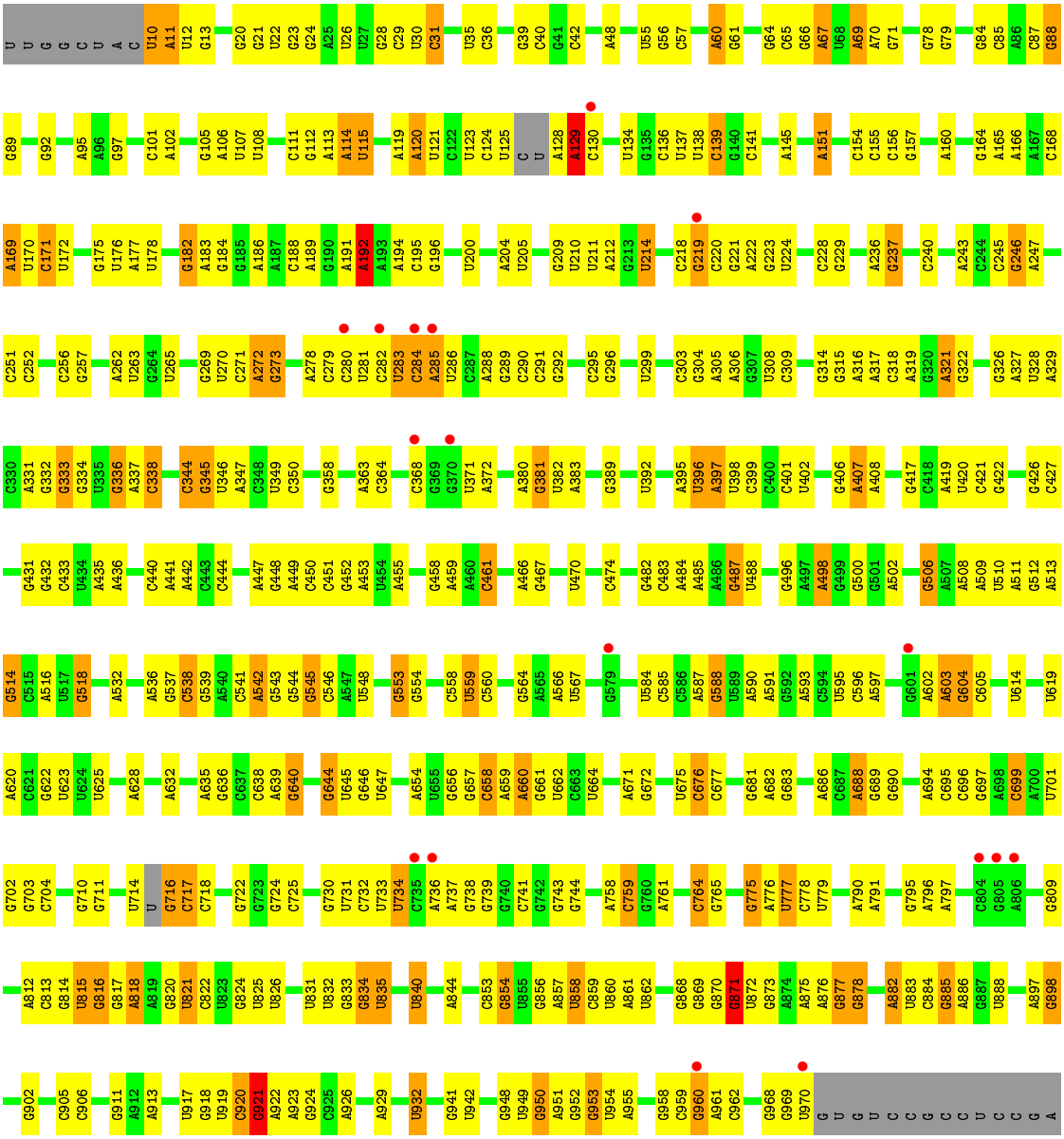
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	X	67	Total O 67 67	0	0
38	Y	28	Total O 28 28	0	0
38	Z	100	Total O 100 100	0	0
38	1	36	Total O 36 36	0	0
38	2	58	Total O 58 58	0	0
38	3	37	Total O 37 37	0	0
38	4	70	Total O 70 70	0	0

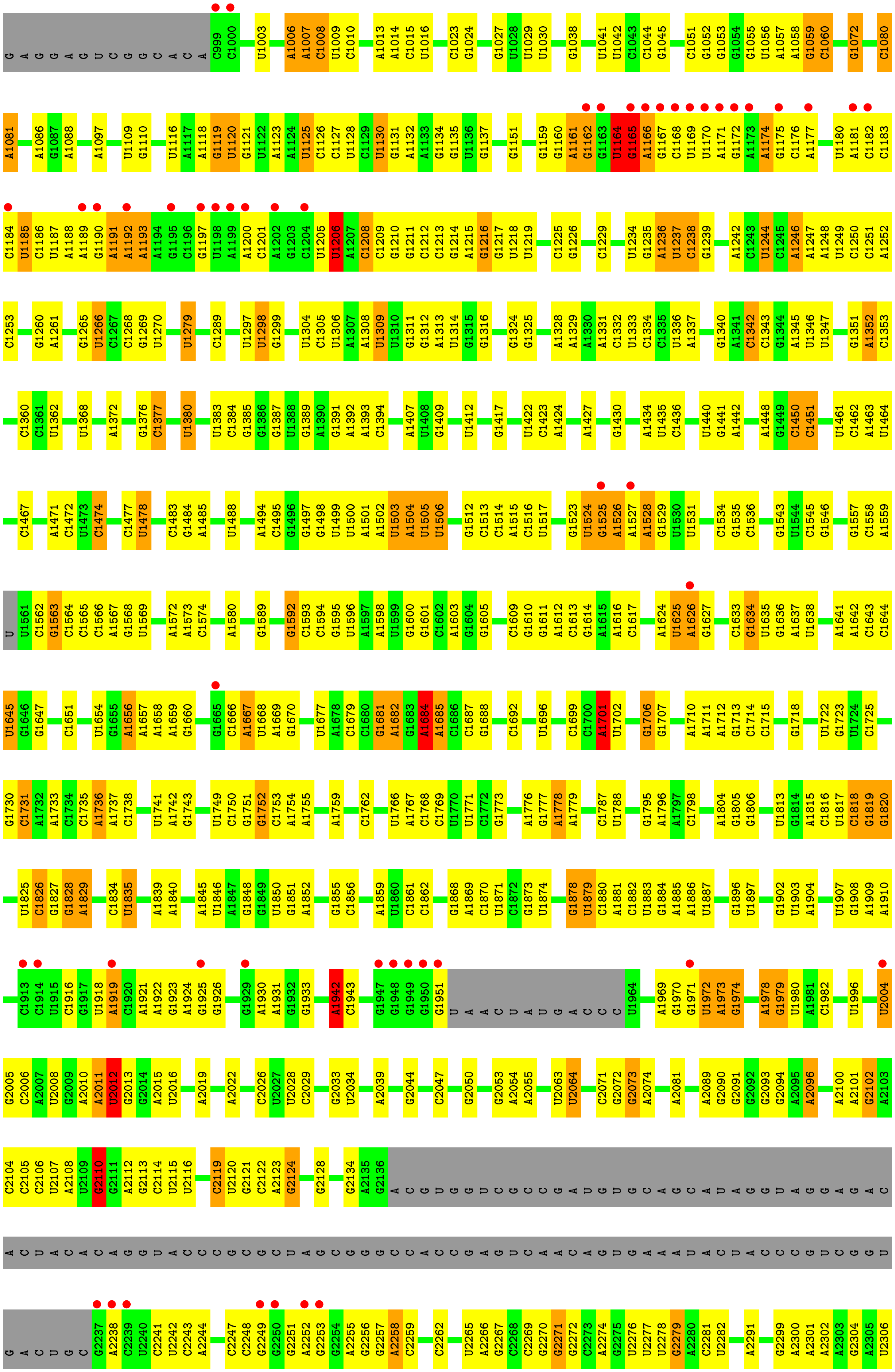
3 Residue-property plots (i)

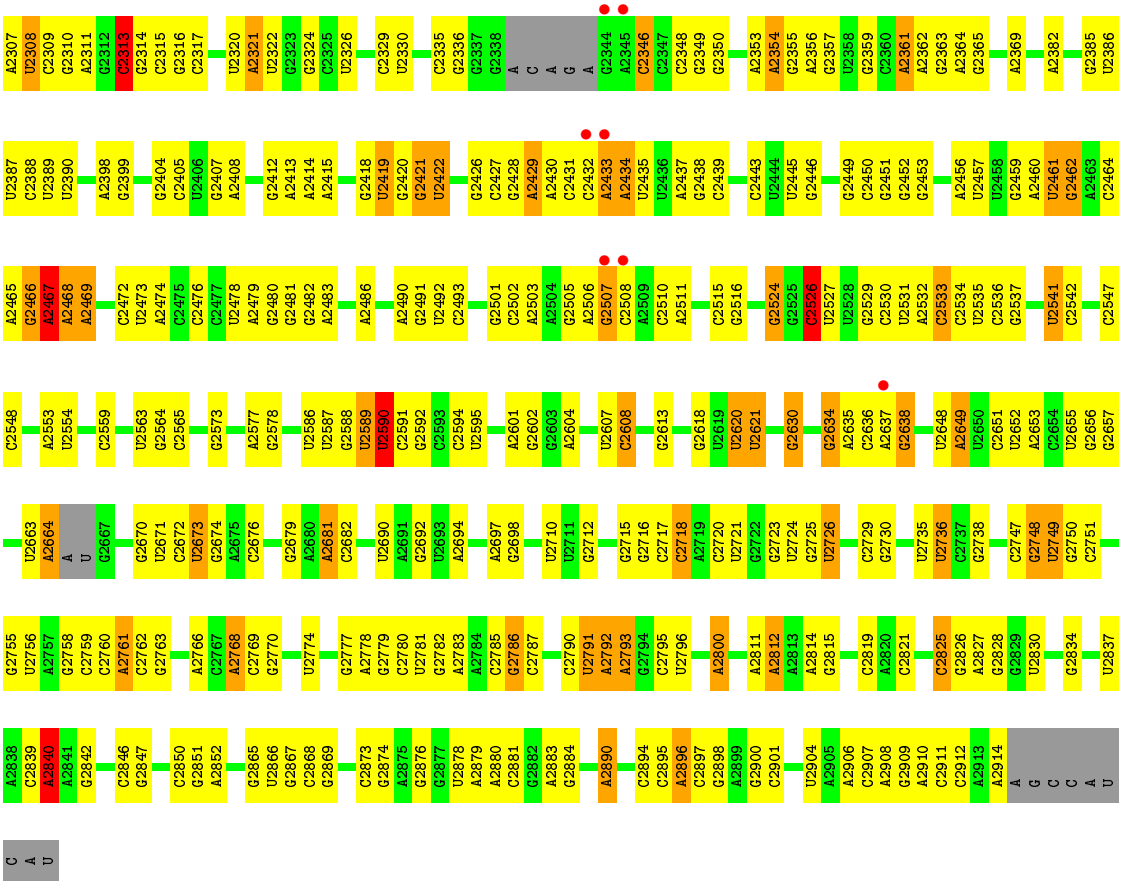
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 23S ribosomal rna

Chain A: 

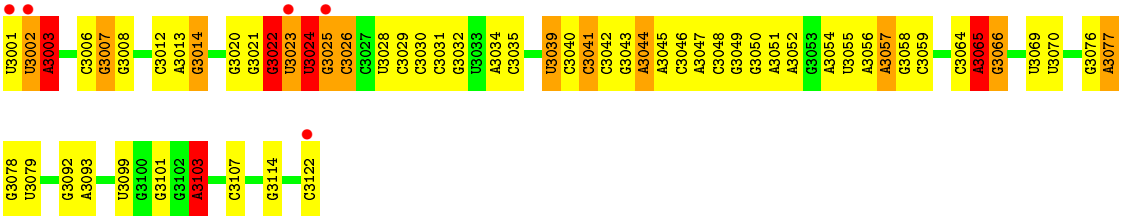






• Molecule 2: 5S ribosomal RNA

Chain B:

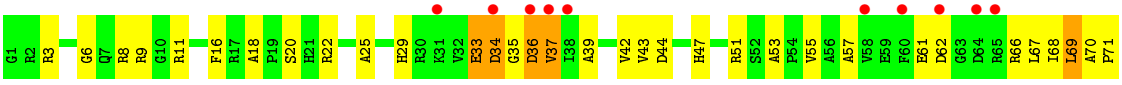


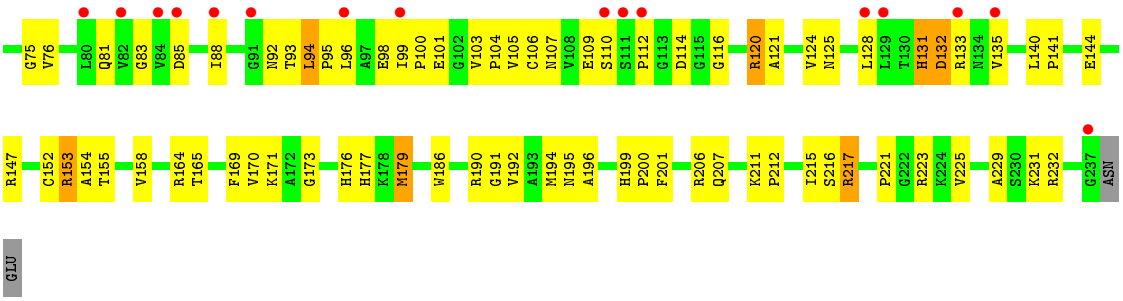
• Molecule 3: CC-puromycin

Chain 5:

• Molecule 4: 50S ribosomal protein L2P

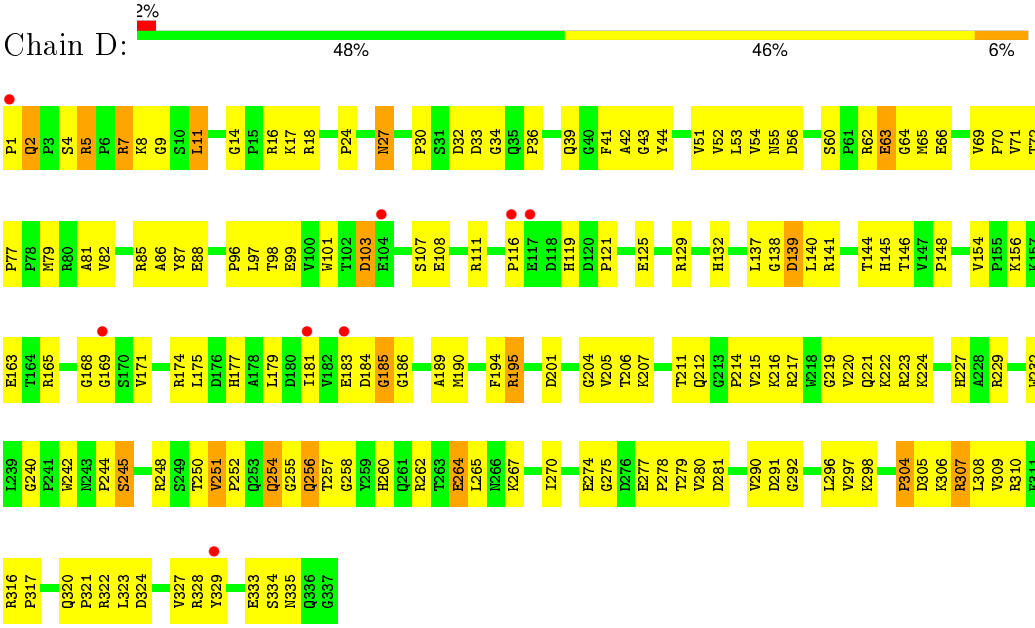
Chain C:





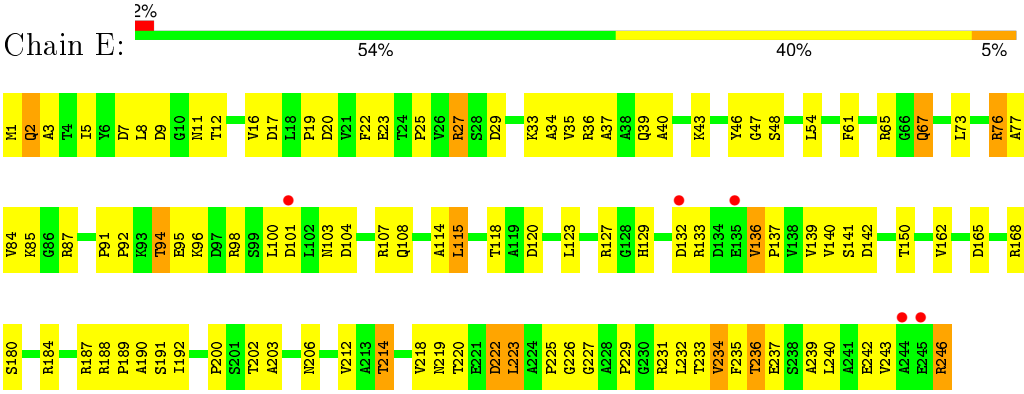
• Molecule 5: 50S ribosomal protein L3P

Chain D:



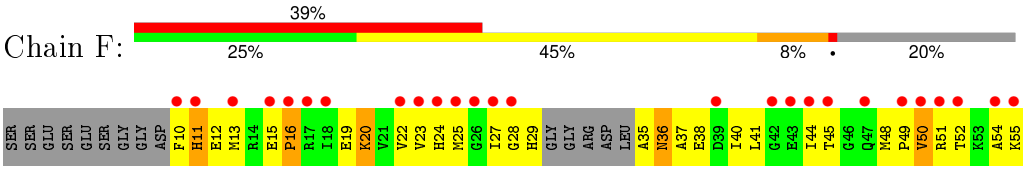
• Molecule 6: 50S ribosomal protein L4E

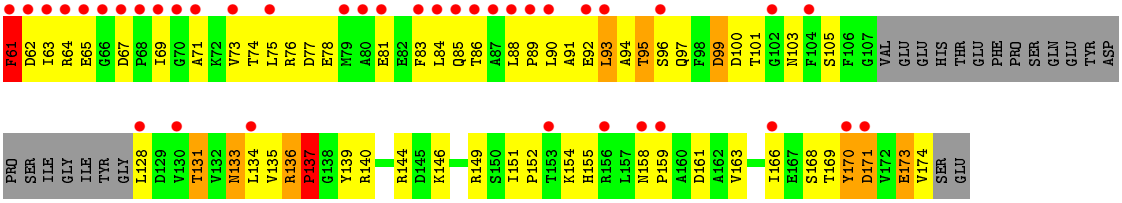
Chain E:



• Molecule 7: 50S ribosomal protein L5P

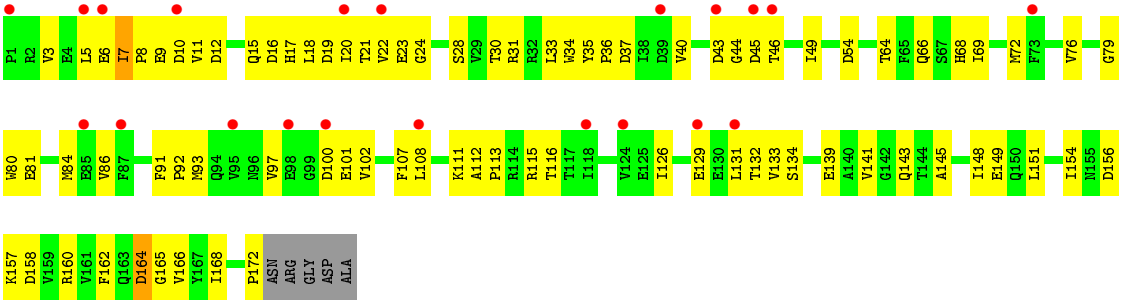
Chain F:





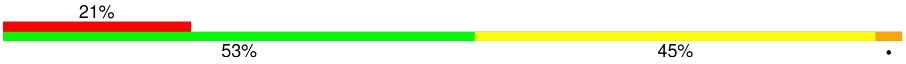
• Molecule 8: 50S ribosomal protein L6P

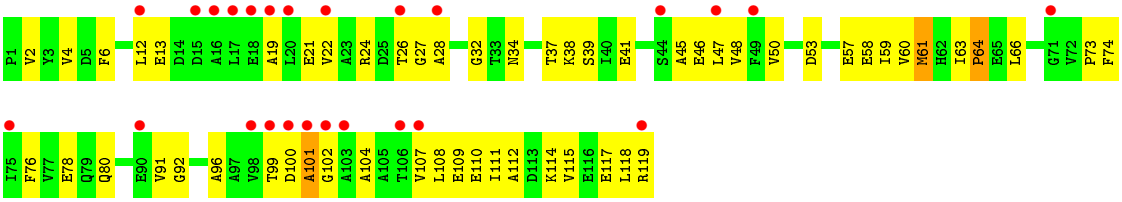
Chain G:



• Molecule 9: 50S ribosomal protein L7Ae

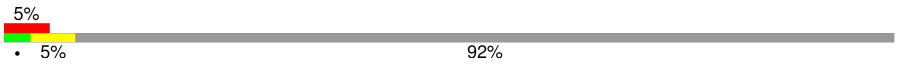
Chain H:

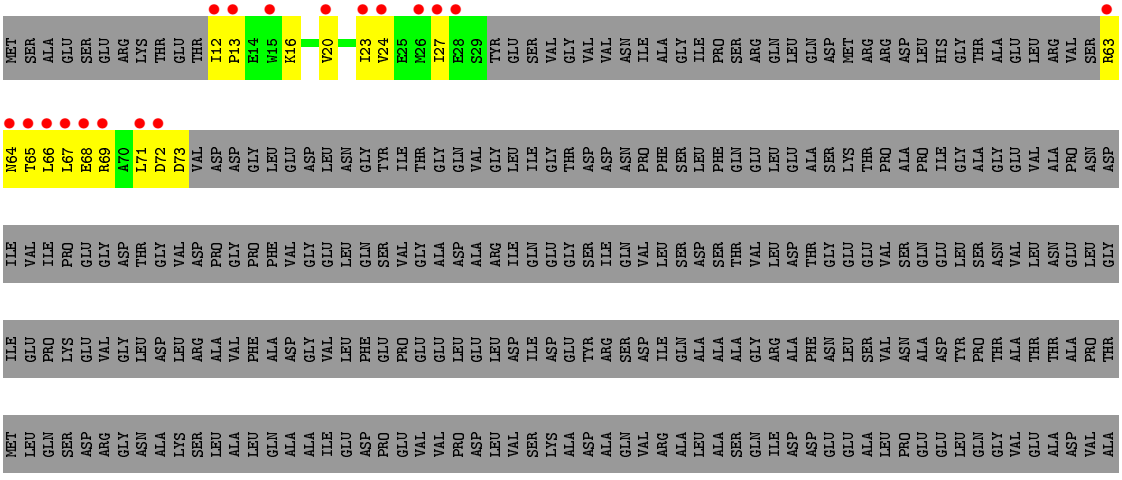




• Molecule 10: Acidic ribosomal protein P0 homolog

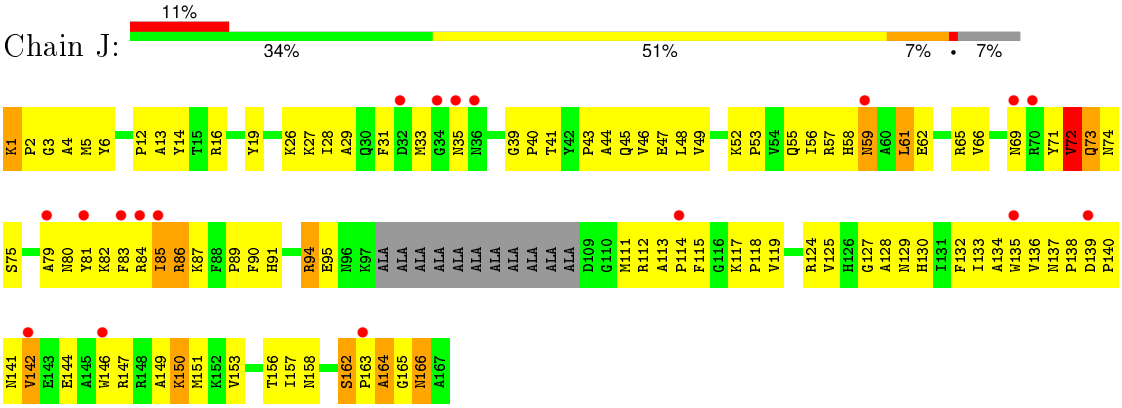
Chain I:





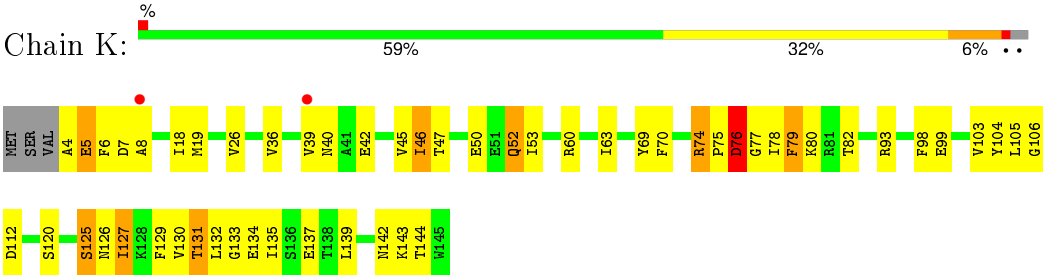
- Molecule 11: L10 Ribosomal Protein

Chain J:



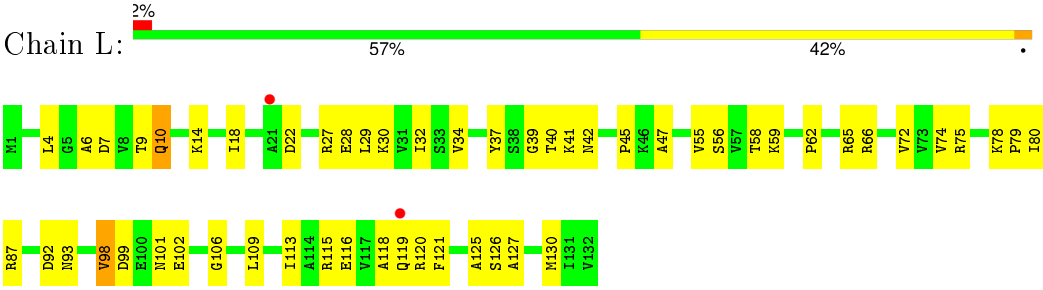
- Molecule 12: 50S ribosomal protein L13P

Chain K:



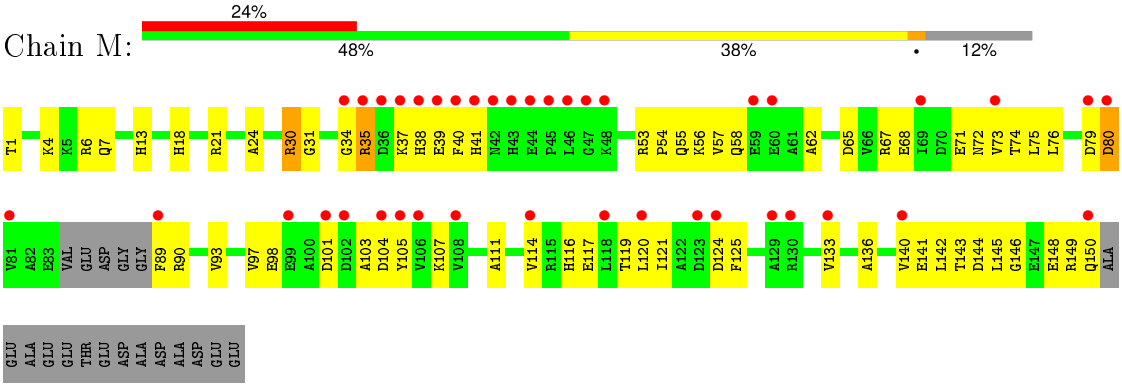
- Molecule 13: 50S ribosomal protein L14P

Chain L:



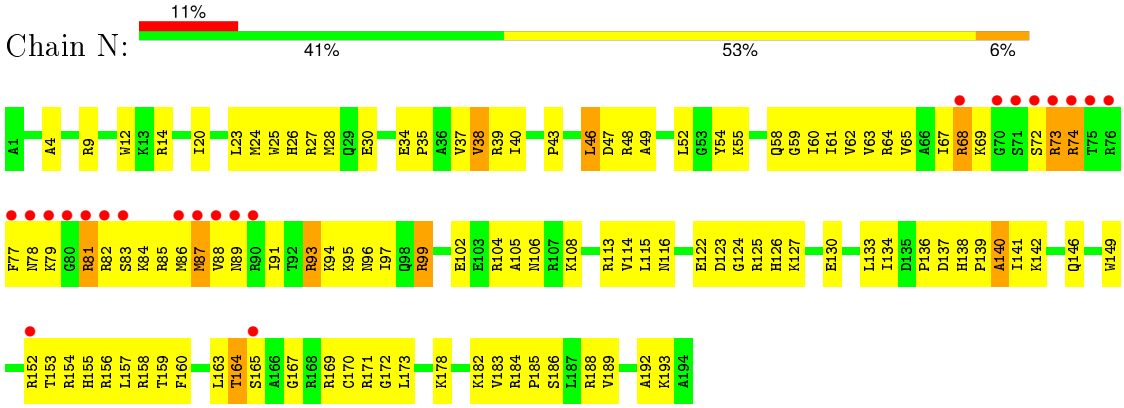
- Molecule 14: 50S ribosomal protein L15P

Chain M:



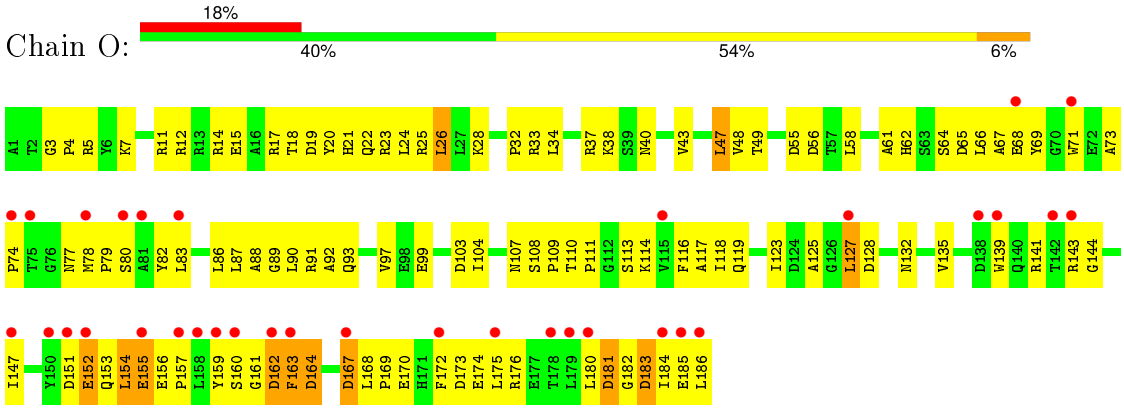
• Molecule 15: L15 Ribosomal Protein

Chain N:



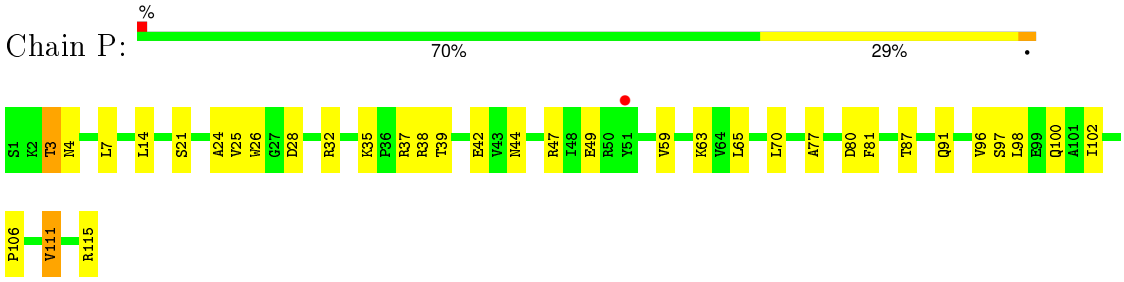
• Molecule 16: 50S ribosomal protein L18P

Chain O:



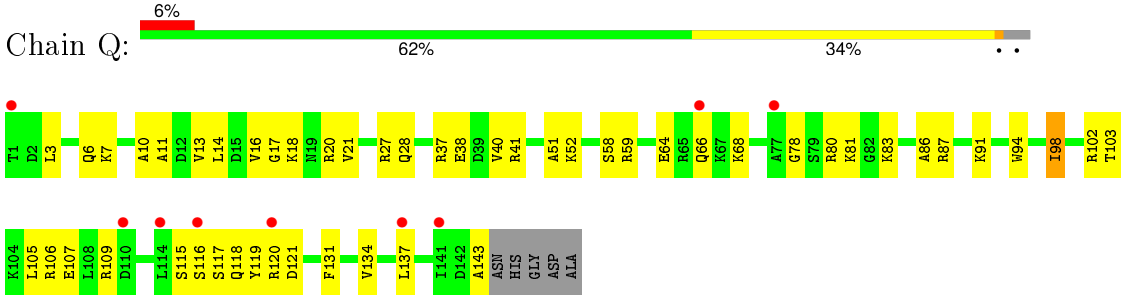
• Molecule 17: 50S ribosomal protein L18e

Chain P:



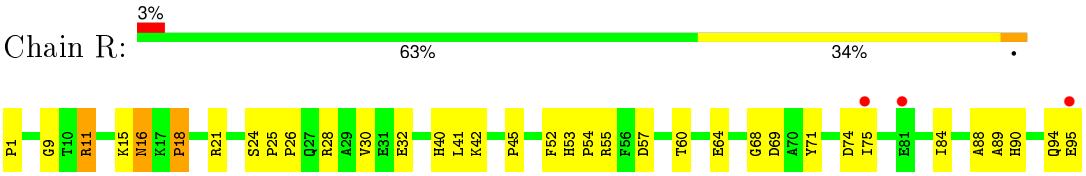
• Molecule 18: 50S ribosomal protein L19E

Chain Q:



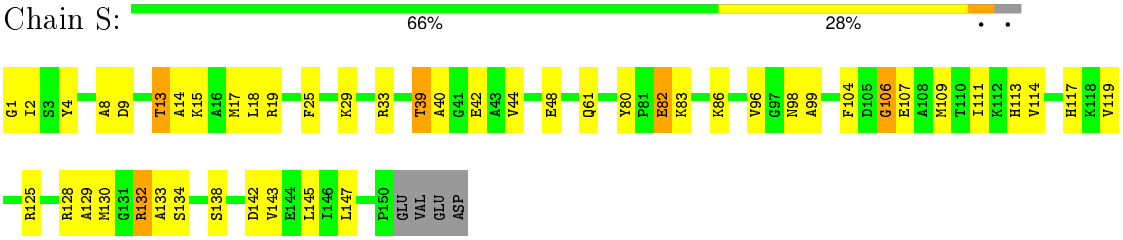
• Molecule 19: 50S ribosomal protein L21e

Chain R:



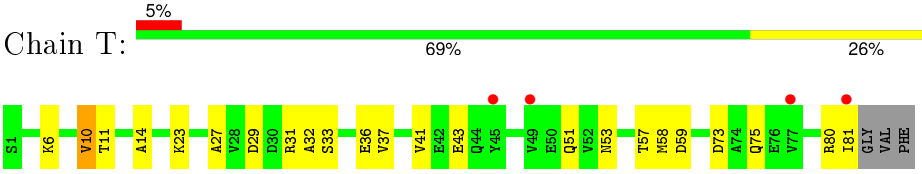
• Molecule 20: 50S ribosomal protein L22P

Chain S:



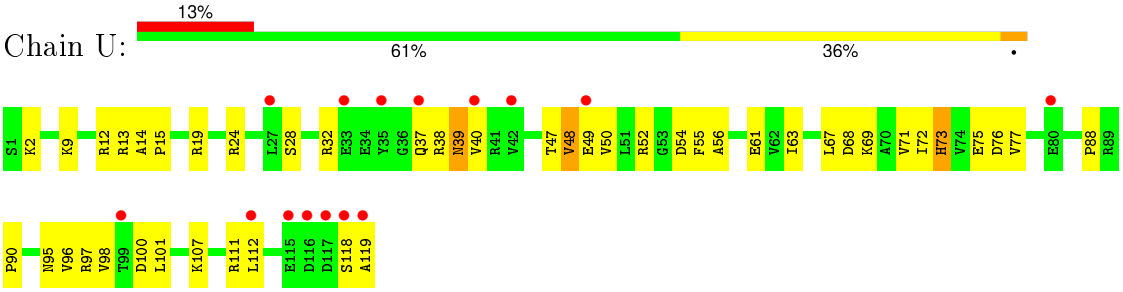
• Molecule 21: 50S ribosomal protein L23P

Chain T:



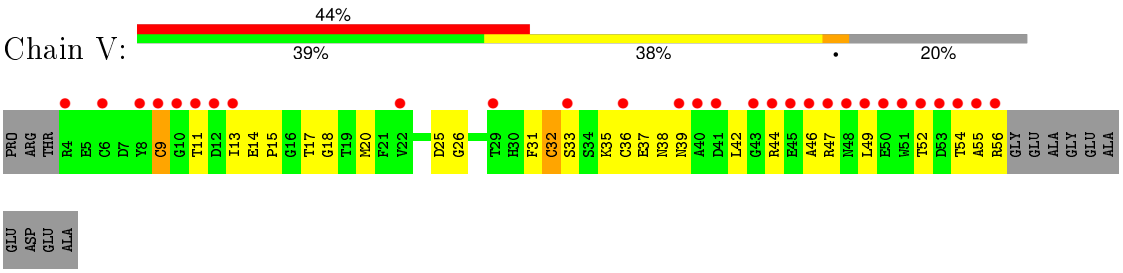
• Molecule 22: 50S ribosomal protein L24P

Chain U:



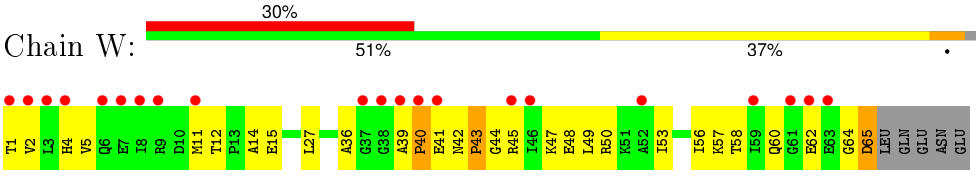
• Molecule 23: 50S ribosomal protein L24E

Chain V:



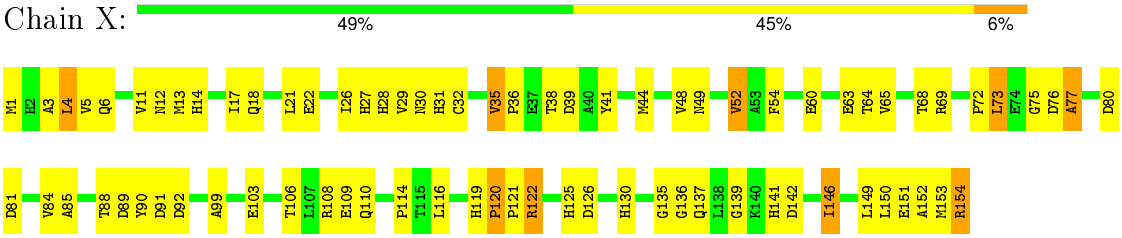
• Molecule 24: 50S ribosomal protein L29P

Chain W:



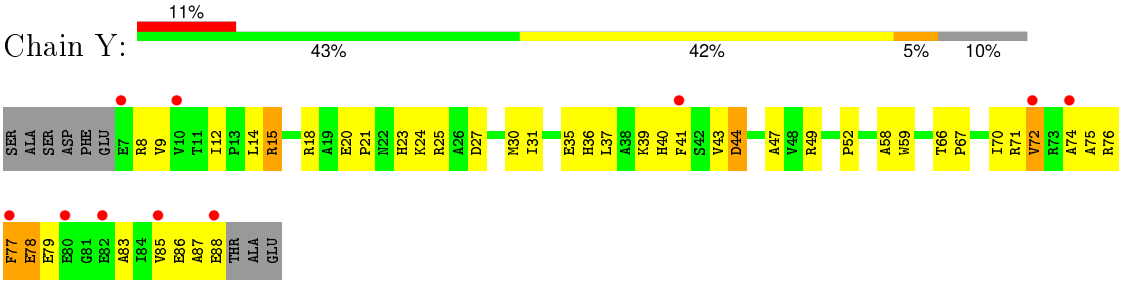
• Molecule 25: 50S ribosomal protein L30P

Chain X:



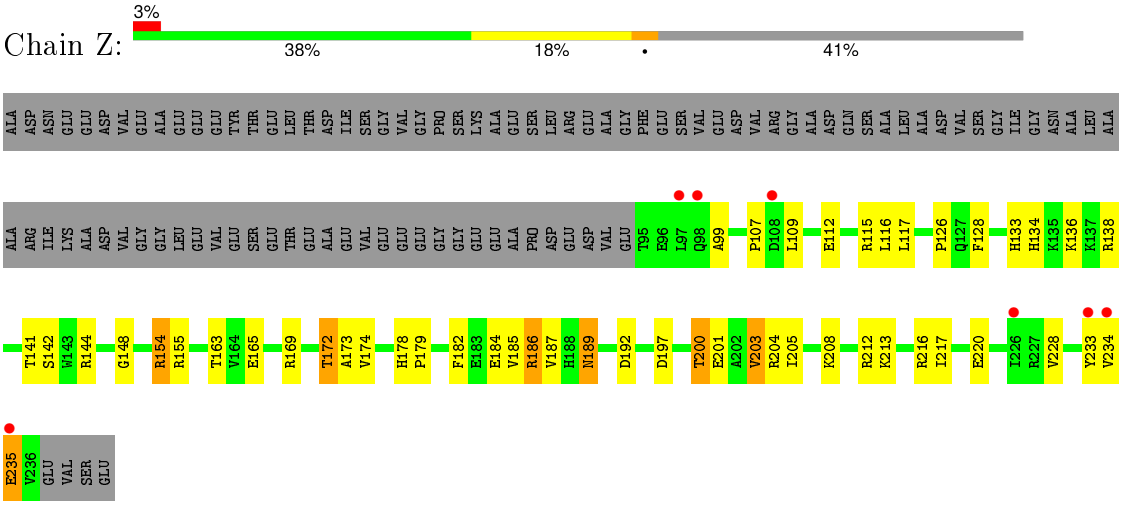
• Molecule 26: 50S ribosomal protein L31e

Chain Y:



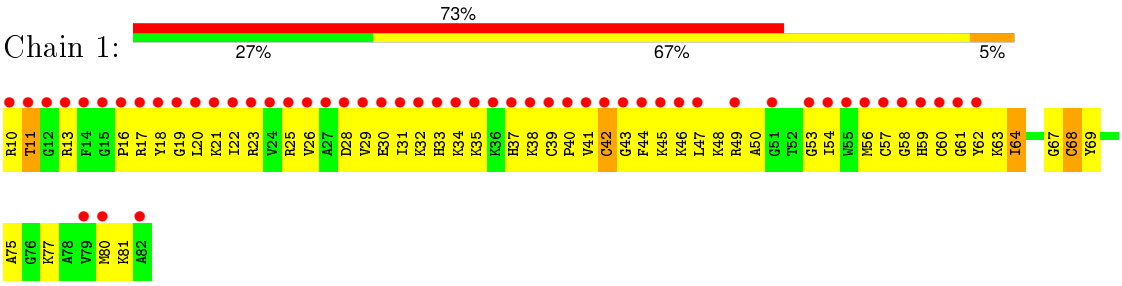
• Molecule 27: 50S ribosomal protein L32E

Chain Z:



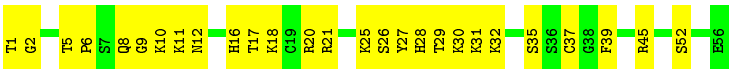
• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:



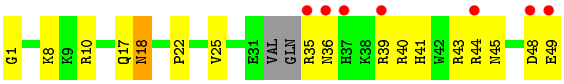
• Molecule 29: 50S ribosomal protein L37e

Chain 2:



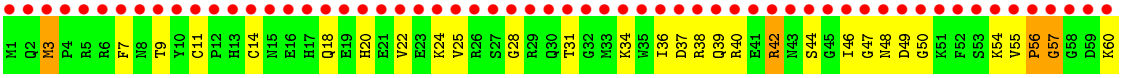
• Molecule 30: 50S ribosomal protein L39e

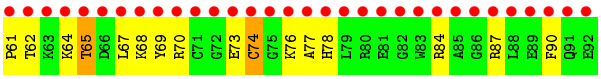
Chain 3:



• Molecule 31: 50S ribosomal protein L44E

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.98 49.62 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.8 (49.62-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.251 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 370643 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, PPU

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	A	0.58	2/66076 (0.0%)	0.76	28/103052 (0.0%)
2	B	0.54	0/2905	0.82	4/4528 (0.1%)
3	5	2.09	1/43 (2.3%)	1.94	0/64
4	C	0.45	0/1787	0.75	0/2409
5	D	0.44	0/2689	0.70	0/3652
6	E	0.48	0/1883	0.72	0/2551
7	F	0.40	0/1111	0.63	0/1498
8	G	0.45	0/1382	0.65	0/1880
9	H	0.39	0/896	0.62	0/1219
10	I	0.38	0/241	0.56	0/324
11	J	0.48	0/1246	0.81	2/1686 (0.1%)
12	K	0.49	0/1135	0.70	0/1530
13	L	0.46	0/1003	0.76	0/1351
14	M	0.49	0/1126	0.76	0/1504
15	N	0.61	0/1633	0.83	2/2180 (0.1%)
16	O	0.40	0/1473	0.71	0/1999
17	P	0.47	0/873	0.70	0/1181
18	Q	0.44	0/1143	0.62	0/1521
19	R	0.44	0/748	0.75	1/1005 (0.1%)
20	S	0.49	0/1172	0.73	0/1578
21	T	0.41	0/648	0.65	0/875
22	U	0.39	0/957	0.70	0/1289
23	V	0.58	0/417	0.74	1/562 (0.2%)
24	W	0.38	0/502	0.60	0/675
25	X	0.50	0/1218	0.72	0/1655
26	Y	0.46	0/664	0.71	0/895
27	Z	0.48	0/1146	0.71	0/1536
28	1	0.77	0/575	0.84	0/763
29	2	0.55	0/437	0.77	0/578
30	3	0.44	0/398	0.61	0/527
31	4	0.93	0/771	0.80	0/1024
All	All	0.56	3/98298 (0.0%)	0.75	38/147091 (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	A	1	143
2	B	1	4
All	All	2	147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1206	U	N1-C2	5.33	1.43	1.38
1	A	1206	U	C3'-O3'	-5.24	1.34	1.42
3	5	75	C	C4'-C3'	-5.04	1.47	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	U	OP1-P-O3'	-18.53	64.43	105.20
1	A	1164	U	OP2-P-O3'	-18.53	64.44	105.20
1	A	1165	G	O5'-P-OP1	-11.90	94.99	105.70
2	B	3024	U	C2'-C3'-O3'	9.55	130.52	109.50
1	A	1563	G	C2'-C3'-O3'	9.10	129.51	109.50
1	A	1979	G	C2'-C3'-O3'	8.54	128.28	109.50
1	A	1206	U	O5'-P-OP1	-8.21	98.31	105.70
1	A	1942	A	C5'-C4'-C3'	7.54	128.07	116.00
2	B	3003	A	O5'-P-OP1	7.40	119.58	110.70
1	A	1942	A	C5'-C4'-O4'	7.19	117.73	109.10
2	B	3103	A	C5'-C4'-O4'	7.07	117.59	109.10
1	A	871	G	C5'-C4'-O4'	-6.56	101.23	109.10
1	A	1504	A	C1'-O4'-C4'	-6.30	104.86	109.90
2	B	3039	U	N1-C1'-C2'	6.18	122.03	114.00
1	A	1165	G	OP1-P-OP2	6.10	128.75	119.60
1	A	1120	U	C5'-C4'-C3'	-6.07	106.29	116.00
1	A	1165	G	O5'-P-OP2	-6.02	100.28	105.70
1	A	389	G	C5'-C4'-C3'	-6.02	106.38	116.00
23	V	36	CYS	CA-CB-SG	-6.00	103.21	114.00
1	A	2419	U	N1-C1'-C2'	5.98	121.77	114.00
1	A	2313	C	C5'-C4'-O4'	5.89	116.17	109.10
1	A	2012	U	N1-C1'-C2'	5.88	121.65	114.00
1	A	2467	A	O5'-P-OP1	-5.79	100.49	105.70
1	A	2726	U	N1-C1'-C2'	5.66	121.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1738	C	O4'-C4'-C3'	-5.61	98.39	104.00
11	J	74	ASN	N-CA-C	-5.56	95.98	111.00
1	A	129	A	C2'-C3'-O3'	5.54	122.56	113.70
1	A	2096	A	N9-C1'-C2'	5.42	121.05	114.00
11	J	156	THR	N-CA-C	-5.38	96.49	111.00
15	N	73	ARG	N-CA-C	-5.35	96.55	111.00
19	R	68	GLY	N-CA-C	-5.28	99.90	113.10
1	A	921	G	N9-C1'-C2'	5.12	120.65	114.00
1	A	192	A	N9-C1'-C2'	5.09	120.62	114.00
1	A	658	C	N1-C1'-C2'	-5.08	106.41	112.00
1	A	2468	A	N9-C1'-C2'	5.04	120.56	114.00
15	N	74	ARG	N-CA-C	5.04	124.60	111.00
1	A	917	U	C5'-C4'-C3'	5.01	124.01	116.00
1	A	1819	G	C5'-C4'-C3'	5.01	124.01	116.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	A	Sidechain
1	A	1027	G	Sidechain
1	A	1030	U	Sidechain
1	A	1038	G	Sidechain
1	A	1125	U	Sidechain
1	A	115	U	Sidechain
1	A	1191	A	Sidechain
1	A	1206	U	Sidechain
1	A	1226	G	Sidechain
1	A	1236	A	Sidechain
1	A	1244	U	Sidechain
1	A	1260	G	Sidechain
1	A	1261	A	Sidechain
1	A	1266	U	Sidechain
1	A	1297	U	Sidechain
1	A	1298	U	Sidechain
1	A	1309	U	Sidechain
1	A	1332	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1347	U	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1387	G	Sidechain
1	A	1412	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1467	C	Sidechain
1	A	1478	U	Sidechain
1	A	1503	U	Sidechain
1	A	1531	U	Sidechain
1	A	1635	U	Sidechain
1	A	1645	U	Sidechain
1	A	1647	G	Sidechain
1	A	1681	G	Sidechain
1	A	1684	A	Sidechain
1	A	1688	G	Sidechain
1	A	1696	U	Sidechain
1	A	1701	A	Sidechain
1	A	1706	G	Sidechain
1	A	171	C	Sidechain
1	A	1736	A	Sidechain
1	A	1750	C	Sidechain
1	A	176	U	Sidechain
1	A	1777	G	Sidechain
1	A	1818	C	Sidechain
1	A	182	G	Sidechain
1	A	1826	C	Sidechain
1	A	1828	G	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1846	U	Sidechain
1	A	1848	G	Sidechain
1	A	1878	G	Sidechain
1	A	1933	G	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	2022	A	Sidechain
1	A	2026	C	Sidechain
1	A	2063	U	Sidechain
1	A	2102	G	Sidechain
1	A	211	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2110	G	Sidechain
1	A	2119	C	Sidechain
1	A	2124	G	Sidechain
1	A	214	U	Sidechain
1	A	22	U	Sidechain
1	A	224	U	Sidechain
1	A	2279	G	Sidechain
1	A	2306	U	Sidechain
1	A	2308	U	Sidechain
1	A	2313	C	Sidechain
1	A	2336	G	Sidechain
1	A	2390	U	Sidechain
1	A	2421	G	Sidechain
1	A	2429	A	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	246	G	Sidechain
1	A	2461	U	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2524	G	Sidechain
1	A	2526	C	Sidechain
1	A	2535	U	Sidechain
1	A	2590	U	Sidechain
1	A	26	U	Sidechain
1	A	2620	U	Sidechain
1	A	2621	U	Sidechain
1	A	2630	G	Sidechain
1	A	2634	G	Sidechain
1	A	265	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2692	G	Sidechain
1	A	2736	U	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	28	G	Sidechain
1	A	2800	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	315	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	321	A	Sidechain
1	A	333	G	Sidechain
1	A	344	C	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	407	A	Sidechain
1	A	435	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	459	A	Sidechain
1	A	48	A	Sidechain
1	A	483	C	Sidechain
1	A	502	A	Sidechain
1	A	506	G	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	55	U	Sidechain
1	A	614	U	Sidechain
1	A	619	U	Sidechain
1	A	640	G	Sidechain
1	A	664	U	Sidechain
1	A	676	C	Sidechain
1	A	722	G	Sidechain
1	A	734	U	Sidechain
1	A	743	G	Sidechain
1	A	761	A	Sidechain
1	A	764	C	Sidechain
1	A	775	G	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	818	A	Sidechain
1	A	854	G	Sidechain
1	A	873	G	Sidechain
1	A	888	U	Sidechain
1	A	897	A	Sidechain
1	A	898	G	Sidechain
1	A	906	C	Sidechain
1	A	919	U	Sidechain
1	A	932	U	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain
2	B	3022	G	Sidechain

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Mol	Chain	Res	Type	Group
2	B	3024	U	Sidechain
2	B	3065	A	Sidechain
2	B	3099	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29798	1217	0
2	B	2600	0	1326	82	0
3	5	40	0	22	5	0
4	C	1754	0	1763	125	0
5	D	2624	0	2533	189	0
6	E	1858	0	1816	137	0
7	F	1094	0	1085	137	0
8	G	1357	0	1266	83	0
9	H	885	0	854	57	0
10	I	240	0	231	25	0
11	J	1215	0	1215	155	0
12	K	1119	0	1098	70	0
13	L	993	0	1027	67	0
14	M	1114	0	1072	67	0
15	N	1605	0	1676	179	0
16	O	1444	0	1401	142	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	60	0
19	R	734	0	728	28	0
20	S	1149	0	1122	56	0
21	T	641	0	605	28	0
22	U	949	0	923	49	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	99	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	63	0
28	1	563	0	601	80	0
29	2	430	0	426	39	0
30	3	393	0	406	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	755	0	732	62	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1	36	0	0	13	0
38	2	58	0	0	4	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	268	0
38	B	146	0	0	15	0
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	20	0
38	G	45	0	0	11	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	20	0
38	K	54	0	0	4	0
38	L	64	0	0	16	0
38	M	86	0	0	15	0
38	N	138	0	0	27	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	4	0
38	S	83	0	0	10	0
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	6	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3185	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 (3185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10
1:A:1751:G:H2'	1:A:1752:G:H5"	1.30	1.10
6:E:236:THR:HG22	6:E:239:ALA:H	1.01	1.09
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.34	1.08
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.34	1.08
28:1:39:CYS:SG	28:1:47:LEU:HD21	1.93	1.08
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.34	1.08
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.38	1.06
1:A:2121:G:OP2	38:A:3007:HOH:O	1.69	1.06
1:A:1160:G:H5'	1:A:1161:A:H5'	1.36	1.04
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.39	1.04
1:A:1134:G:H4'	11:J:151:MET:HE1	1.41	1.03
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.39	1.03
1:A:156:C:H5"	15:N:171:ARG:HD3	1.39	1.03
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.40	1.02
1:A:870:G:H2'	1:A:871:G:H5"	1.40	1.02
1:A:2426:G:H1'	38:A:5552:HOH:O	1.57	1.02
15:N:74:ARG:O	15:N:88:VAL:HG13	1.56	1.02
25:X:88:THR:HB	38:X:6679:HOH:O	1.60	1.01
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.39	1.00
1:A:1835:U:H5	1:A:1840:A:N7	1.58	1.00
7:F:105:SER:HB2	7:F:131:THR:HG23	1.43	1.00
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.77	0.99
1:A:2466:G:H5"	38:A:3142:HOH:O	1.61	0.99
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.42	0.98
5:D:86:ALA:HA	38:D:8583:HOH:O	1.64	0.98
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.42	0.98
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.77	0.97
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.82	0.97
1:A:1886:A:N3	38:A:4297:HOH:O	1.95	0.97
14:M:68:GLU:HA	38:M:8548:HOH:O	1.62	0.97
1:A:1474:C:H6	1:A:1474:C:H5'	1.30	0.97
2:B:3056:A:H2'	2:B:3057:A:H5"	1.45	0.96
21:T:57:THR:HG22	21:T:59:ASP:H	1.24	0.96
13:L:10:GLN:NE2	13:L:10:GLN:H	1.62	0.96
1:A:2717:C:H2'	1:A:2718:C:H5"	1.47	0.96
18:Q:115:SER:H	18:Q:118:GLN:HE21	0.99	0.96
1:A:2467:A:H2'	38:A:4927:HOH:O	1.64	0.95
5:D:321:PRO:HA	38:D:8657:HOH:O	1.66	0.95
1:A:962:C:H1'	16:O:5:ARG:NH1	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:G:H5'	1:A:871:G:H8	1.31	0.94
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.50	0.94
21:T:57:THR:HG22	21:T:59:ASP:N	1.82	0.93
38:A:4337:HOH:O	15:N:14:ARG:HG2	1.65	0.93
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.47	0.93
11:J:142:VAL:HG13	38:J:8381:HOH:O	1.68	0.93
7:F:25:MET:HE2	7:F:41:LEU:HG	1.50	0.93
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.83	0.93
1:A:2533:C:H5'	1:A:2533:C:H6	1.32	0.93
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.33	0.93
2:B:3023:U:H4'	2:B:3024:U:OP2	1.69	0.93
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.49	0.92
1:A:856:G:H2'	38:A:4898:HOH:O	1.68	0.92
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.52	0.91
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.52	0.91
1:A:1116:U:HO2'	1:A:1118:A:H2	0.92	0.91
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.53	0.91
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.50	0.91
13:L:10:GLN:HE21	13:L:10:GLN:H	1.10	0.91
6:E:2:GLN:HB3	38:E:8338:HOH:O	1.70	0.91
6:E:236:THR:HG22	6:E:239:ALA:N	1.85	0.90
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.01	0.90
27:Z:212:ARG:HD2	38:Z:8605:HOH:O	1.70	0.90
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.53	0.90
1:A:1372:A:H3'	38:A:6651:HOH:O	1.68	0.90
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.36	0.90
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.54	0.90
15:N:69:LYS:O	15:N:73:ARG:NH2	2.04	0.90
1:A:2122:C:OP2	38:A:6038:HOH:O	1.88	0.90
1:A:871:G:H5'	1:A:871:G:C8	2.06	0.90
15:N:87:MET:CG	31:4:46:ILE:HG21	2.02	0.90
2:B:3076:G:H3'	2:B:3077:A:H5"	1.54	0.89
1:A:506:G:H22	1:A:509:A:H5'	1.35	0.89
11:J:27:LYS:H	11:J:58:HIS:HD2	1.14	0.89
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.51	0.89
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.55	0.89
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.38	0.89
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.38	0.89
26:Y:25:ARG:HD2	38:Y:3861:HOH:O	1.73	0.88
1:A:1679:C:H5'	38:A:8834:HOH:O	1.74	0.88
30:3:41:HIS:H	30:3:45:ASN:HD22	1.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.54	0.88
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.37	0.88
1:A:2717:C:C2'	1:A:2718:C:H5"	2.04	0.88
6:E:132:ASP:HB3	38:E:8364:HOH:O	1.74	0.88
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.56	0.88
15:N:164:THR:HG22	15:N:167:GLY:N	1.88	0.87
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.56	0.87
16:O:144:GLY:O	16:O:147:ILE:HG22	1.73	0.87
5:D:62:ARG:HA	5:D:65:MET:HE3	1.56	0.87
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.38	0.87
4:C:223:ARG:HG3	38:C:8616:HOH:O	1.73	0.87
1:A:1242:A:H5'	12:K:82:THR:HG23	1.53	0.87
25:X:88:THR:HG22	25:X:89:ASP:H	1.39	0.87
6:E:236:THR:HG21	38:E:8375:HOH:O	1.74	0.86
1:A:2123:A:OP2	38:A:4762:HOH:O	1.91	0.86
26:Y:15:ARG:HH11	26:Y:15:ARG:HB3	1.40	0.86
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.75	0.86
12:K:19:MET:CE	12:K:132:LEU:HD11	2.05	0.86
2:B:3025:G:H3'	2:B:3026:C:H5'	1.55	0.86
1:A:21:G:H5'	20:S:2:ILE:HA	1.56	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
1:A:542:A:H8	1:A:542:A:H5'	1.38	0.86
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.57	0.86
1:A:870:G:C2'	1:A:871:G:H5"	2.06	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
20:S:9:ASP:O	20:S:13:THR:HB	1.76	0.86
1:A:545:G:H5'	1:A:545:G:H8	1.40	0.86
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.06	0.85
5:D:140:LEU:HA	38:D:8583:HOH:O	1.75	0.85
1:A:1244:U:OP1	12:K:18:ILE:HD13	1.76	0.85
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.41	0.85
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.74	0.85
1:A:2420:G:O2'	1:A:2421:G:H5'	1.75	0.85
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.58	0.85
1:A:1474:C:C6	1:A:1474:C:H5'	2.12	0.85
15:N:164:THR:HG23	15:N:165:SER:N	1.90	0.85
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.57	0.85
11:J:162:SER:HB2	11:J:163:PRO:CD	2.07	0.85
6:E:246:ARG:NH1	6:E:246:ARG:HB3	1.91	0.85
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.77	0.84
1:A:506:G:H22	1:A:509:A:C5'	1.88	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:140:VAL:HB	38:E:8457:HOH:O	1.77	0.84
1:A:1450:C:H4'	1:A:1451:C:OP2	1.76	0.84
1:A:645:U:OP2	14:M:4:LYS:HE2	1.77	0.84
2:B:3025:G:H3'	2:B:3026:C:C5'	2.07	0.84
25:X:122:ARG:NH2	25:X:154:ARG:HD2	1.92	0.84
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.60	0.84
15:N:52:LEU:HD11	38:N:8616:HOH:O	1.76	0.84
29:2:8:GLN:HE22	29:2:11:LYS:NZ	1.74	0.84
38:B:8459:HOH:O	19:R:25:PRO:HB2	1.78	0.84
11:J:59:ASN:HD22	11:J:59:ASN:H	1.21	0.84
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.40	0.84
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.93	0.83
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.23	0.83
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.17	0.83
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.13	0.83
1:A:2459:G:P	31:4:64:LYS:HB2	2.18	0.83
38:A:3219:HOH:O	15:N:157:LEU:HD11	1.77	0.83
14:M:79:ASP:HB3	38:M:8564:HOH:O	1.78	0.83
1:A:960:G:H4'	38:A:6886:HOH:O	1.76	0.83
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.61	0.83
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.60	0.83
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.59	0.83
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.59	0.83
13:L:10:GLN:HE21	13:L:10:GLN:N	1.77	0.83
7:F:27:ILE:HG22	7:F:28:GLY:H	1.43	0.83
1:A:1603:A:H5'	1:A:1605:G:O4'	1.78	0.82
15:N:74:ARG:NH2	38:N:8632:HOH:O	2.11	0.82
16:O:7:LYS:HE3	19:R:21:ARG:O	1.79	0.82
12:K:76:ASP:HA	38:K:5907:HOH:O	1.79	0.82
4:C:121:ALA:O	4:C:124:VAL:HG22	1.79	0.82
28:1:46:LYS:HB2	28:1:57:CYS:SG	2.19	0.82
16:O:113:SER:HB2	38:O:8556:HOH:O	1.77	0.82
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.60	0.82
7:F:154:LYS:H	7:F:154:LYS:HD2	1.44	0.82
38:A:7015:HOH:O	31:4:60:LYS:HG3	1.79	0.81
29:2:25:LYS:HE2	38:3:7213:HOH:O	1.79	0.81
38:A:8631:HOH:O	15:N:82:ARG:HD2	1.80	0.81
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.61	0.81
8:G:100:ASP:HB2	38:G:2789:HOH:O	1.79	0.81
11:J:26:LYS:HG2	11:J:28:ILE:H	1.44	0.81
1:A:2506:A:HO2'	1:A:2507:G:H8	0.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:U:C5	1:A:1840:A:N7	2.48	0.81
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.28	0.81
38:A:4426:HOH:O	2:B:3103:A:H4'	1.81	0.81
1:A:1184:C:H1'	38:A:6922:HOH:O	1.81	0.81
11:J:2:PRO:HB2	38:J:8365:HOH:O	1.81	0.80
4:C:192:VAL:HB	38:C:8606:HOH:O	1.81	0.80
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.62	0.80
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.12	0.80
7:F:20:LYS:HA	7:F:75:LEU:O	1.82	0.80
1:A:1974:G:OP1	38:A:6321:HOH:O	1.99	0.80
28:1:47:LEU:HD23	28:1:57:CYS:HB2	1.63	0.80
1:A:2506:A:O2'	1:A:2507:G:H8	1.62	0.80
11:J:5:MET:HG3	38:J:8365:HOH:O	1.80	0.80
1:A:1205:U:H2'	1:A:1206:U:H5'	1.62	0.80
1:A:560:C:H42	1:A:597:A:H61	1.29	0.80
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.62	0.80
9:H:91:VAL:HG12	9:H:92:GLY:H	1.47	0.80
23:V:9:CYS:SG	23:V:11:THR:HG23	2.21	0.79
1:A:289:G:H22	1:A:363:A:H2	1.30	0.79
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.79
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.47	0.79
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.79
1:A:1165:G:H4'	1:A:1174:A:O2'	1.81	0.79
1:A:2466:G:OP1	38:A:3142:HOH:O	2.00	0.79
14:M:133:VAL:HA	38:M:8577:HOH:O	1.80	0.79
12:K:26:VAL:HG13	12:K:36:VAL:HG11	1.65	0.79
1:A:346:U:H4'	38:A:6302:HOH:O	1.83	0.79
38:A:3278:HOH:O	15:N:189:VAL:HG21	1.83	0.78
1:A:31:C:H4'	38:A:6880:HOH:O	1.83	0.78
13:L:30:LYS:O	13:L:55:VAL:HG13	1.82	0.78
38:A:6460:HOH:O	19:R:9:GLY:HA2	1.82	0.78
6:E:246:ARG:HH11	6:E:246:ARG:HB3	1.45	0.78
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.49	0.78
12:K:99:GLU:HA	38:K:7377:HOH:O	1.84	0.78
7:F:19:GLU:O	7:F:20:LYS:HG2	1.84	0.78
1:A:381:G:H5"	38:A:3807:HOH:O	1.84	0.78
27:Z:185:VAL:HA	38:Z:8566:HOH:O	1.84	0.78
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.65	0.78
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.65	0.78
15:N:87:MET:HG2	31:4:46:ILE:CG2	2.14	0.78
11:J:139:ASP:N	11:J:140:PRO:HD3	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.48	0.78
27:Z:216:ARG:HD3	38:Z:8574:HOH:O	1.83	0.78
5:D:145:HIS:HD2	5:D:146:THR:O	1.67	0.78
6:E:107:ARG:NH1	6:E:107:ARG:HB3	1.99	0.77
11:J:150:LYS:HE2	38:J:8383:HOH:O	1.84	0.77
1:A:2468:A:H61	31:4:48:ASN:HD21	1.27	0.77
1:A:2812:A:H2	1:A:2814:A:H62	1.32	0.77
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.48	0.77
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.66	0.77
1:A:1160:G:C5'	1:A:1161:A:H5'	2.14	0.77
9:H:91:VAL:HG12	9:H:92:GLY:N	2.00	0.77
1:A:288:A:H61	1:A:364:C:H42	1.32	0.77
38:A:5753:HOH:O	7:F:99:ASP:HA	1.84	0.77
9:H:96:ALA:HA	38:H:3111:HOH:O	1.84	0.77
12:K:103:VAL:HG12	38:K:5907:HOH:O	1.84	0.77
15:N:157:LEU:HA	35:N:8518:CL:CL	2.22	0.77
1:A:1118:A:H3'	1:A:1118:A:H8	1.48	0.77
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.20	0.77
27:Z:220:GLU:HG2	38:Z:8553:HOH:O	1.85	0.77
12:K:133:GLY:O	12:K:137:GLU:HG3	1.85	0.76
1:A:338:C:H4'	6:E:174:ILE:CD1	2.15	0.76
8:G:97:VAL:HG12	38:G:4191:HOH:O	1.84	0.76
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.85	0.76
2:B:3023:U:H6	2:B:3023:U:H5"	1.50	0.76
2:B:3014:G:H8	2:B:3014:G:H5'	1.50	0.76
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.82	0.76
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.80	0.76
1:A:1058:A:H2'	1:A:1060:C:H5"	1.68	0.76
1:A:871:G:C5'	1:A:871:G:H8	1.98	0.76
1:A:2466:G:C5'	38:A:3142:HOH:O	2.23	0.76
28:1:29:VAL:O	28:1:33:HIS:HB2	1.86	0.76
1:A:962:C:H1'	16:O:5:ARG:HH12	1.50	0.76
2:B:3023:U:H3'	38:B:8482:HOH:O	1.85	0.76
1:A:559:U:H6	1:A:559:U:H5'	1.51	0.76
1:A:450:C:OP1	6:E:184:ARG:NH2	2.17	0.76
11:J:59:ASN:HD22	11:J:59:ASN:N	1.83	0.76
1:A:2578:G:H5'	1:A:2578:G:H8	1.49	0.76
5:D:258:GLY:H	5:D:260:HIS:CE1	2.03	0.76
11:J:141:ASN:HA	38:J:8366:HOH:O	1.84	0.76
1:A:31:C:H2'	38:A:7147:HOH:O	1.86	0.76
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.16	0.76
1:A:2467:A:H3'	38:A:4927:HOH:O	1.85	0.75
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.65	0.75
1:A:2271:G:OP2	38:A:8940:HOH:O	2.05	0.75
14:M:120:LEU:HD12	14:M:133:VAL:HG21	1.69	0.75
8:G:6:GLU:HA	8:G:46:THR:HG22	1.69	0.75
20:S:99:ALA:HB1	20:S:109:MET:CE	2.15	0.75
11:J:27:LYS:N	11:J:58:HIS:HD2	1.84	0.75
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.68	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
1:A:1741:U:O2'	1:A:2723:G:H4'	1.87	0.75
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.85	0.75
13:L:39:GLY:HA2	38:L:4183:HOH:O	1.86	0.75
4:C:35:GLY:O	4:C:36:ASP:HB3	1.86	0.75
1:A:711:G:H1'	38:A:6554:HOH:O	1.87	0.75
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.67	0.75
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.67	0.75
24:W:1:THR:HG23	24:W:2:VAL:H	1.51	0.75
1:A:2094:G:H4'	5:D:245:SER:HB3	1.66	0.75
28:1:46:LYS:HB2	28:1:57:CYS:HG	1.52	0.75
1:A:1191:A:H3'	1:A:1192:A:H5"	1.68	0.75
1:A:2508:C:H2'	38:A:6213:HOH:O	1.86	0.75
11:J:28:ILE:HA	11:J:62:GLU:OE1	1.87	0.75
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.86	0.75
1:A:2433:A:H2'	1:A:2434:A:C8	2.22	0.75
6:E:76:ARG:HD2	38:E:8439:HOH:O	1.85	0.75
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.22	0.75
28:1:18:TYR:HB3	28:1:22:ILE:HG21	1.68	0.74
14:M:67:ARG:O	14:M:71:GLU:HG3	1.87	0.74
1:A:1751:G:C2'	1:A:1752:G:H5"	2.11	0.74
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.69	0.74
15:N:87:MET:CB	31:4:46:ILE:HG21	2.17	0.74
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.68	0.74
8:G:166:VAL:HG12	38:G:3134:HOH:O	1.87	0.74
31:4:65:THR:HG23	31:4:67:LEU:HG	1.69	0.74
1:A:2812:A:N7	38:A:6974:HOH:O	2.20	0.74
23:V:13:ILE:HG12	23:V:32:CYS:CB	2.17	0.74
15:N:152:ARG:HG3	38:N:8559:HOH:O	1.87	0.74
7:F:95:THR:O	7:F:97:GLN:N	2.18	0.74
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.69	0.74
38:B:8467:HOH:O	16:O:147:ILE:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:49:ARG:HD2	38:1:8426:HOH:O	1.87	0.73
2:B:3056:A:C2'	2:B:3057:A:H5"	2.18	0.73
4:C:36:ASP:OD2	4:C:85:ASP:HB2	1.87	0.73
23:V:47:ARG:HG3	38:V:4381:HOH:O	1.88	0.73
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.71	0.73
1:A:2755:G:H1'	38:A:4164:HOH:O	1.88	0.73
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.70	0.73
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.36	0.73
1:A:2748:G:H2'	38:A:6999:HOH:O	1.88	0.73
1:A:820:G:OP1	28:1:17:ARG:NH2	2.20	0.73
15:N:79:LYS:HD3	38:N:8563:HOH:O	1.88	0.73
1:A:1701:A:H5'	38:A:5741:HOH:O	1.87	0.73
1:A:1209:C:H4'	38:A:4753:HOH:O	1.88	0.73
1:A:1829:A:H61	28:1:18:TYR:HA	1.54	0.73
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.52	0.73
1:A:1130:U:H2'	1:A:1131:G:O4'	1.89	0.73
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.70	0.73
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.54	0.73
2:B:3024:U:O2'	2:B:3025:G:H4'	1.88	0.73
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.72
7:F:35:ALA:N	38:F:5576:HOH:O	2.22	0.72
38:A:3951:HOH:O	15:N:146:GLN:HG2	1.89	0.72
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.71	0.72
4:C:135:VAL:HG21	4:C:147:ARG:NH1	2.04	0.72
20:S:39:THR:HG23	20:S:107:GLU:O	1.89	0.72
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.03	0.72
1:A:2404:G:O3'	38:A:6058:HOH:O	2.06	0.72
31:4:74:CYS:SG	31:4:76:LYS:HB2	2.28	0.72
15:N:87:MET:CB	31:4:46:ILE:HD13	2.20	0.72
10:I:12:ILE:N	10:I:13:PRO:HD3	2.04	0.72
1:A:182:G:H5'	38:A:4632:HOH:O	1.87	0.72
38:A:4311:HOH:O	12:K:47:THR:HB	1.89	0.72
8:G:101:GLU:HB2	8:G:116:THR:O	1.90	0.72
15:N:72:SER:O	38:N:8655:HOH:O	2.06	0.72
5:D:179:LEU:O	5:D:183:GLU:HG2	1.90	0.72
11:J:137:ASN:O	11:J:139:ASP:N	2.22	0.72
1:A:2620:U:O2'	38:A:6629:HOH:O	2.06	0.72
20:S:39:THR:HG22	20:S:42:GLU:H	1.53	0.72
1:A:1666:C:H2'	1:A:1667:A:H5'	1.70	0.72
1:A:172:U:OP2	38:A:5669:HOH:O	2.07	0.72
1:A:113:A:OP2	1:A:114:A:H2'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:139:PRO:O	15:N:140:ALA:HB3	1.89	0.72
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.71	0.72
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.70	0.72
14:M:114:VAL:HG11	38:M:8577:HOH:O	1.89	0.72
15:N:59:GLY:HA3	15:N:141:ILE:CD1	2.19	0.72
38:A:6880:HOH:O	22:U:9:LYS:HB2	1.89	0.72
19:R:64:GLU:HG3	19:R:74:ASP:OD2	1.89	0.72
10:I:12:ILE:HA	38:I:4499:HOH:O	1.89	0.71
17:P:32:ARG:O	17:P:32:ARG:HD3	1.87	0.71
15:N:68:ARG:HD3	15:N:68:ARG:O	1.89	0.71
1:A:2346:C:H6	1:A:2346:C:O5'	1.73	0.71
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.55	0.71
8:G:11:VAL:HG12	8:G:12:ASP:N	2.05	0.71
1:A:272:A:H3'	38:A:6987:HOH:O	1.88	0.71
13:L:106:GLY:HA3	38:L:5264:HOH:O	1.89	0.71
1:A:2467:A:C2'	38:A:4927:HOH:O	2.31	0.71
24:W:12:THR:HG22	24:W:15:GLU:CG	2.19	0.71
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.56	0.71
1:A:284:C:H4'	1:A:285:A:O5'	1.88	0.71
11:J:162:SER:CB	11:J:163:PRO:HD3	2.20	0.71
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.73	0.71
4:C:179:MET:HG2	4:C:186:TRP:CB	2.20	0.71
11:J:139:ASP:HA	38:J:8370:HOH:O	1.88	0.71
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.73	0.71
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.72	0.71
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.22	0.71
1:A:2638:G:H1'	38:A:7218:HOH:O	1.90	0.71
1:A:2310:G:OP2	11:J:114:PRO:HD2	1.89	0.71
5:D:190:MET:HE2	5:D:194:PHE:CD1	2.25	0.71
1:A:2291:A:C8	1:A:2309:C:H5'	2.25	0.71
1:A:1701:A:H4'	1:A:1702:U:H5"	1.72	0.71
6:E:12:THR:HB	38:E:8447:HOH:O	1.89	0.71
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.70	0.71
38:A:3555:HOH:O	5:D:27:ASN:HB2	1.90	0.71
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.71
25:X:81:ASP:OD1	25:X:92:ASP:HB2	1.91	0.71
1:A:877:G:H5'	1:A:878:G:OP1	1.91	0.71
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.71
14:M:34:GLY:HA3	14:M:38:HIS:CE1	2.25	0.71
13:L:81:ARG:HB2	13:L:87:ARG:NH1	2.04	0.71
1:A:113:A:H3'	1:A:114:A:H5"	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:C:C2'	1:A:2503:A:H5'	2.21	0.70
1:A:1741:U:H5'	1:A:1742:A:OP1	1.90	0.70
1:A:2346:C:O2'	7:F:52:THR:HG21	1.91	0.70
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.70
6:E:46:TYR:CE2	6:E:98:ARG:NH1	2.59	0.70
1:A:2421:G:H4'	38:A:4257:HOH:O	1.91	0.70
1:A:1666:C:O2'	1:A:1667:A:H5"	1.91	0.70
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.72	0.70
38:A:5258:HOH:O	15:N:170:CYS:SG	2.48	0.70
15:N:122:GLU:OE2	15:N:127:LYS:HE2	1.91	0.70
15:N:164:THR:CG2	15:N:167:GLY:H	1.95	0.70
6:E:236:THR:H	6:E:239:ALA:HB3	1.55	0.70
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.06	0.70
7:F:91:ALA:HB1	38:F:5198:HOH:O	1.91	0.70
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.72	0.70
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.73	0.70
1:A:2467:A:OP1	38:A:8560:HOH:O	2.09	0.70
1:A:1119:G:N2	1:A:1246:A:C2	2.59	0.70
11:J:14:TYR:H	11:J:91:HIS:CE1	2.09	0.70
1:A:1164:U:H3	1:A:1192:A:H2	1.38	0.70
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.21	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.72	0.70
2:B:3006:C:H5"	16:O:37:ARG:HH12	1.55	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.91	0.70
1:A:2281:C:C2'	1:A:2282:U:H5'	2.20	0.70
11:J:75:SER:O	11:J:79:ALA:HB2	1.92	0.70
38:A:9293:HOH:O	13:L:39:GLY:HA3	1.90	0.70
6:E:78:ARG:HH11	6:E:78:ARG:HG3	1.56	0.70
6:E:25:PRO:HG2	38:E:8325:HOH:O	1.92	0.70
2:B:3023:U:C6	2:B:3023:U:H5"	2.27	0.70
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.73	0.70
26:Y:18:ARG:NH1	38:Y:4132:HOH:O	2.16	0.70
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.02	0.70
11:J:140:PRO:HB3	38:J:8381:HOH:O	1.92	0.70
11:J:27:LYS:H	11:J:58:HIS:CD2	2.04	0.70
12:K:107:ASN:ND2	12:K:109:TYR:H	1.90	0.70
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.27	0.70
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.72	0.69
38:A:6913:HOH:O	6:E:188:ARG:HD3	1.92	0.69
1:A:2837:U:H2'	38:A:6298:HOH:O	1.92	0.69
1:A:299:U:H5'	38:A:6794:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:39:THR:HB	20:S:42:GLU:HG3	1.73	0.69
1:A:2526:C:O2'	1:A:2527:U:H5'	1.92	0.69
5:D:148:PRO:HD2	38:D:8584:HOH:O	1.91	0.69
1:A:541:C:C2'	1:A:542:A:H5"	2.22	0.69
1:A:1377:C:H5'	1:A:1377:C:H6	1.57	0.69
1:A:2249:G:OP2	38:A:4912:HOH:O	2.10	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.90	0.69
1:A:461:C:H2'	38:A:3491:HOH:O	1.92	0.69
6:E:139:VAL:HG13	38:E:8454:HOH:O	1.90	0.69
1:A:1625:U:H4'	38:A:4149:HOH:O	1.92	0.69
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.10	0.69
1:A:182:G:H4'	15:N:157:LEU:HD13	1.75	0.69
4:C:199:HIS:CD2	4:C:201:PHE:H	2.10	0.69
25:X:88:THR:HG22	25:X:89:ASP:N	2.08	0.69
1:A:2433:A:H2'	1:A:2434:A:H8	1.56	0.69
16:O:164:ASP:CG	16:O:167:ASP:HA	2.13	0.69
1:A:1380:U:OP1	38:A:7331:HOH:O	2.09	0.69
1:A:541:C:H2'	1:A:542:A:C5'	2.22	0.69
4:C:33:GLU:O	4:C:34:ASP:HB2	1.92	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.41	0.69
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.74	0.69
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.75	0.69
24:W:39:ALA:N	24:W:40:PRO:HD2	2.08	0.69
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.57	0.69
1:A:2100:A:H5'	38:A:6844:HOH:O	1.92	0.69
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.75	0.69
2:B:3025:G:C3'	2:B:3026:C:H5'	2.22	0.69
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.08	0.69
17:P:47:ARG:NH1	38:P:4564:HOH:O	2.24	0.69
1:A:69:A:H5'	1:A:69:A:C8	2.28	0.69
30:3:39:ARG:HG2	38:3:3143:HOH:O	1.93	0.69
1:A:214:U:H5'	38:A:5600:HOH:O	1.91	0.69
9:H:110:GLU:HG2	38:H:6926:HOH:O	1.92	0.69
11:J:69:ASN:O	11:J:72:VAL:HG12	1.92	0.69
1:A:447:A:OP1	22:U:2:LYS:HG2	1.92	0.69
38:A:6913:HOH:O	6:E:188:ARG:CD	2.41	0.68
11:J:41:THR:HA	38:J:8396:HOH:O	1.91	0.68
28:1:47:LEU:CD2	28:1:57:CYS:HB2	2.23	0.68
1:A:1160:G:N3	38:A:5102:HOH:O	2.26	0.68
30:3:41:HIS:N	30:3:45:ASN:HD22	1.89	0.68
5:D:254:GLN:HG3	38:D:8530:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1743:G:N7	38:A:8768:HOH:O	2.25	0.68
1:A:2467:A:C3'	38:A:4927:HOH:O	2.42	0.68
2:B:3039:U:H1'	2:B:3044:A:H61	1.57	0.68
1:A:542:A:H5'	1:A:542:A:C8	2.27	0.68
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.41	0.68
16:O:151:ASP:O	16:O:154:LEU:HB2	1.94	0.68
1:A:371:U:H2'	1:A:372:A:H8	1.58	0.68
15:N:37:VAL:HG21	15:N:108:LYS:HG3	1.74	0.68
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.06	0.68
1:A:1909:A:N1	1:A:2128:G:H1'	2.08	0.68
6:E:242:GLU:HG3	38:E:8383:HOH:O	1.92	0.68
1:A:2316:G:H8	38:A:5124:HOH:O	1.76	0.68
22:U:61:GLU:HG3	38:U:3851:HOH:O	1.93	0.68
1:A:516:A:OP2	38:A:5115:HOH:O	2.10	0.68
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.76	0.68
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.23	0.68
25:X:13:MET:HE1	25:X:18:GLN:HA	1.75	0.68
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.29	0.68
1:A:541:C:H2'	1:A:542:A:H5"	1.75	0.68
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.94	0.68
21:T:37:VAL:O	21:T:41:VAL:HG23	1.93	0.68
1:A:21:G:C5'	20:S:2:ILE:HA	2.23	0.68
1:A:2716:G:H5"	5:D:206:THR:HG21	1.76	0.68
1:A:2301:A:H5"	1:A:2302:A:H5'	1.75	0.68
2:B:3013:A:O2'	2:B:3014:G:H5"	1.94	0.68
1:A:485:A:N3	1:A:487:G:H5"	2.09	0.68
9:H:99:THR:HA	38:H:3461:HOH:O	1.94	0.68
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.28	0.68
1:A:2830:U:H3'	38:A:4703:HOH:O	1.92	0.68
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.59	0.67
1:A:739:G:C5	38:A:7001:HOH:O	2.47	0.67
1:A:545:G:C8	1:A:545:G:H5'	2.28	0.67
15:N:78:ASN:ND2	38:N:8651:HOH:O	2.26	0.67
2:B:3092:G:H2'	2:B:3093:A:C8	2.29	0.67
27:Z:155:ARG:NH1	38:Z:8562:HOH:O	2.26	0.67
1:A:918:G:N7	38:A:9993:HOH:O	2.27	0.67
1:A:2748:G:H5'	38:A:6999:HOH:O	1.94	0.67
1:A:69:A:H8	1:A:69:A:H5'	1.59	0.67
1:A:689:G:N3	38:A:8933:HOH:O	2.26	0.67
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.58	0.67
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2464:C:H5"	1:A:2465:A:OP1	1.93	0.67
1:A:281:U:H2'	1:A:282:C:O4'	1.95	0.67
16:O:73:ALA:N	38:O:8563:HOH:O	2.28	0.67
16:O:119:GLN:O	16:O:123:ILE:HG13	1.94	0.67
1:A:1172:G:H1'	38:A:4448:HOH:O	1.93	0.67
26:Y:41:PHE:O	26:Y:43:VAL:HG23	1.94	0.67
15:N:89:ASN:HA	38:N:8557:HOH:O	1.94	0.67
7:F:105:SER:CB	7:F:131:THR:HG23	2.21	0.67
17:P:42:GLU:HB2	38:P:2176:HOH:O	1.92	0.67
12:K:19:MET:HE2	12:K:79:PHE:HA	1.76	0.67
1:A:544:G:H2'	1:A:545:G:H5"	1.77	0.67
4:C:8:ARG:HG2	38:C:8558:HOH:O	1.94	0.67
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.77	0.67
17:P:38:ARG:NH1	38:P:7674:HOH:O	2.27	0.67
1:A:236:A:H4'	1:A:237:G:H5'	1.77	0.67
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.77	0.67
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.75	0.67
7:F:97:GLN:O	7:F:97:GLN:HG2	1.95	0.67
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.67
1:A:902:G:N7	14:M:18:HIS:HD2	1.92	0.67
23:V:14:GLU:O	23:V:17:THR:HB	1.95	0.67
13:L:55:VAL:HG12	13:L:56:SER:N	2.09	0.67
5:D:297:VAL:HB	38:D:8606:HOH:O	1.95	0.67
15:N:169:ARG:HD2	38:N:8591:HOH:O	1.95	0.67
1:A:2851:G:O2'	1:A:2852:A:H5'	1.94	0.67
1:A:2502:C:H2'	1:A:2503:A:H5'	1.77	0.66
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.58	0.66
11:J:127:GLY:O	11:J:128:ALA:HB3	1.95	0.66
1:A:2635:A:O2'	1:A:2636:C:H5'	1.94	0.66
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.30	0.66
5:D:51:VAL:HG23	5:D:329:TYR:O	1.95	0.66
1:A:111:C:O2'	29:2:20:ARG:HG2	1.95	0.66
7:F:55:LYS:HA	38:F:6752:HOH:O	1.95	0.66
15:N:164:THR:CG2	15:N:165:SER:N	2.58	0.66
1:A:2533:C:H5'	1:A:2533:C:C6	2.23	0.66
1:A:1667:A:H5'	1:A:1667:A:H8	1.60	0.66
5:D:41:PHE:HA	5:D:79:MET:HE2	1.76	0.66
13:L:115:ARG:HG3	13:L:116:GLU:N	2.08	0.66
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.76	0.66
1:A:2780:C:H1'	8:G:143:GLN:NE2	2.09	0.66
1:A:2459:G:OP2	31:4:64:LYS:HD2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.30	0.66
1:A:1829:A:N6	28:1:18:TYR:HA	2.10	0.66
9:H:2:VAL:HG22	9:H:57:GLU:OE1	1.94	0.66
4:C:94:LEU:N	4:C:94:LEU:HD23	2.10	0.66
25:X:149:LEU:HG	25:X:153:MET:HE2	1.78	0.66
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.76	0.66
15:N:172:GLY:O	15:N:183:VAL:HG11	1.96	0.66
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.77	0.66
7:F:51:ARG:HD3	38:F:7636:HOH:O	1.96	0.66
5:D:141:ARG:HD2	5:D:163:GLU:OE2	1.95	0.66
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.60	0.66
1:A:2502:C:H4'	11:J:151:MET:HG2	1.78	0.66
1:A:1119:G:H22	1:A:1246:A:H2	1.42	0.66
1:A:2505:G:O2'	1:A:2506:A:H5'	1.95	0.66
1:A:1874:U:OP1	38:A:3810:HOH:O	2.14	0.66
20:S:44:VAL:O	20:S:48:GLU:HG3	1.96	0.66
28:1:53:GLY:HA2	28:1:67:GLY:O	1.96	0.66
1:A:2768:A:H2'	1:A:2769:C:O4'	1.94	0.66
1:A:2271:G:P	38:A:8940:HOH:O	2.54	0.65
1:A:282:C:O2'	1:A:283:U:H5'	1.96	0.65
13:L:28:GLU:OE2	13:L:58:THR:HG21	1.96	0.65
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.78	0.65
28:1:30:GLU:HA	28:1:33:HIS:CB	2.26	0.65
6:E:1:MET:HG2	6:E:2:GLN:H	1.61	0.65
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.10	0.65
2:B:3001:U:O3'	2:B:3003:A:H5"	1.96	0.65
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.61	0.65
1:A:814:G:H4'	38:A:9628:HOH:O	1.96	0.65
15:N:30:GLU:O	15:N:34:GLU:HG3	1.97	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.31	0.65
1:A:1130:U:H5'	38:A:7130:HOH:O	1.95	0.65
27:Z:142:SER:OG	38:Z:8616:HOH:O	2.15	0.65
1:A:1681:G:H5"	1:A:1682:A:H5'	1.79	0.65
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.12	0.65
5:D:238:ASN:HD22	5:D:240:GLY:H	1.44	0.65
7:F:136:ARG:HD2	7:F:155:HIS:O	1.95	0.65
4:C:191:GLY:HA2	4:C:194:MET:CE	2.27	0.65
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.26	0.65
16:O:91:ARG:HG3	16:O:186:LEU:HD23	1.79	0.65
25:X:149:LEU:HG	25:X:153:MET:CE	2.27	0.65
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.78	0.65
13:L:27:ARG:HD2	38:L:4747:HOH:O	1.97	0.65
18:Q:87:ARG:HG2	38:Q:190:HOH:O	1.96	0.65
1:A:1477:C:O2'	1:A:1478:U:H5'	1.96	0.65
6:E:127:ARG:HG2	6:E:127:ARG:HH11	1.61	0.65
5:D:140:LEU:HD23	38:D:8583:HOH:O	1.96	0.65
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.11	0.65
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.77	0.65
1:A:2414:A:H2'	1:A:2415:A:C8	2.31	0.65
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.78	0.65
1:A:1886:A:H4'	38:1:8405:HOH:O	1.97	0.65
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.78	0.65
1:A:2618:G:N7	38:A:3140:HOH:O	2.30	0.65
31:4:11:CYS:SG	38:4:8534:HOH:O	2.54	0.65
15:N:84:LYS:HA	31:4:46:ILE:O	1.96	0.65
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.77	0.65
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.00	0.65
1:A:2432:C:O2'	1:A:2433:A:H5'	1.96	0.65
11:J:118:PRO:HD2	38:J:8340:HOH:O	1.97	0.65
1:A:2064:U:H5'	1:A:2652:U:O3'	1.97	0.65
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.11	0.64
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.79	0.64
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.27	0.64
2:B:3029:C:H2'	2:B:3030:C:H5'	1.77	0.64
1:A:733:U:OP2	38:A:5671:HOH:O	2.14	0.64
8:G:11:VAL:HG13	8:G:23:GLU:O	1.97	0.64
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.12	0.64
1:A:2054:A:N3	20:S:128:ARG:NH2	2.45	0.64
27:Z:141:THR:HG23	38:Z:8594:HOH:O	1.96	0.64
1:A:2276:U:H2'	1:A:2277:U:C6	2.33	0.64
1:A:2064:U:H4'	1:A:2653:A:OP1	1.97	0.64
28:1:42:CYS:SG	28:1:43:GLY:N	2.70	0.64
1:A:2428:G:C5	38:A:3276:HOH:O	2.50	0.64
28:1:30:GLU:HB2	38:1:8413:HOH:O	1.98	0.64
12:K:74:ARG:CB	12:K:74:ARG:HH11	2.10	0.64
4:C:88:ILE:O	4:C:88:ILE:HG22	1.97	0.64
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.80	0.64
1:A:777:U:OP1	38:A:6954:HOH:O	2.14	0.64
25:X:65:VAL:HA	25:X:68:THR:HG22	1.80	0.64
1:A:1187:U:H2'	38:A:6356:HOH:O	1.98	0.64
28:1:31:ILE:O	28:1:35:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1773:G:C8	28:1:16:PRO:HA	2.32	0.64
1:A:558:C:O2'	1:A:559:U:H5"	1.97	0.64
2:B:3023:U:H3'	2:B:3024:U:H5"	1.78	0.64
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.27	0.64
13:L:22:ASP:HB2	38:L:5264:HOH:O	1.96	0.64
1:A:2769:C:H2'	1:A:2770:G:O4'	1.98	0.64
5:D:248:ARG:NH2	38:D:8524:HOH:O	2.31	0.64
1:A:2119:C:O2'	1:A:2120:U:H5'	1.97	0.64
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.38	0.64
1:A:1441:G:O2'	1:A:1442:A:H5'	1.98	0.64
6:E:115:LEU:O	6:E:118:THR:HB	1.97	0.64
1:A:1942:A:H3'	38:A:6804:HOH:O	1.98	0.64
15:N:59:GLY:HA3	15:N:141:ILE:HD11	1.78	0.64
4:C:93:THR:C	4:C:94:LEU:HD23	2.18	0.64
11:J:71:TYR:C	11:J:73:GLN:H	2.01	0.64
1:A:2314:G:C2'	1:A:2315:C:H5'	2.28	0.64
15:N:84:LYS:HE2	38:N:8580:HOH:O	1.97	0.63
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.79	0.63
4:C:131:HIS:O	4:C:132:ASP:HB2	1.96	0.63
13:L:58:THR:HG22	13:L:59:LYS:HG3	1.80	0.63
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.80	0.63
25:X:38:THR:HG22	38:X:3580:HOH:O	1.97	0.63
7:F:101:THR:HG22	38:F:7400:HOH:O	1.97	0.63
14:M:89:PHE:N	38:M:8575:HOH:O	2.32	0.63
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.20	0.63
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.78	0.63
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.80	0.63
2:B:3049:G:H5"	38:B:8467:HOH:O	1.99	0.63
13:L:92:ASP:OD1	38:L:5638:HOH:O	2.15	0.63
1:A:2465:A:H3'	38:A:3142:HOH:O	1.97	0.63
1:A:544:G:C2'	1:A:545:G:H5"	2.28	0.63
8:G:79:GLY:HA3	38:G:7046:HOH:O	1.98	0.63
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.80	0.63
15:N:60:ILE:C	15:N:61:ILE:HD12	2.17	0.63
24:W:64:GLY:O	24:W:65:ASP:HB2	1.99	0.63
1:A:1923:G:H4'	31:4:31:THR:O	1.98	0.63
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.98	0.63
31:4:55:VAL:HG22	38:4:8510:HOH:O	1.99	0.63
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.79	0.63
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.79	0.63
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:101:GLU:OE2	4:C:131:HIS:HB2	1.99	0.63
7:F:69:ILE:O	7:F:69:ILE:HG22	1.97	0.63
32:A:8011:MG:MG	38:A:3800:HOH:O	1.40	0.63
1:A:157:G:H4'	15:N:95:LYS:HE3	1.80	0.63
6:E:168:ARG:NH2	6:E:190:ALA:O	2.31	0.63
1:A:1329:A:H2	38:A:4165:HOH:O	1.80	0.63
1:A:2467:A:P	38:A:8560:HOH:O	2.57	0.63
8:G:7:ILE:HG22	8:G:45:ASP:O	1.98	0.63
11:J:53:PRO:HG3	11:J:127:GLY:H	1.63	0.63
9:H:107:VAL:O	9:H:111:ILE:HG13	1.98	0.63
5:D:280:VAL:CG1	5:D:334:SER:HA	2.29	0.63
17:P:87:THR:O	17:P:91:GLN:HG3	1.99	0.63
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.80	0.63
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.80	0.63
2:B:3028:U:H5"	16:O:40:ASN:ND2	2.14	0.63
1:A:1595:G:O2'	1:A:1596:U:H5'	1.98	0.63
14:M:143:THR:HG22	14:M:145:LEU:H	1.63	0.63
8:G:20:ILE:CD1	8:G:33:LEU:HD12	2.29	0.63
1:A:396:U:OP2	31:4:38:ARG:NH1	2.32	0.63
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.28	0.63
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.81	0.63
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.81	0.63
1:A:2890:A:H1'	23:V:56:ARG:NH2	2.14	0.63
21:T:23:LYS:HE2	38:T:8330:HOH:O	1.99	0.63
22:U:71:VAL:HG11	22:U:90:PRO:CB	2.22	0.63
5:D:175:LEU:C	5:D:175:LEU:HD23	2.19	0.63
30:3:35:ARG:HB2	38:3:2691:HOH:O	1.98	0.63
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.14	0.63
1:A:2105:C:H2'	1:A:2106:C:C6	2.33	0.63
5:D:138:GLY:O	5:D:139:ASP:O	2.16	0.63
12:K:131:THR:HG22	12:K:134:GLU:H	1.63	0.62
11:J:166:ASN:N	11:J:166:ASN:HD22	1.96	0.62
12:K:45:VAL:HG23	12:K:130:VAL:O	1.98	0.62
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.80	0.62
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.29	0.62
6:E:233:THR:HG22	6:E:234:VAL:N	2.13	0.62
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.32	0.62
7:F:25:MET:HE1	7:F:37:ALA:O	1.99	0.62
1:A:1116:U:O2'	1:A:1118:A:H2	1.72	0.62
1:A:240:C:H4'	15:N:146:GLN:NE2	2.15	0.62
10:I:12:ILE:N	10:I:13:PRO:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:235:GLU:CD	27:Z:235:GLU:H	2.03	0.62
1:A:2004:U:H4'	38:A:4780:HOH:O	1.98	0.62
7:F:23:VAL:HG23	7:F:23:VAL:O	1.99	0.62
6:E:78:ARG:NH1	6:E:78:ARG:HG3	2.13	0.62
9:H:46:GLU:N	38:H:3461:HOH:O	2.32	0.62
38:C:8627:HOH:O	28:1:75:ALA:HB3	1.98	0.62
15:N:91:ILE:HG23	38:N:8649:HOH:O	1.99	0.62
6:E:107:ARG:HH11	6:E:107:ARG:HB3	1.64	0.62
20:S:104:PHE:HB2	20:S:109:MET:HE1	1.81	0.62
38:A:4556:HOH:O	5:D:216:LYS:HA	2.00	0.62
1:A:189:A:OP1	15:N:171:ARG:NH2	2.32	0.62
7:F:37:ALA:O	7:F:40:ILE:HG12	1.99	0.62
15:N:64:ARG:HD2	38:N:8587:HOH:O	1.98	0.62
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.15	0.62
1:A:714:U:H3'	38:A:6403:HOH:O	2.00	0.62
1:A:56:G:H5"	24:W:50:ARG:NH1	2.13	0.62
15:N:104:ARG:O	15:N:108:LYS:HE2	2.00	0.62
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.28	0.62
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.99	0.62
5:D:41:PHE:HB3	5:D:190:MET:HE1	1.82	0.62
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.00	0.62
1:A:280:C:H2'	1:A:281:U:O4'	2.00	0.62
1:A:488:U:H2'	38:A:3497:HOH:O	1.99	0.62
29:2:28:HIS:HD2	29:2:30:LYS:H	1.48	0.62
22:U:48:VAL:HG22	22:U:97:ARG:O	2.00	0.62
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.82	0.62
25:X:26:ILE:O	25:X:26:ILE:HG13	1.97	0.62
5:D:145:HIS:CD2	5:D:146:THR:O	2.52	0.62
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.30	0.62
32:A:8011:MG:MG	38:A:3470:HOH:O	1.42	0.62
28:1:23:ARG:NH1	38:1:8404:HOH:O	2.32	0.62
1:A:558:C:H5'	38:A:4732:HOH:O	1.99	0.62
1:A:1213:C:O2'	1:A:1214:G:H5'	2.00	0.62
1:A:1713:G:H1'	38:A:4547:HOH:O	2.00	0.62
1:A:2421:G:H3'	1:A:2422:U:H5"	1.82	0.61
1:A:2506:A:O2'	1:A:2507:G:O5'	2.18	0.61
23:V:44:ARG:HB3	38:V:3805:HOH:O	1.99	0.61
1:A:603:A:H5"	1:A:604:G:OP1	1.99	0.61
1:A:1534:C:N3	38:A:8988:HOH:O	2.31	0.61
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.30	0.61
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:G:H5”	24:W:50:ARG:HH12	1.63	0.61
1:A:671:A:O2’	1:A:672:G:H2’	2.00	0.61
24:W:42:ASN:HB3	38:W:7247:HOH:O	2.00	0.61
1:A:1669:A:H2’	1:A:1670:G:C8	2.35	0.61
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.81	0.61
5:D:36:PRO:HA	5:D:168:GLY:CA	2.31	0.61
1:A:1120:U:C6	1:A:1120:U:H5”	2.36	0.61
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.98	0.61
1:A:1886:A:O2’	28:1:20:LEU:HB2	1.99	0.61
1:A:183:A:H5’	15:N:157:LEU:HD12	1.82	0.61
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.35	0.61
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.81	0.61
1:A:948:G:N7	38:A:5313:HOH:O	2.30	0.61
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.83	0.61
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.61
11:J:62:GLU:O	11:J:66:VAL:HG23	2.00	0.61
1:A:1884:G:O6	4:C:190:ARG:HD2	2.00	0.61
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.18	0.61
14:M:21:ARG:N	38:M:8534:HOH:O	2.34	0.61
1:A:1086:A:C6	25:X:11:VAL:HG11	2.34	0.61
1:A:1234:U:N3	5:D:244:PRO:HB3	2.16	0.61
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.81	0.61
11:J:141:ASN:CA	38:J:8366:HOH:O	2.46	0.61
10:I:12:ILE:HD12	38:I:692:HOH:O	2.00	0.61
21:T:80:ARG:HG2	38:T:8337:HOH:O	2.01	0.61
16:O:80:SER:HB2	38:O:8536:HOH:O	2.01	0.61
18:Q:143:ALA:HA	38:Q:170:HOH:O	2.00	0.61
28:1:39:CYS:CB	28:1:47:LEU:HD21	2.30	0.61
16:O:89:GLY:O	16:O:92:ALA:HB3	2.00	0.61
26:Y:15:ARG:NH1	26:Y:15:ARG:HB3	2.15	0.61
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.82	0.61
6:E:118:THR:O	6:E:136:VAL:HG13	2.01	0.61
28:1:19:GLY:O	28:1:23:ARG:HG2	2.01	0.61
2:B:3039:U:H1’	2:B:3044:A:N6	2.15	0.61
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.98	0.61
1:A:338:C:H4’	6:E:174:ILE:HD11	1.83	0.61
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.83	0.61
1:A:1878:G:H1’	38:A:5581:HOH:O	2.01	0.61
5:D:204:GLY:HA3	38:D:8653:HOH:O	2.00	0.61
5:D:305:ASP:O	5:D:306:LYS:HB2	2.01	0.61
1:A:1862:C:H1’	38:A:6681:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.83	0.61
5:D:312:ARG:HD3	5:D:315:VAL:HG13	1.83	0.61
8:G:7:ILE:HD11	8:G:11:VAL:C	2.21	0.61
8:G:7:ILE:HD11	8:G:11:VAL:O	2.01	0.61
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.83	0.61
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.36	0.61
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.83	0.61
1:A:1972:U:H2'	1:A:1973:A:H5'	1.82	0.61
6:E:219:ASN:O	6:E:222:ASP:OD1	2.18	0.61
12:K:74:ARG:O	12:K:78:ILE:HG12	2.00	0.61
20:S:132:ARG:HG2	20:S:133:ALA:N	2.16	0.61
2:B:3002:U:H4'	2:B:3002:U:OP2	2.01	0.61
1:A:1919:A:H4'	38:A:4324:HOH:O	1.99	0.61
11:J:150:LYS:CB	11:J:157:ILE:HD12	2.27	0.60
25:X:84:VAL:HG12	38:X:6679:HOH:O	2.01	0.60
11:J:136:VAL:HG22	11:J:137:ASN:O	2.00	0.60
15:N:149:TRP:O	15:N:152:ARG:HG2	1.99	0.60
1:A:2717:C:H2'	1:A:2718:C:C5'	2.27	0.60
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.30	0.60
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.01	0.60
1:A:2827:A:H2'	1:A:2828:G:O4'	2.00	0.60
1:A:871:G:C5'	1:A:871:G:C8	2.77	0.60
31:4:48:ASN:ND2	31:4:50:GLY:H	1.99	0.60
1:A:2405:C:P	38:A:6058:HOH:O	2.58	0.60
2:B:3007:G:H4'	16:O:55:ASP:OD2	2.00	0.60
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.31	0.60
1:A:558:C:C2'	1:A:559:U:H5"	2.31	0.60
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.31	0.60
5:D:81:ALA:O	5:D:186:GLY:HA3	2.01	0.60
1:A:2710:U:H1'	38:A:7082:HOH:O	2.01	0.60
4:C:105:VAL:HG13	4:C:155:THR:O	2.02	0.60
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.49	0.60
28:1:39:CYS:HA	28:1:47:LEU:CD1	2.29	0.60
22:U:69:LYS:O	22:U:71:VAL:HG23	2.02	0.60
7:F:38:GLU:HB3	7:F:49:PRO:HG2	1.83	0.60
25:X:26:ILE:O	25:X:26:ILE:CG1	2.49	0.60
5:D:85:ARG:NH1	38:D:8634:HOH:O	2.34	0.60
1:A:553:G:P	27:Z:204:ARG:HH22	2.24	0.60
38:B:8477:HOH:O	16:O:23:ARG:HD3	2.00	0.60
18:Q:78:GLY:O	38:Q:157:HOH:O	2.17	0.60
1:A:659:A:H5"	38:A:6557:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.81	0.60
1:A:2419:U:H5"	1:A:2420:G:H5'	1.84	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.01	0.60
8:G:23:GLU:HG2	8:G:28:SER:CB	2.32	0.60
1:A:2908:A:H2'	1:A:2909:G:O4'	2.01	0.60
1:A:2089:A:O2'	1:A:2090:G:H5'	2.01	0.60
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.60
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.84	0.60
1:A:1185:U:H2'	1:A:1186:C:C6	2.36	0.60
15:N:138:HIS:ND1	15:N:139:PRO:O	2.32	0.60
1:A:1730:G:H5'	1:A:1731:C:C5	2.36	0.60
15:N:74:ARG:O	15:N:88:VAL:CG1	2.43	0.60
7:F:50:VAL:O	7:F:71:ALA:HA	2.02	0.60
6:E:104:ASP:O	6:E:108:GLN:HG3	2.02	0.60
15:N:52:LEU:HD21	38:N:8616:HOH:O	2.01	0.60
9:H:58:GLU:HA	9:H:61:MET:HG3	1.82	0.60
1:A:282:C:H1'	1:A:368:C:H42	1.65	0.60
1:A:134:U:C2	1:A:145:A:C2	2.90	0.60
1:A:2019:A:H5'	38:A:4024:HOH:O	2.01	0.60
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.00	0.60
1:A:281:U:H3'	38:A:6668:HOH:O	2.02	0.60
12:K:39:VAL:HG13	12:K:106:GLY:O	2.01	0.60
22:U:48:VAL:HG23	22:U:98:VAL:HA	1.84	0.60
24:W:4:HIS:HB3	38:W:6622:HOH:O	2.02	0.60
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.83	0.60
1:A:821:U:H2'	1:A:822:C:H6	1.67	0.60
7:F:25:MET:CE	7:F:41:LEU:HG	2.29	0.59
13:L:109:LEU:HD13	13:L:113:ILE:HD11	1.84	0.59
38:A:9444:HOH:O	26:Y:23:HIS:HD2	1.84	0.59
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
25:X:4:LEU:O	25:X:32:CYS:HA	2.02	0.59
23:V:9:CYS:CA	23:V:52:THR:HG23	2.32	0.59
1:A:263:U:O4'	9:H:59:ILE:HD13	2.03	0.59
1:A:639:A:H2'	1:A:640:G:C8	2.37	0.59
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.01	0.59
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.83	0.59
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.83	0.59
13:L:28:GLU:HG2	13:L:58:THR:HB	1.84	0.59
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.83	0.59
6:E:180:SER:HB2	38:E:8451:HOH:O	2.02	0.59
5:D:1:PRO:O	5:D:2:GLN:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2408:A:H2	38:A:9595:HOH:O	1.84	0.59
5:D:43:GLY:O	5:D:308:LEU:HD12	2.02	0.59
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.84	0.59
9:H:46:GLU:O	9:H:73:PRO:HD2	2.02	0.59
1:A:824:G:C8	38:A:3800:HOH:O	2.51	0.59
5:D:2:GLN:HA	38:D:8622:HOH:O	2.02	0.59
22:U:47:THR:HB	22:U:100:ASP:HB3	1.83	0.59
1:A:2428:G:O6	1:A:2464:C:H1'	2.03	0.59
16:O:37:ARG:NE	38:O:8534:HOH:O	2.34	0.59
1:A:289:G:N2	1:A:363:A:H2	1.98	0.59
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.84	0.59
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.59
7:F:135:VAL:HG22	7:F:136:ARG:H	1.66	0.59
4:C:109:GLU:HG2	4:C:116:GLY:N	2.17	0.59
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.38	0.59
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.84	0.59
16:O:182:GLY:N	38:O:8567:HOH:O	2.32	0.59
1:A:182:G:O3'	15:N:157:LEU:CD1	2.51	0.59
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.18	0.59
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.02	0.59
1:A:738:G:H3'	38:A:6507:HOH:O	2.03	0.59
1:A:1170:U:O2'	1:A:1172:G:N7	2.27	0.59
28:1:28:ASP:O	28:1:31:ILE:HG22	2.02	0.59
14:M:37:LYS:O	38:M:8525:HOH:O	2.17	0.59
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.33	0.59
14:M:136:ALA:HB3	38:M:8577:HOH:O	2.03	0.59
16:O:154:LEU:O	16:O:155:GLU:HB3	2.03	0.59
1:A:20:G:H21	20:S:117:HIS:HD2	1.51	0.59
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.50	0.59
1:A:2429:A:O2'	1:A:2430:A:H5'	2.03	0.59
7:F:11:HIS:O	7:F:12:GLU:HB3	2.02	0.59
38:A:4990:HOH:O	5:D:298:LYS:HD3	2.02	0.59
2:B:3040:C:N4	7:F:51:ARG:HB2	2.18	0.59
7:F:170:TYR:O	7:F:171:ASP:HB3	2.01	0.59
1:A:449:A:N7	6:E:43:LYS:HG2	2.18	0.59
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.85	0.59
1:A:775:G:OP1	29:2:16:HIS:HE1	1.85	0.59
1:A:2896:A:H5"	38:A:5559:HOH:O	2.02	0.59
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.83	0.59
1:A:1666:C:C2'	1:A:1667:A:H5'	2.32	0.59
15:N:59:GLY:HA3	15:N:141:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:152:GLU:C	16:O:154:LEU:H	2.05	0.59
27:Z:144:ARG:CZ	38:Z:8616:HOH:O	2.51	0.59
10:I:64:ASN:N	10:I:64:ASN:HD22	2.00	0.59
38:A:6333:HOH:O	15:N:178:LYS:HB2	2.02	0.59
1:A:1918:U:OP2	38:A:3513:HOH:O	2.17	0.59
1:A:157:G:H4'	15:N:95:LYS:CE	2.33	0.58
1:A:2413:A:N7	16:O:109:PRO:HB3	2.18	0.58
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.85	0.58
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.32	0.58
16:O:163:PHE:HA	38:O:8520:HOH:O	2.02	0.58
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.33	0.58
20:S:132:ARG:NH2	38:S:8582:HOH:O	2.35	0.58
24:W:49:LEU:O	24:W:53:ILE:HG13	2.03	0.58
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.37	0.58
29:2:10:LYS:HG3	38:2:2979:HOH:O	2.02	0.58
1:A:1183:C:N4	38:A:3888:HOH:O	2.32	0.58
15:N:72:SER:OG	15:N:74:ARG:HB2	2.02	0.58
1:A:371:U:H2'	1:A:372:A:C8	2.37	0.58
1:A:120:A:H2'	1:A:120:A:N3	2.18	0.58
2:B:3057:A:N6	38:B:8444:HOH:O	2.36	0.58
2:B:3044:A:O4'	7:F:76:ARG:NE	2.36	0.58
6:E:107:ARG:CB	6:E:107:ARG:HH11	2.16	0.58
13:L:37:TYR:CD2	38:L:7169:HOH:O	2.52	0.58
5:D:264:GLU:HG2	5:D:267:LYS:CE	2.28	0.58
27:Z:187:VAL:HB	38:Z:8575:HOH:O	2.03	0.58
1:A:1759:A:N3	1:A:1818:C:H2'	2.17	0.58
38:A:3680:HOH:O	27:Z:186:ARG:HD2	2.03	0.58
15:N:48:ARG:NH2	38:N:8567:HOH:O	2.35	0.58
6:E:237:GLU:HB2	38:E:8436:HOH:O	2.01	0.58
27:Z:187:VAL:HG23	27:Z:192:ASP:HB3	1.85	0.58
1:A:567:U:H5"	38:A:5862:HOH:O	2.03	0.58
4:C:25:ALA:HA	38:C:8573:HOH:O	2.03	0.58
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.52	0.58
5:D:62:ARG:HA	5:D:65:MET:CE	2.33	0.58
2:B:3047:A:C2	2:B:3048:C:C2	2.91	0.58
1:A:739:G:N7	38:A:7001:HOH:O	2.36	0.58
20:S:14:ALA:HB3	20:S:147:LEU:HB2	1.86	0.58
1:A:1168:C:H2'	1:A:1169:U:O4'	2.03	0.58
6:E:103:ASN:HB3	38:E:8308:HOH:O	2.02	0.58
1:A:184:G:H5"	15:N:153:THR:HG22	1.86	0.58
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:G:N7	31:4:60:LYS:NZ	2.45	0.58
1:A:2578:G:H5'	1:A:2578:G:C8	2.36	0.58
16:O:169:PRO:O	16:O:172:PHE:HB3	2.04	0.58
1:A:29:C:O2'	1:A:30:U:H5'	2.04	0.58
1:A:661:G:C5	1:A:686:A:C2	2.91	0.58
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.61	0.58
12:K:130:VAL:HG12	12:K:131:THR:N	2.18	0.58
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.32	0.58
11:J:75:SER:C	11:J:79:ALA:HB2	2.24	0.58
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.68	0.58
1:A:646:G:H2'	1:A:647:U:C6	2.38	0.58
2:B:3051:A:H5'	16:O:160:SER:HB3	1.86	0.58
1:A:820:G:C6	4:C:171:LYS:HB2	2.39	0.58
1:A:2316:G:H2'	38:A:4385:HOH:O	2.02	0.58
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.36	0.58
1:A:1053:G:OP1	11:J:12:PRO:HG3	2.02	0.58
1:A:2274:A:H1'	15:N:86:MET:SD	2.43	0.58
1:A:1123:A:C6	1:A:1238:C:H5'	2.39	0.58
1:A:1351:G:O2'	38:A:4032:HOH:O	2.17	0.58
18:Q:64:GLU:HG2	38:Q:171:HOH:O	2.04	0.58
1:A:2073:G:OP2	1:A:2490:A:H5'	2.02	0.58
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.86	0.58
11:J:44:ALA:HA	11:J:163:PRO:O	2.03	0.58
1:A:542:A:H1'	38:A:4158:HOH:O	2.04	0.58
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.51	0.58
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.84	0.58
1:A:2427:C:OP2	31:4:84:ARG:HD2	2.03	0.58
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.39	0.58
1:A:2878:U:H2'	1:A:2879:A:O4'	2.04	0.58
15:N:35:PRO:O	38:N:8539:HOH:O	2.17	0.57
1:A:1942:A:O2'	1:A:1943:C:H5'	2.04	0.57
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.33	0.57
5:D:205:VAL:O	5:D:307:ARG:NE	2.37	0.57
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.86	0.57
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.85	0.57
15:N:61:ILE:HG13	38:N:8624:HOH:O	2.03	0.57
38:B:8477:HOH:O	16:O:20:TYR:CE2	2.53	0.57
4:C:109:GLU:HG2	4:C:116:GLY:H	1.69	0.57
5:D:82:VAL:HG12	5:D:82:VAL:O	2.04	0.57
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.57
7:F:166:ILE:HD12	38:F:6326:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2763:G:OP1	13:L:9:THR:OG1	2.20	0.57
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.86	0.57
15:N:186:SER:O	15:N:189:VAL:HG12	2.03	0.57
16:O:141:ARG:HB3	38:O:8566:HOH:O	2.05	0.57
1:A:1162:G:H2'	38:A:6045:HOH:O	2.04	0.57
14:M:104:ASP:O	14:M:105:TYR:HB3	2.04	0.57
1:A:820:G:C5	4:C:171:LYS:HB2	2.40	0.57
1:A:2421:G:H3'	1:A:2422:U:C5'	2.35	0.57
4:C:179:MET:HG2	4:C:186:TRP:HB2	1.86	0.57
14:M:143:THR:CG2	14:M:144:ASP:N	2.67	0.57
1:A:2324:G:H4'	1:A:2418:G:O2'	2.04	0.57
1:A:128:A:H3'	1:A:128:A:C8	2.38	0.57
1:A:2866:U:C2	38:A:6955:HOH:O	2.53	0.57
21:T:43:GLU:HB3	38:T:8345:HOH:O	2.04	0.57
25:X:21:LEU:HD22	25:X:26:ILE:HD13	1.86	0.57
9:H:57:GLU:O	9:H:61:MET:HG3	2.05	0.57
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.21	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
1:A:2011:A:P	38:A:5418:HOH:O	2.63	0.57
1:A:2783:A:H3'	38:A:4707:HOH:O	2.02	0.57
1:A:1753:C:O2	5:D:229:ARG:NH2	2.38	0.57
38:A:9660:HOH:O	15:N:87:MET:HE3	2.03	0.57
1:A:1474:C:H6	1:A:1474:C:C5'	2.11	0.57
5:D:320:GLN:HG3	5:D:321:PRO:HD2	1.87	0.57
4:C:211:LYS:NZ	38:C:8635:HOH:O	2.38	0.57
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.19	0.57
1:A:1500:U:P	18:Q:41:ARG:HH22	2.27	0.57
1:A:1497:G:H4'	1:A:1627:G:O2'	2.04	0.57
17:P:59:VAL:HG23	17:P:111:VAL:HG23	1.86	0.57
1:A:2365:G:H4'	19:R:45:PRO:O	2.04	0.57
4:C:29:HIS:CE1	4:C:107:ASN:ND2	2.73	0.57
28:1:47:LEU:HD23	28:1:57:CYS:CB	2.34	0.57
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.33	0.57
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.86	0.57
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.74	0.57
10:I:12:ILE:HG13	38:I:6833:HOH:O	2.04	0.57
1:A:1299:G:O6	14:M:6:ARG:HD3	2.05	0.57
1:A:1669:A:H2'	1:A:1670:G:H8	1.69	0.57
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.40	0.57
1:A:138:U:H5"	1:A:139:C:OP2	2.05	0.57
25:X:4:LEU:HD21	25:X:52:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:C:H2'	1:A:639:A:C8	2.40	0.57
27:Z:115:ARG:NE	38:Z:8560:HOH:O	2.37	0.57
38:A:4879:HOH:O	4:C:164:ARG:NE	2.36	0.57
29:2:52:SER:HA	38:2:4248:HOH:O	2.04	0.57
1:A:105:G:O2'	1:A:106:A:H5'	2.04	0.57
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.56
30:3:18:ASN:HD21	30:3:40:ARG:H	1.52	0.56
15:N:186:SER:OG	15:N:189:VAL:HG12	2.05	0.56
9:H:110:GLU:O	9:H:114:LYS:HG3	2.04	0.56
1:A:396:U:H1'	38:A:7089:HOH:O	2.03	0.56
1:A:1086:A:N6	25:X:11:VAL:HG11	2.20	0.56
1:A:2793:A:N3	38:A:3982:HOH:O	2.33	0.56
16:O:33:ARG:NH1	16:O:103:ASP:OD2	2.30	0.56
1:A:2359:G:N7	38:A:3196:HOH:O	2.32	0.56
9:H:21:GLU:O	9:H:24:ARG:HG3	2.05	0.56
1:A:825:U:H5"	1:A:826:U:OP1	2.05	0.56
1:A:1766:U:O2	1:A:1778:A:H5'	2.05	0.56
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.25	0.56
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.35	0.56
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.30	0.56
12:K:39:VAL:HG11	12:K:107:ASN:HB2	1.85	0.56
8:G:69:ILE:HA	8:G:72:MET:CE	2.35	0.56
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.39	0.56
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.18	0.56
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.05	0.56
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.40	0.56
30:3:41:HIS:H	30:3:45:ASN:ND2	1.96	0.56
11:J:13:ALA:CA	11:J:91:HIS:HE1	2.15	0.56
1:A:595:U:O2'	1:A:596:C:H5'	2.05	0.56
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.35	0.56
24:W:39:ALA:N	24:W:40:PRO:CD	2.69	0.56
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.03	0.56
1:A:2314:G:H2'	1:A:2315:C:H5'	1.87	0.56
25:X:38:THR:HB	38:X:5390:HOH:O	2.06	0.56
14:M:104:ASP:HB3	38:M:8570:HOH:O	2.05	0.56
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.40	0.56
5:D:55:ASN:HB3	5:D:64:GLY:H	1.70	0.56
25:X:60:GLU:O	25:X:63:GLU:HB2	2.05	0.56
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.03	0.56
31:4:38:ARG:O	31:4:42:ARG:HB2	2.06	0.56
27:Z:186:ARG:HH11	27:Z:186:ARG:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:A:H4'	38:A:4801:HOH:O	2.06	0.56
1:A:2718:C:H6	1:A:2718:C:H5'	1.70	0.56
1:A:2620:U:O4	36:5:76:PPU:C	2.54	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
1:A:2814:A:OP2	38:A:4548:HOH:O	2.17	0.56
6:E:162:VAL:HG12	6:E:162:VAL:O	2.04	0.56
1:A:272:A:H5'	1:A:273:G:OP2	2.05	0.56
16:O:154:LEU:HG	16:O:155:GLU:H	1.70	0.56
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.06	0.56
1:A:2529:G:O2'	1:A:2530:C:H5'	2.05	0.56
1:A:2241:C:O2'	1:A:2242:U:H5'	2.05	0.56
20:S:29:LYS:HB3	38:S:8531:HOH:O	2.05	0.56
24:W:58:THR:O	24:W:62:GLU:HG3	2.05	0.56
6:E:133:ARG:HD2	38:E:8414:HOH:O	2.05	0.56
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.69	0.56
1:A:283:U:H5"	1:A:284:C:P	2.45	0.56
14:M:148:GLU:HA	38:M:8576:HOH:O	2.05	0.56
18:Q:58:SER:HB3	38:Q:186:HOH:O	2.04	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
9:H:19:ALA:O	9:H:22:VAL:HG22	2.06	0.56
6:E:214:THR:HG21	38:E:8407:HOH:O	2.05	0.56
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.36	0.56
1:A:316:A:H5'	22:U:54:ASP:OD2	2.05	0.56
2:B:3049:G:O2'	2:B:3050:G:H5'	2.06	0.56
31:4:74:CYS:SG	31:4:76:LYS:CB	2.94	0.56
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.88	0.56
16:O:80:SER:CB	38:O:8536:HOH:O	2.53	0.56
16:O:58:LEU:HD12	16:O:58:LEU:N	2.21	0.56
1:A:2502:C:C4'	11:J:151:MET:HG2	2.35	0.56
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.88	0.56
12:K:19:MET:HE1	12:K:132:LEU:HD11	1.85	0.56
5:D:280:VAL:HG13	5:D:334:SER:HA	1.88	0.56
15:N:87:MET:CG	31:4:46:ILE:HD13	2.36	0.56
29:2:8:GLN:NE2	29:2:11:LYS:NZ	2.52	0.56
22:U:48:VAL:HG22	22:U:97:ARG:C	2.27	0.56
1:A:2664:A:OP1	1:A:2664:A:H8	1.89	0.56
1:A:2093:G:H5"	38:D:8526:HOH:O	2.06	0.56
1:A:154:C:H2'	1:A:155:C:H6	1.70	0.56
8:G:31:ARG:NH1	38:G:5919:HOH:O	2.38	0.56
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.87	0.56
12:K:126:ASN:O	12:K:129:PHE:HE2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:59:ASN:ND2	11:J:59:ASN:H	1.97	0.56
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.88	0.56
1:A:2507:G:H2'	1:A:2510:C:H42	1.71	0.56
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.71	0.56
11:J:39:GLY:O	11:J:41:THR:N	2.39	0.56
17:P:7:LEU:HD22	38:P:5650:HOH:O	2.05	0.56
7:F:144:ARG:NH2	38:F:3839:HOH:O	2.39	0.56
9:H:107:VAL:HG23	38:H:6617:HOH:O	2.05	0.55
1:A:2672:C:H1'	38:D:8634:HOH:O	2.06	0.55
1:A:121:U:OP2	30:3:10:ARG:NH2	2.39	0.55
21:T:32:ALA:HA	21:T:36:GLU:OE1	2.06	0.55
15:N:104:ARG:O	15:N:108:LYS:HG2	2.06	0.55
1:A:113:A:H3'	1:A:114:A:C5'	2.36	0.55
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.21	0.55
8:G:133:VAL:HG12	8:G:141:VAL:HG13	1.88	0.55
18:Q:109:ARG:NH1	18:Q:119:TYR:CE2	2.74	0.55
8:G:21:THR:HG23	8:G:30:THR:OG1	2.06	0.55
6:E:236:THR:CG2	6:E:239:ALA:H	1.95	0.55
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.72	0.55
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.55
1:A:1682:A:H5"	38:A:8961:HOH:O	2.06	0.55
2:B:3028:U:H2'	2:B:3029:C:C6	2.42	0.55
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.41	0.55
4:C:215:ILE:HG13	4:C:216:SER:N	2.22	0.55
31:4:44:SER:HA	31:4:49:ASP:OD1	2.06	0.55
14:M:1:THR:HA	38:M:8526:HOH:O	2.06	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.55
1:A:1393:A:H2'	1:A:1394:C:C6	2.41	0.55
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.20	0.55
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.71	0.55
7:F:27:ILE:HG22	7:F:28:GLY:N	2.15	0.55
27:Z:216:ARG:CD	38:Z:8574:HOH:O	2.47	0.55
1:A:338:C:H5"	38:E:8426:HOH:O	2.06	0.55
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.88	0.55
27:Z:133:HIS:HD2	38:Z:8588:HOH:O	1.88	0.55
23:V:33:SER:O	23:V:37:GLU:HG3	2.07	0.55
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.20	0.55
1:A:506:G:N2	1:A:509:A:H5'	2.16	0.55
15:N:114:VAL:HB	15:N:159:THR:HG23	1.87	0.55
24:W:64:GLY:O	24:W:65:ASP:CB	2.55	0.55
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:2:GLY:O	29:2:6:PRO:HG2	2.07	0.55
1:A:635:A:H2'	1:A:636:G:H5"	1.87	0.55
1:A:182:G:O3'	15:N:157:LEU:HD13	2.07	0.55
14:M:145:LEU:O	14:M:148:GLU:HG3	2.07	0.55
9:H:100:ASP:HB3	38:H:5691:HOH:O	2.07	0.55
1:A:2361:A:H5"	38:A:8523:HOH:O	2.06	0.55
19:R:11:ARG:HD3	38:R:5620:HOH:O	2.07	0.55
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.35	0.55
5:D:119:HIS:O	5:D:121:PRO:HD3	2.06	0.55
31:4:34:LYS:HB2	31:4:37:ASP:OD2	2.06	0.55
1:A:57:C:H5"	38:A:6218:HOH:O	2.06	0.55
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
6:E:236:THR:O	6:E:237:GLU:C	2.45	0.55
1:A:1191:A:C3'	1:A:1192:A:H5"	2.37	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.21	0.55
7:F:140:ARG:O	7:F:144:ARG:HG2	2.06	0.55
1:A:2326:U:H4'	1:A:2412:G:C4'	2.37	0.55
4:C:140:LEU:HB3	4:C:141:PRO:HD2	1.88	0.55
7:F:23:VAL:CG2	7:F:73:VAL:HB	2.36	0.55
4:C:211:LYS:NZ	38:C:8582:HOH:O	2.39	0.55
1:A:777:U:O2'	29:2:11:LYS:HG2	2.06	0.55
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.42	0.55
2:B:3029:C:C2'	2:B:3030:C:H5'	2.36	0.55
20:S:82:GLU:O	20:S:86:LYS:HG3	2.07	0.55
8:G:34:TRP:O	12:K:127:ILE:HD11	2.06	0.55
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.89	0.55
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.07	0.55
1:A:970:U:H2'	38:A:5786:HOH:O	2.06	0.55
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.88	0.55
1:A:2478:U:H2'	1:A:2479:A:C8	2.41	0.55
21:T:6:LYS:HB2	21:T:27:ALA:O	2.06	0.55
22:U:37:GLN:OE1	22:U:118:SER:HA	2.06	0.55
2:B:3023:U:H6	2:B:3023:U:C5'	2.20	0.54
1:A:1165:G:H3'	1:A:1165:G:OP1	2.08	0.54
1:A:1159:G:P	38:A:3782:HOH:O	2.65	0.54
8:G:11:VAL:CG1	8:G:12:ASP:N	2.70	0.54
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.88	0.54
31:4:3:MET:O	31:4:90:PHE:HA	2.07	0.54
1:A:125:U:H2'	38:A:3261:HOH:O	2.07	0.54
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.72	0.54
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:C:C1'	16:O:5:ARG:NH1	2.64	0.54
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.15	0.54
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.38	0.54
4:C:192:VAL:O	4:C:192:VAL:HG12	2.07	0.54
1:A:1187:U:O2'	1:A:1189:A:H2	1.91	0.54
13:L:4:LEU:HD22	13:L:116:GLU:HB3	1.89	0.54
1:A:2415:A:N3	16:O:26:LEU:HD13	2.22	0.54
20:S:132:ARG:CZ	38:S:8582:HOH:O	2.55	0.54
1:A:514:G:O5'	1:A:514:G:H8	1.90	0.54
1:A:1512:G:O2'	1:A:1513:C:H5'	2.06	0.54
16:O:132:ASN:O	16:O:135:VAL:HG12	2.06	0.54
12:K:42:GLU:O	12:K:131:THR:HG23	2.07	0.54
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.37	0.54
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.36	0.54
15:N:61:ILE:N	15:N:61:ILE:HD12	2.21	0.54
22:U:32:ARG:NH1	22:U:38:ARG:HH12	2.05	0.54
15:N:46:LEU:HG	38:N:8622:HOH:O	2.07	0.54
2:B:3042:C:H2'	38:B:8505:HOH:O	2.07	0.54
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.36	0.54
2:B:3023:U:C3'	2:B:3024:U:H5"	2.38	0.54
1:A:21:G:H4'	20:S:2:ILE:HG22	1.88	0.54
1:A:711:G:C2	1:A:718:C:C2	2.96	0.54
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.40	0.54
4:C:199:HIS:HD2	4:C:201:PHE:H	1.52	0.54
9:H:101:ALA:HA	38:H:5413:HOH:O	2.07	0.54
1:A:2320:U:H4'	1:A:2321:A:O4'	2.08	0.54
1:A:204:A:H2'	1:A:205:U:H5'	1.88	0.54
1:A:1422:U:H2'	1:A:1423:C:C6	2.42	0.54
19:R:40:HIS:HD2	19:R:60:THR:OG1	1.90	0.54
5:D:75:GLU:C	5:D:77:PRO:HD3	2.28	0.54
11:J:136:VAL:HG23	38:J:8344:HOH:O	2.07	0.54
2:B:3020:G:O2'	2:B:3021:G:H5'	2.07	0.54
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.40	0.54
1:A:1120:U:H6	1:A:1120:U:H5"	1.70	0.54
14:M:149:ARG:O	14:M:150:GLN:HB2	2.07	0.54
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.37	0.54
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.88	0.54
1:A:541:C:H2'	1:A:542:A:H5'	1.88	0.54
28:1:42:CYS:SG	28:1:44:PHE:N	2.61	0.54
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.71	0.54
38:A:6231:HOH:O	16:O:4:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:G:N7	38:A:3800:HOH:O	2.39	0.54
1:A:2429:A:H2'	1:A:2430:A:C8	2.42	0.54
4:C:164:ARG:HA	28:1:69:TYR:CE1	2.43	0.54
1:A:1951:G:N2	38:A:5718:HOH:O	2.40	0.54
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.42	0.54
6:E:16:VAL:HG12	6:E:17:ASP:N	2.22	0.54
1:A:2761:A:C4	1:A:2763:G:C8	2.95	0.54
1:A:2349:G:OP1	7:F:20:LYS:NZ	2.36	0.54
1:A:951:A:C2'	1:A:952:G:H5'	2.38	0.54
10:I:64:ASN:O	10:I:68:GLU:HG3	2.08	0.54
31:4:87:ARG:HG3	38:4:8570:HOH:O	2.06	0.54
4:C:173:GLY:O	4:C:176:HIS:HB3	2.07	0.54
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.89	0.54
1:A:2437:A:H2'	1:A:2438:G:C8	2.43	0.54
1:A:2758:G:H2'	1:A:2759:C:C6	2.43	0.54
5:D:66:GLU:OE1	5:D:328:ARG:HD2	2.08	0.54
11:J:166:ASN:N	11:J:166:ASN:ND2	2.56	0.54
15:N:164:THR:HB	38:N:8520:HOH:O	2.08	0.54
1:A:2717:C:O2'	1:A:2718:C:H5"	2.06	0.54
12:K:131:THR:HG22	12:K:133:GLY:N	2.23	0.54
5:D:168:GLY:N	5:D:174:ARG:HD3	2.22	0.54
23:V:44:ARG:CB	38:V:3805:HOH:O	2.54	0.54
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.89	0.54
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.54
1:A:2015:A:H2'	1:A:2016:U:O4'	2.07	0.54
6:E:236:THR:HA	38:E:8457:HOH:O	2.08	0.54
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.56	0.54
1:A:1829:A:H5"	38:A:9578:HOH:O	2.07	0.54
13:L:34:VAL:HB	38:L:7169:HOH:O	2.08	0.54
1:A:506:G:H22	1:A:509:A:H5"	1.70	0.54
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.90	0.54
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.21	0.54
7:F:65:GLU:HG3	38:F:6752:HOH:O	2.06	0.54
1:A:1713:G:C2'	38:A:4547:HOH:O	2.56	0.54
1:A:1527:A:H1'	1:A:1528:A:C8	2.43	0.54
1:A:1887:U:OP1	28:1:21:LYS:HG3	2.08	0.54
38:A:7138:HOH:O	15:N:154:ARG:HB2	2.07	0.54
38:A:5970:HOH:O	30:3:1:GLY:HA3	2.07	0.54
2:B:3035:C:H5"	38:B:8456:HOH:O	2.08	0.54
25:X:110:GLN:HA	25:X:110:GLN:NE2	2.24	0.53
15:N:87:MET:SD	31:4:46:ILE:HD13	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:A:C5	1:A:1201:C:H4'	2.43	0.53
13:L:75:ARG:CZ	38:L:4172:HOH:O	2.56	0.53
17:P:39:THR:O	17:P:115:ARG:NH2	2.41	0.53
1:A:447:A:O2'	1:A:448:G:H5'	2.08	0.53
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.38	0.53
6:E:43:LYS:NZ	38:E:8392:HOH:O	2.41	0.53
1:A:2265:U:H2'	1:A:2266:A:C8	2.43	0.53
1:A:329:A:OP2	6:E:206:ASN:HB2	2.08	0.53
1:A:1641:A:H2'	1:A:1642:A:H5'	1.89	0.53
1:A:778:C:C4	1:A:779:U:C4	2.96	0.53
21:T:57:THR:CG2	21:T:58:MET:N	2.71	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.91	0.53
23:V:9:CYS:HA	23:V:52:THR:CG2	2.38	0.53
15:N:172:GLY:C	15:N:183:VAL:HG11	2.29	0.53
10:I:12:ILE:HG22	10:I:12:ILE:O	2.08	0.53
10:I:12:ILE:N	38:I:4714:HOH:O	2.41	0.53
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.48	0.53
17:P:4:ASN:HB3	17:P:7:LEU:HB3	1.90	0.53
1:A:816:G:H5'	1:A:1598:A:H4'	1.90	0.53
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.53
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.90	0.53
29:2:25:LYS:HD2	30:3:49:GLU:H	1.72	0.53
1:A:113:A:OP1	38:A:9242:HOH:O	2.19	0.53
1:A:1909:A:H2'	1:A:1910:A:C8	2.42	0.53
5:D:72:THR:HB	38:D:8606:HOH:O	2.09	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.56	0.53
22:U:24:ARG:HH21	22:U:39:ASN:ND2	2.06	0.53
8:G:69:ILE:HA	8:G:72:MET:HE3	1.90	0.53
1:A:644:G:H5'	1:A:644:G:N3	2.24	0.53
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.43	0.53
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.90	0.53
1:A:1097:A:H5"	25:X:125:HIS:NE2	2.24	0.53
7:F:99:ASP:CB	7:F:103:ASN:H	2.22	0.53
1:A:1666:C:O2'	1:A:1667:A:C5'	2.56	0.53
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.39	0.53
9:H:28:ALA:HB3	9:H:99:THR:O	2.08	0.53
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.89	0.53
1:A:1730:G:H5'	1:A:1731:C:C6	2.44	0.53
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.89	0.53
38:L:408:HOH:O	23:V:37:GLU:HB3	2.08	0.53
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2791:U:H1'	1:A:2792:A:H5"	1.90	0.53
1:A:2028:U:H2'	1:A:2029:C:C6	2.43	0.53
16:O:43:VAL:HG13	16:O:118:ILE:HD11	1.89	0.53
9:H:91:VAL:CG1	9:H:92:GLY:H	2.18	0.53
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.90	0.53
4:C:95:PRO:HA	4:C:153:ARG:HA	1.91	0.53
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.39	0.53
1:A:681:G:N3	1:A:681:G:H5'	2.24	0.53
1:A:1617:C:C4	1:A:1643:C:H4'	2.43	0.53
1:A:42:C:H1'	38:A:4157:HOH:O	2.08	0.53
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.73	0.53
15:N:108:LYS:HE3	38:N:8614:HOH:O	2.08	0.53
1:A:1192:A:H3'	1:A:1193:A:H5'	1.90	0.53
9:H:91:VAL:CG1	9:H:92:GLY:N	2.70	0.53
4:C:37:VAL:HG22	38:C:8610:HOH:O	2.08	0.53
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.90	0.53
15:N:61:ILE:HA	38:N:8624:HOH:O	2.09	0.53
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.53
24:W:44:GLY:O	24:W:48:GLU:HG2	2.08	0.53
1:A:344:C:H2'	1:A:345:G:O4'	2.08	0.53
1:A:1268:C:O2'	1:A:1269:G:H5'	2.09	0.53
1:A:1362:U:H5'	38:A:9762:HOH:O	2.09	0.53
1:A:1242:A:OP2	12:K:60:ARG:NH2	2.38	0.53
10:I:12:ILE:HB	38:I:4714:HOH:O	2.07	0.53
9:H:99:THR:O	9:H:100:ASP:HB2	2.08	0.53
1:A:902:G:N7	14:M:18:HIS:CD2	2.75	0.53
1:A:1200:A:H4'	38:A:6798:HOH:O	2.09	0.53
4:C:217:ARG:HG2	4:C:229:ALA:HB2	1.91	0.53
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.92	0.53
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.91	0.53
13:L:55:VAL:HG12	13:L:56:SER:H	1.73	0.53
1:A:1185:U:H5'	38:A:6922:HOH:O	2.09	0.53
18:Q:10:ALA:CA	18:Q:13:VAL:HG12	2.39	0.53
24:W:39:ALA:O	24:W:41:GLU:N	2.41	0.53
38:A:5778:HOH:O	7:F:55:LYS:HB2	2.07	0.53
15:N:87:MET:HB2	15:N:91:ILE:CD1	2.39	0.53
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.53
1:A:2459:G:OP1	31:4:64:LYS:N	2.21	0.53
6:E:77:ALA:O	6:E:78:ARG:HG3	2.08	0.53
38:A:4311:HOH:O	12:K:47:THR:CB	2.51	0.53
1:A:212:A:O4'	1:A:214:U:C6	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.24	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.91	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.09	0.53
18:Q:115:SER:O	18:Q:117:SER:N	2.42	0.53
12:K:131:THR:HB	12:K:134:GLU:HG3	1.91	0.53
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.91	0.53
9:H:100:ASP:O	9:H:101:ALA:O	2.27	0.53
1:A:776:A:OP1	29:2:28:HIS:HE1	1.92	0.53
7:F:11:HIS:C	7:F:13:MET:H	2.12	0.53
38:A:9566:HOH:O	20:S:83:LYS:HB3	2.08	0.53
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.44	0.53
38:A:9733:HOH:O	4:C:221:PRO:HA	2.07	0.53
1:A:1328:A:OP1	27:Z:169:ARG:HD2	2.08	0.53
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.44	0.53
16:O:157:PRO:HA	38:O:8526:HOH:O	2.09	0.53
1:A:2594:C:O2'	1:A:2595:U:H5'	2.09	0.53
28:1:10:ARG:HG3	28:1:11:THR:N	2.25	0.52
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.52
7:F:174:VAL:HG13	38:F:6555:HOH:O	2.08	0.52
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.90	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.57	0.52
1:A:2107:U:O2'	1:A:2108:A:H5'	2.09	0.52
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.77	0.52
6:E:95:GLU:N	6:E:95:GLU:OE1	2.39	0.52
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.91	0.52
1:A:1014:A:H5"	2:B:3101:G:O2'	2.09	0.52
31:4:40:ARG:HD2	38:4:8547:HOH:O	2.07	0.52
11:J:4:ALA:HB3	38:J:8365:HOH:O	2.08	0.52
1:A:1701:A:H4'	1:A:1702:U:C5'	2.39	0.52
8:G:20:ILE:HD12	8:G:33:LEU:CD1	2.40	0.52
1:A:1819:G:H2'	1:A:1820:G:C5'	2.39	0.52
20:S:82:GLU:HG3	20:S:83:LYS:N	2.24	0.52
1:A:2478:U:H2'	1:A:2479:A:H8	1.74	0.52
25:X:125:HIS:HE1	38:X:3071:HOH:O	1.92	0.52
28:1:46:LYS:NZ	38:1:8439:HOH:O	2.43	0.52
1:A:2123:A:H5'	15:N:89:ASN:HD21	1.74	0.52
1:A:1834:C:H2'	1:A:1840:A:N6	2.24	0.52
28:1:26:VAL:O	28:1:30:GLU:HG3	2.09	0.52
2:B:3041:C:H4'	7:F:48:MET:HB2	1.90	0.52
5:D:62:ARG:CA	5:D:65:MET:HE3	2.33	0.52
1:A:559:U:H2'	1:A:560:C:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2435:U:H1'	38:A:4900:HOH:O	2.08	0.52
1:A:1505:U:H6	1:A:1505:U:H5'	1.73	0.52
1:A:88:G:H8	1:A:88:G:H5'	1.75	0.52
1:A:1333:U:H2'	1:A:1334:C:C6	2.44	0.52
11:J:117:LYS:O	11:J:119:VAL:HG13	2.09	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52
7:F:58:VAL:HG12	7:F:59:GLY:N	2.24	0.52
4:C:18:ALA:O	4:C:20:SER:N	2.39	0.52
11:J:150:LYS:NZ	38:J:8379:HOH:O	2.40	0.52
2:B:3025:G:H5"	2:B:3026:C:C6	2.45	0.52
1:A:1205:U:H2'	1:A:1206:U:C5'	2.38	0.52
15:N:184:ARG:HG3	15:N:185:PRO:HA	1.92	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.56	0.52
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.57	0.52
1:A:1015:C:H2'	1:A:1016:U:C6	2.44	0.52
10:I:69:ARG:NH1	38:I:3513:HOH:O	2.42	0.52
28:1:50:ALA:HB3	28:1:54:ILE:HG22	1.91	0.52
17:P:96:VAL:HA	38:P:4258:HOH:O	2.08	0.52
20:S:61:GLN:NE2	38:S:8539:HOH:O	2.42	0.52
6:E:127:ARG:HG2	6:E:127:ARG:NH1	2.24	0.52
1:A:2467:A:O2'	1:A:2468:A:H2'	2.08	0.52
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.57	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.09	0.52
1:A:401:C:H2'	1:A:402:U:C6	2.45	0.52
1:A:2276:U:H2'	1:A:2277:U:H6	1.74	0.52
1:A:380:A:OP2	15:N:9:ARG:HD2	2.09	0.52
1:A:657:G:OP1	6:E:27:ARG:NH2	2.40	0.52
6:E:150:THR:HA	6:E:203:ALA:O	2.09	0.52
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.44	0.52
1:A:622:G:O2'	1:A:623:U:H5'	2.09	0.52
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.24	0.52
1:A:2587:U:H2'	1:A:2589:U:H5"	1.91	0.52
1:A:1008:C:O2'	1:A:1009:U:H5'	2.09	0.52
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.38	0.52
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.40	0.52
8:G:11:VAL:HG12	8:G:12:ASP:H	1.74	0.52
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.22	0.52
1:A:2769:C:C2'	1:A:2770:G:H5'	2.40	0.52
1:A:2064:U:H5'	1:A:2652:U:H4'	1.90	0.52
5:D:305:ASP:O	5:D:306:LYS:CB	2.56	0.52
1:A:566:A:H2'	1:A:567:U:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.74	0.52
1:A:1176:C:H1'	38:A:3422:HOH:O	2.10	0.52
6:E:142:ASP:OD1	6:E:236:THR:HG23	2.09	0.52
1:A:797:A:O4'	28:1:10:ARG:N	2.42	0.52
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.39	0.52
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.39	0.52
5:D:162:MET:CE	5:D:308:LEU:HD21	2.40	0.52
14:M:73:VAL:HG23	14:M:74:THR:H	1.73	0.52
12:K:93:ARG:HH11	12:K:93:ARG:HB3	1.74	0.52
16:O:64:SER:C	16:O:66:LEU:H	2.12	0.52
6:E:37:ALA:HB2	38:E:8382:HOH:O	2.09	0.52
1:A:513:A:N3	38:A:3157:HOH:O	2.33	0.52
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.74	0.52
11:J:46:VAL:O	11:J:146:TRP:HH2	1.93	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.52
1:A:2505:G:H8	38:A:5108:HOH:O	1.93	0.52
5:D:144:THR:HG22	5:D:145:HIS:N	2.25	0.52
1:A:401:C:P	38:A:5258:HOH:O	2.68	0.52
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.75	0.52
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.40	0.52
1:A:1718:G:OP2	18:Q:20:ARG:HD2	2.09	0.52
1:A:2630:G:O6	4:C:206:ARG:NH2	2.43	0.52
28:1:37:HIS:O	28:1:45:LYS:HA	2.10	0.52
25:X:88:THR:CG2	25:X:89:ASP:H	2.19	0.52
1:A:2715:G:N2	5:D:264:GLU:OE1	2.43	0.52
30:3:40:ARG:HH11	30:3:40:ARG:HG2	1.74	0.52
1:A:1188:A:C5	1:A:1189:A:C2	2.98	0.52
4:C:99:ILE:O	4:C:131:HIS:CE1	2.63	0.52
1:A:431:G:P	15:N:48:ARG:HH12	2.33	0.52
17:P:25:VAL:HG23	17:P:26:TRP:N	2.25	0.52
11:J:144:GLU:HA	11:J:144:GLU:OE1	2.10	0.52
1:A:625:U:H5"	1:A:1044:C:N4	2.25	0.52
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.24	0.52
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.45	0.52
11:J:48:LEU:CD1	11:J:157:ILE:HG21	2.39	0.52
11:J:139:ASP:N	11:J:140:PRO:CD	2.72	0.52
5:D:162:MET:CE	5:D:310:ARG:HD3	2.40	0.52
16:O:154:LEU:HG	16:O:155:GLU:N	2.24	0.52
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.25	0.52
1:A:218:C:OP2	1:A:220:C:N4	2.42	0.52
14:M:35:ARG:O	14:M:40:PHE:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:U:H2'	1:A:833:G:C8	2.45	0.52
10:I:23:ILE:O	10:I:27:ILE:HG13	2.10	0.51
1:A:2896:A:H2'	1:A:2896:A:N3	2.25	0.51
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.74	0.51
7:F:92:GLU:O	7:F:93:LEU:O	2.28	0.51
1:A:2724:U:H2'	1:A:2725:G:O4'	2.10	0.51
1:A:1055:G:OP2	11:J:94:ARG:NH1	2.43	0.51
13:L:125:ALA:C	13:L:127:ALA:H	2.12	0.51
1:A:2781:U:H2'	1:A:2782:G:H5'	1.91	0.51
25:X:122:ARG:HG2	25:X:152:ALA:O	2.09	0.51
1:A:2756:U:H3	1:A:2896:A:H2	1.56	0.51
1:A:2115:U:H2'	1:A:2116:U:C6	2.45	0.51
1:A:2524:G:H21	1:A:2526:C:N4	2.08	0.51
23:V:14:GLU:OE1	23:V:15:PRO:HD2	2.10	0.51
11:J:127:GLY:O	11:J:128:ALA:CB	2.58	0.51
6:E:178:GLN:O	6:E:179:GLY:C	2.48	0.51
14:M:57:VAL:HG12	14:M:57:VAL:O	2.10	0.51
25:X:90:TYR:CD1	25:X:90:TYR:N	2.78	0.51
1:A:2307:A:C2	1:A:2308:U:N3	2.78	0.51
1:A:920:C:H5"	1:A:921:G:O5'	2.10	0.51
1:A:2533:C:H6	1:A:2533:C:C5'	2.15	0.51
1:A:542:A:H2'	1:A:543:G:O4'	2.10	0.51
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.40	0.51
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.41	0.51
22:U:111:ARG:HB3	22:U:119:ALA:HB2	1.93	0.51
4:C:125:ASN:ND2	38:C:8542:HOH:O	2.39	0.51
1:A:2121:G:O2'	31:4:47:GLY:HA2	2.11	0.51
25:X:154:ARG:C	38:X:4276:HOH:O	2.47	0.51
1:A:1874:U:P	4:C:51:ARG:HD2	2.50	0.51
1:A:1056:U:H2'	1:A:1057:A:O4'	2.11	0.51
1:A:2432:C:H2'	1:A:2433:A:H8	1.75	0.51
1:A:926:A:O2'	14:M:41:HIS:CD2	2.63	0.51
31:4:39:GLN:HA	31:4:42:ARG:NH2	2.26	0.51
7:F:169:THR:O	7:F:170:TYR:HB2	2.11	0.51
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.51
1:A:2749:U:O2'	1:A:2751:C:OP2	2.17	0.51
1:A:911:G:H5'	1:A:932:U:OP1	2.10	0.51
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.92	0.51
1:A:797:A:C4'	28:1:10:ARG:N	2.73	0.51
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.75	0.51
4:C:192:VAL:O	4:C:207:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:52:THR:HG22	23:V:54:THR:N	2.26	0.51
16:O:162:ASP:O	38:O:8520:HOH:O	2.18	0.51
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.41	0.51
2:B:3030:C:OP1	7:F:137:PRO:O	2.28	0.51
20:S:25:PHE:CE2	20:S:29:LYS:HE2	2.46	0.51
16:O:180:LEU:O	16:O:181:ASP:HB3	2.10	0.51
38:A:6167:HOH:O	27:Z:165:GLU:HB3	2.10	0.51
1:A:2039:A:H4'	1:A:2760:C:O2'	2.11	0.51
1:A:1568:G:O2'	1:A:1569:U:H5'	2.09	0.51
28:1:25:ARG:O	28:1:29:VAL:HG23	2.10	0.51
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.38	0.51
23:V:52:THR:HG22	23:V:54:THR:H	1.76	0.51
1:A:289:G:O2'	1:A:290:C:H5'	2.11	0.51
1:A:711:G:N2	1:A:718:C:C2	2.79	0.51
15:N:59:GLY:CA	15:N:141:ILE:HD11	2.41	0.51
8:G:7:ILE:CG2	8:G:45:ASP:O	2.58	0.51
25:X:14:HIS:HB2	25:X:17:ILE:HG13	1.93	0.51
1:A:111:C:H2'	1:A:112:G:O4'	2.11	0.51
7:F:135:VAL:HG22	7:F:136:ARG:N	2.25	0.51
6:E:39:GLN:O	6:E:43:LYS:HD3	2.11	0.51
1:A:2256:G:C2'	1:A:2257:G:H5'	2.41	0.51
10:I:66:LEU:O	10:I:69:ARG:HB3	2.10	0.51
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.91	0.51
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.46	0.51
1:A:245:C:H2'	1:A:246:G:H5'	1.92	0.51
1:A:2787:C:H5	38:A:4115:HOH:O	1.93	0.51
28:1:57:CYS:O	28:1:61:GLY:N	2.41	0.51
1:A:1589:G:N2	1:A:1605:G:H1'	2.26	0.51
29:2:25:LYS:HD2	30:3:49:GLU:N	2.25	0.51
29:2:25:LYS:HG3	30:3:49:GLU:H	1.76	0.51
9:H:99:THR:HG23	9:H:99:THR:O	2.10	0.51
1:A:2363:G:O2'	19:R:11:ARG:HG3	2.11	0.51
5:D:204:GLY:C	38:D:8653:HOH:O	2.49	0.51
1:A:2055:A:H4'	20:S:132:ARG:NH2	2.25	0.51
7:F:10:PHE:CG	7:F:11:HIS:N	2.79	0.51
1:A:470:U:O2'	29:2:16:HIS:HD2	1.93	0.51
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.26	0.51
1:A:1882:C:O2'	1:A:2012:U:OP2	2.26	0.51
1:A:306:A:P	22:U:38:ARG:HH21	2.33	0.51
8:G:92:PRO:HB2	38:G:4917:HOH:O	2.11	0.51
1:A:1052:G:H2'	1:A:1052:G:N3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:56:ILE:HG21	11:J:61:LEU:HD13	1.93	0.51
25:X:31:HIS:HB3	38:X:5420:HOH:O	2.11	0.51
7:F:86:THR:O	7:F:90:LEU:HG	2.11	0.51
5:D:211:THR:HA	5:D:255:GLY:O	2.11	0.51
1:A:1787:C:H4'	1:A:2883:A:O4'	2.10	0.51
1:A:2897:C:H2'	1:A:2898:G:H8	1.75	0.51
6:E:140:VAL:HG12	6:E:141:SER:N	2.26	0.51
21:T:58:MET:SD	30:3:8:LYS:HE3	2.50	0.51
1:A:960:G:N3	1:A:960:G:H2'	2.26	0.51
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.93	0.51
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.74	0.51
38:A:4879:HOH:O	4:C:164:ARG:CZ	2.59	0.51
20:S:29:LYS:HD3	38:S:8531:HOH:O	2.11	0.51
1:A:305:A:C5	1:A:329:A:C2	2.99	0.51
1:A:1008:C:OP1	11:J:16:ARG:NH2	2.40	0.51
19:R:30:VAL:O	19:R:30:VAL:HG12	2.11	0.51
5:D:125:GLU:O	5:D:129:ARG:HG3	2.10	0.51
16:O:82:TYR:OH	16:O:176:ARG:NH1	2.44	0.51
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.55	0.51
1:A:2779:G:H21	8:G:143:GLN:NE2	2.09	0.51
1:A:737:A:H2'	1:A:738:G:O4'	2.11	0.51
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.76	0.51
16:O:3:GLY:HA3	38:O:8512:HOH:O	2.10	0.51
5:D:32:ASP:HA	38:D:8575:HOH:O	2.10	0.51
31:4:24:LYS:HG2	35:4:8504:CL:CL	2.48	0.51
21:T:57:THR:CG2	21:T:59:ASP:HB2	2.40	0.50
1:A:2094:G:C4'	5:D:245:SER:HB3	2.39	0.50
11:J:71:TYR:C	11:J:73:GLN:N	2.63	0.50
1:A:204:A:C2'	1:A:205:U:H5'	2.40	0.50
1:A:2795:C:O2'	1:A:2796:U:H5'	2.11	0.50
1:A:1699:C:H4'	38:A:5901:HOH:O	2.10	0.50
28:1:58:GLY:HA3	38:1:8437:HOH:O	2.10	0.50
1:A:2112:A:H2'	1:A:2113:G:C8	2.46	0.50
6:E:33:LYS:HE2	38:E:8361:HOH:O	2.10	0.50
1:A:1197:G:N2	38:A:5692:HOH:O	2.43	0.50
5:D:235:ARG:HA	38:D:8596:HOH:O	2.10	0.50
26:Y:20:GLU:CD	26:Y:21:PRO:HD2	2.31	0.50
1:A:2897:C:O2'	1:A:2898:G:H5'	2.11	0.50
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.46	0.50
5:D:189:ALA:HB1	38:D:8566:HOH:O	2.10	0.50
6:E:5:ILE:CD1	6:E:16:VAL:HG23	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:127:ARG:HD2	6:E:229:PRO:O	2.11	0.50
1:A:1119:G:H8	12:K:52:GLN:HE22	1.59	0.50
8:G:15:GLN:HG2	8:G:19:ASP:O	2.11	0.50
1:A:2004:U:H1'	38:A:9690:HOH:O	2.10	0.50
1:A:821:U:O2'	1:A:822:C:H5'	2.12	0.50
26:Y:8:ARG:NH1	38:Y:2479:HOH:O	2.23	0.50
1:A:2266:A:H2'	1:A:2267:G:H8	1.76	0.50
38:A:4057:HOH:O	15:N:83:SER:HA	2.10	0.50
38:A:5651:HOH:O	30:3:44:ARG:HG2	2.11	0.50
15:N:24:MET:HE2	15:N:28:MET:HE3	1.94	0.50
1:A:1559:A:H1'	38:A:5328:HOH:O	2.11	0.50
1:A:192:A:N6	1:A:194:A:C2	2.80	0.50
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.41	0.50
7:F:49:PRO:HG3	38:F:5828:HOH:O	2.10	0.50
1:A:1205:U:C2'	1:A:1206:U:H5'	2.36	0.50
15:N:52:LEU:HD13	15:N:116:ASN:CG	2.31	0.50
23:V:52:THR:CG2	23:V:54:THR:HB	2.42	0.50
7:F:95:THR:C	7:F:97:GLN:H	2.07	0.50
15:N:173:LEU:HD23	15:N:183:VAL:CG1	2.41	0.50
7:F:64:ARG:O	7:F:67:ASP:OD2	2.29	0.50
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.41	0.50
25:X:11:VAL:O	25:X:12:ASN:HB2	2.11	0.50
1:A:220:C:OP2	1:A:2431:C:H1'	2.12	0.50
1:A:2266:A:H2'	1:A:2267:G:C8	2.46	0.50
1:A:1015:C:O5'	1:A:1015:C:H6	1.93	0.50
14:M:72:ASN:O	14:M:76:LEU:HG	2.11	0.50
1:A:564:G:H1'	38:A:5768:HOH:O	2.12	0.50
1:A:1829:A:C8	1:A:1885:A:C8	2.99	0.50
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.40	0.50
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.42	0.50
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.94	0.50
14:M:73:VAL:HG23	14:M:74:THR:N	2.26	0.50
20:S:119:VAL:O	20:S:119:VAL:HG12	2.11	0.50
31:4:18:GLN:OE1	31:4:73:GLU:HB3	2.12	0.50
1:A:858:U:H2'	1:A:859:C:C6	2.47	0.50
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.50
6:E:79:ARG:O	6:E:87:ARG:HG2	2.11	0.50
2:B:3076:G:C3'	2:B:3077:A:H5"	2.35	0.50
1:A:646:G:H2'	1:A:647:U:H6	1.77	0.50
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.40	0.50
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:G:H2'	1:A:1524:U:C6	2.47	0.50
8:G:37:ASP:OD1	12:K:125:SER:HB3	2.11	0.50
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.93	0.50
29:2:25:LYS:O	29:2:25:LYS:HG2	2.12	0.50
4:C:51:ARG:HB2	38:C:8620:HOH:O	2.11	0.50
9:H:32:GLY:N	38:H:3111:HOH:O	2.44	0.50
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.41	0.50
1:A:128:A:H3'	1:A:128:A:H8	1.77	0.50
5:D:103:ASP:HB2	38:D:8594:HOH:O	2.11	0.50
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.50
1:A:419:A:C2	1:A:2449:G:C2	3.00	0.50
11:J:65:ARG:NH1	38:J:8385:HOH:O	2.44	0.50
1:A:2404:G:OP1	19:R:69:ASP:N	2.38	0.50
4:C:75:GLY:HA2	28:1:63:LYS:O	2.12	0.50
7:F:65:GLU:HA	38:F:6752:HOH:O	2.12	0.50
5:D:4:SER:O	5:D:5:ARG:HB2	2.12	0.50
1:A:2531:U:O2'	1:A:2532:A:H5'	2.12	0.50
31:4:7:PHE:HE2	31:4:22:VAL:HG21	1.76	0.50
1:A:2256:G:H2'	1:A:2257:G:C5'	2.42	0.50
1:A:702:G:O2'	1:A:703:G:H5'	2.12	0.50
1:A:858:U:H2'	1:A:859:C:H6	1.77	0.50
15:N:85:ARG:NE	38:N:8519:HOH:O	2.34	0.50
8:G:93:MET:HE1	8:G:165:GLY:N	2.27	0.50
1:A:2382:A:H5'	38:4:8531:HOH:O	2.11	0.50
1:A:1636:G:O2'	1:A:1637:A:H5'	2.11	0.50
1:A:1557:G:O2'	1:A:1558:C:H5'	2.12	0.50
22:U:19:ARG:HD3	22:U:67:LEU:O	2.11	0.50
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.93	0.50
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.42	0.50
25:X:122:ARG:CG	25:X:152:ALA:O	2.60	0.50
21:T:53:ASN:ND2	38:T:8321:HOH:O	2.44	0.50
9:H:27:GLY:HA3	38:H:5413:HOH:O	2.12	0.50
21:T:81:ILE:HG23	38:T:8337:HOH:O	2.11	0.50
1:A:832:U:H2'	1:A:833:G:H8	1.76	0.50
9:H:117:GLU:C	9:H:119:ARG:H	2.15	0.50
1:A:2911:C:H2'	1:A:2912:C:C6	2.47	0.50
1:A:303:C:O2'	1:A:304:G:H5'	2.12	0.50
1:A:2304:G:H5'	38:R:1719:HOH:O	2.10	0.50
4:C:53:ALA:HB3	38:C:8620:HOH:O	2.11	0.49
20:S:39:THR:HB	20:S:42:GLU:CG	2.41	0.49
1:A:2361:A:H2'	1:A:2362:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:105:VAL:HG12	4:C:106:CYS:N	2.27	0.49
14:M:140:VAL:HG23	38:M:8562:HOH:O	2.11	0.49
1:A:119:A:H2'	1:A:120:A:H5"	1.94	0.49
1:A:656:G:OP2	17:P:37:ARG:HD2	2.11	0.49
8:G:18:LEU:HD13	8:G:34:TRP:CD1	2.47	0.49
18:Q:7:LYS:HD3	18:Q:21:VAL:HG21	1.94	0.49
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.10	0.49
1:A:2278:U:H2'	38:A:7060:HOH:O	2.11	0.49
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.46	0.49
5:D:223:ARG:HG3	5:D:232:TRP:O	2.12	0.49
9:H:34:ASN:HA	15:N:4:ALA:HB2	1.94	0.49
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.47	0.49
1:A:820:G:O2'	1:A:856:G:H4'	2.12	0.49
6:E:246:ARG:CB	6:E:246:ARG:HH11	2.18	0.49
1:A:922:A:N7	1:A:2281:C:H5'	2.27	0.49
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.10	0.49
1:A:821:U:H2'	1:A:822:C:C6	2.47	0.49
1:A:734:U:O2'	1:A:737:A:N6	2.45	0.49
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.12	0.49
1:A:883:U:O2	1:A:883:U:C2'	2.60	0.49
19:R:24:SER:O	38:R:2847:HOH:O	2.19	0.49
1:A:1127:C:H2'	1:A:1128:U:H5'	1.93	0.49
11:J:59:ASN:ND2	11:J:59:ASN:N	2.56	0.49
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.93	0.49
15:N:122:GLU:HB2	15:N:126:HIS:O	2.12	0.49
1:A:1495:C:H1'	1:A:1573:A:H1'	1.94	0.49
1:A:2453:G:H5'	38:A:4173:HOH:O	2.11	0.49
10:I:63:ARG:N	38:I:2569:HOH:O	2.45	0.49
2:B:3031:C:H1'	38:B:8392:HOH:O	2.11	0.49
12:K:52:GLN:HG3	12:K:53:ILE:N	2.28	0.49
1:A:484:A:N1	1:A:506:G:H4'	2.28	0.49
6:E:162:VAL:CG1	6:E:192:ILE:HD11	2.42	0.49
14:M:143:THR:HG22	14:M:144:ASP:H	1.77	0.49
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.26	0.49
1:A:1015:C:H2'	1:A:1016:U:H6	1.75	0.49
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.32	0.49
1:A:61:G:OP1	30:3:17:GLN:HG2	2.12	0.49
26:Y:36:HIS:CE1	26:Y:40:HIS:CD2	3.01	0.49
1:A:2123:A:H3'	1:A:2124:G:H8	1.77	0.49
1:A:1160:G:HO2'	1:A:1190:G:H8	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:U:H3	1:A:1246:A:N6	2.00	0.49
1:A:2419:U:H5"	1:A:2420:G:C5'	2.41	0.49
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.42	0.49
1:A:2505:G:C2'	1:A:2506:A:H5'	2.42	0.49
1:A:2004:U:H2'	1:A:2004:U:O2	2.11	0.49
1:A:1819:G:H5'	38:A:5281:HOH:O	2.12	0.49
1:A:1778:A:H2'	1:A:1779:A:H5'	1.94	0.49
1:A:921:G:H4'	1:A:924:G:C6	2.47	0.49
1:A:251:C:H1'	15:N:58:GLN:HE22	1.76	0.49
1:A:1762:C:H4'	38:A:4138:HOH:O	2.11	0.49
4:C:57:ALA:HA	4:C:67:LEU:HD23	1.94	0.49
21:T:29:ASP:OD2	21:T:31:ARG:NH1	2.46	0.49
38:A:9103:HOH:O	15:N:165:SER:HB3	2.12	0.49
6:E:118:THR:HG23	38:E:8305:HOH:O	2.12	0.49
21:T:57:THR:C	21:T:59:ASP:H	2.15	0.49
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.27	0.49
1:A:283:U:H5"	1:A:284:C:OP2	2.13	0.49
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.94	0.49
15:N:95:LYS:HG2	15:N:99:ARG:HB3	1.94	0.49
5:D:2:GLN:CD	38:D:8622:HOH:O	2.50	0.49
31:4:62:THR:HB	38:4:8549:HOH:O	2.11	0.49
31:4:84:ARG:HB3	38:4:8549:HOH:O	2.11	0.49
17:P:77:ALA:HA	17:P:96:VAL:O	2.13	0.49
9:H:6:PHE:CD1	9:H:6:PHE:O	2.66	0.49
1:A:1132:A:N6	1:A:1229:C:H2'	2.28	0.49
9:H:13:GLU:OE2	9:H:78:GLU:HG2	2.12	0.49
12:K:142:ASN:O	12:K:144:THR:N	2.45	0.49
6:E:141:SER:HB3	38:E:8421:HOH:O	2.13	0.49
16:O:34:LEU:HD13	16:O:47:LEU:HD21	1.94	0.49
12:K:79:PHE:HB3	12:K:103:VAL:HG11	1.94	0.49
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.38	0.49
23:V:52:THR:HG22	23:V:54:THR:HB	1.95	0.49
1:A:2712:G:H5'	38:L:4183:HOH:O	2.13	0.49
1:A:1189:A:H1'	1:A:1209:C:C1'	2.43	0.49
1:A:1883:U:O2'	1:A:1884:G:H5'	2.13	0.49
1:A:219:G:O5'	1:A:220:C:H5"	2.13	0.49
1:A:228:C:H2'	1:A:229:G:H5'	1.95	0.49
1:A:500:G:H21	20:S:98:ASN:HD21	1.60	0.49
1:A:1125:U:H2'	1:A:1126:C:H5'	1.95	0.49
8:G:43:ASP:HA	38:G:5864:HOH:O	2.12	0.49
7:F:35:ALA:HB1	38:F:3279:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:C:C2'	1:A:542:A:C5'	2.88	0.49
25:X:3:ALA:O	25:X:54:PHE:HA	2.12	0.49
25:X:139:GLY:O	25:X:141:HIS:HD2	1.95	0.49
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.95	0.49
1:A:553:G:O4'	1:A:1325:G:H5'	2.13	0.49
29:2:17:THR:N	29:2:27:TYR:O	2.38	0.49
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.95	0.49
23:V:35:LYS:NZ	38:V:6621:HOH:O	2.39	0.49
16:O:170:GLU:O	16:O:174:GLU:HG3	2.13	0.49
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.13	0.49
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.49
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.76	0.49
1:A:2815:G:N7	12:K:80:LYS:NZ	2.61	0.49
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.48	0.49
1:A:2262:C:O5'	1:A:2262:C:H6	1.95	0.49
1:A:1535:G:H2'	1:A:1536:C:C6	2.48	0.49
1:A:1813:U:O2'	18:Q:81:LYS:HE3	2.13	0.49
1:A:834:G:H4'	1:A:835:U:OP2	2.13	0.49
1:A:1651:C:OP1	38:A:4986:HOH:O	2.20	0.49
14:M:65:ASP:CG	14:M:111:ALA:HB3	2.33	0.49
30:3:48:ASP:O	30:3:49:GLU:HB2	2.13	0.49
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.49
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.95	0.49
38:A:6913:HOH:O	6:E:188:ARG:HD2	2.11	0.49
11:J:81:TYR:CD1	11:J:81:TYR:C	2.86	0.49
27:Z:144:ARG:NH2	38:Z:8616:HOH:O	2.45	0.49
1:A:1299:G:N2	38:A:4165:HOH:O	2.46	0.49
8:G:80:TRP:O	8:G:134:SER:HA	2.12	0.49
1:A:314:G:N2	1:A:316:A:H3'	2.27	0.49
31:4:73:GLU:HB3	38:4:8559:HOH:O	2.12	0.49
10:I:20:VAL:O	10:I:24:VAL:HG23	2.13	0.49
20:S:114:VAL:O	20:S:114:VAL:HG13	2.13	0.49
29:2:26:SER:HB3	29:2:35:SER:OG	2.11	0.49
1:A:1218:U:H2'	1:A:1219:U:C6	2.48	0.49
25:X:6:GLN:HA	25:X:52:VAL:HG23	1.93	0.48
1:A:401:C:C5'	38:A:5258:HOH:O	2.61	0.48
5:D:44:TYR:OH	5:D:148:PRO:HG3	2.13	0.48
16:O:154:LEU:O	16:O:155:GLU:CB	2.61	0.48
8:G:20:ILE:HD11	8:G:33:LEU:HD12	1.93	0.48
16:O:18:THR:HA	38:O:8525:HOH:O	2.12	0.48
23:V:31:PHE:CG	23:V:37:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:C:O2'	1:A:66:G:H5'	2.13	0.48
15:N:77:PHE:HD2	38:N:8526:HOH:O	1.96	0.48
5:D:108:GLU:HB3	5:D:111:ARG:HD2	1.94	0.48
1:A:1735:C:O2'	1:A:1736:A:H5'	2.13	0.48
2:B:3025:G:N2	38:B:8512:HOH:O	2.45	0.48
25:X:122:ARG:HH22	25:X:154:ARG:C	2.17	0.48
1:A:1733:A:H4'	5:D:212:GLN:HA	1.94	0.48
13:L:86:THR:HG22	13:L:87:ARG:N	2.29	0.48
14:M:143:THR:CG2	14:M:144:ASP:H	2.26	0.48
1:A:926:A:O2'	14:M:41:HIS:HD2	1.96	0.48
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.44	0.48
31:4:42:ARG:HH11	31:4:42:ARG:HG3	1.78	0.48
1:A:2010:A:H2'	38:A:5418:HOH:O	2.12	0.48
1:A:2053:G:OP1	20:S:138:SER:OG	2.27	0.48
8:G:132:THR:HG23	8:G:132:THR:O	2.12	0.48
1:A:2251:G:H2'	1:A:2252:A:C8	2.49	0.48
5:D:177:HIS:O	5:D:181:ILE:HG13	2.13	0.48
1:A:2559:C:H4'	38:A:6714:HOH:O	2.13	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.14	0.48
14:M:101:ASP:C	14:M:103:ALA:H	2.15	0.48
11:J:48:LEU:HD13	11:J:146:TRP:HB3	1.95	0.48
7:F:35:ALA:O	7:F:37:ALA:N	2.46	0.48
7:F:49:PRO:HA	7:F:73:VAL:HG22	1.95	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.31	0.48
1:A:1166:A:H61	1:A:1180:U:H3	1.60	0.48
7:F:154:LYS:H	7:F:154:LYS:CD	2.19	0.48
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.95	0.48
5:D:148:PRO:HB2	5:D:156:LYS:O	2.13	0.48
1:A:1494:A:H1'	1:A:1495:C:C6	2.48	0.48
1:A:2542:C:H5"	1:A:2608:C:N4	2.27	0.48
28:1:77:LYS:HA	28:1:80:MET:CE	2.43	0.48
7:F:62:ASP:HA	38:F:4233:HOH:O	2.13	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.14	0.48
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.77	0.48
1:A:2620:U:H1'	38:A:6629:HOH:O	2.13	0.48
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.95	0.48
1:A:338:C:H4'	6:E:174:ILE:HD12	1.95	0.48
7:F:146:LYS:HZ3	16:O:107:ASN:HD21	1.58	0.48
16:O:155:GLU:O	16:O:156:GLU:HG3	2.14	0.48
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.48	0.48
5:D:251:VAL:HG23	5:D:252:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:154:ARG:HD3	38:N:8646:HOH:O	2.12	0.48
1:A:2906:A:H5'	1:A:2907:C:O4'	2.13	0.48
19:R:32:GLU:HA	19:R:71:TYR:OH	2.13	0.48
1:A:1706:G:C5	1:A:1707:G:C6	3.02	0.48
7:F:36:ASN:HA	38:F:7500:HOH:O	2.12	0.48
16:O:32:PRO:HD2	16:O:99:GLU:O	2.14	0.48
1:A:870:G:C3'	1:A:871:G:H5"	2.43	0.48
2:B:3054:A:O2'	2:B:3055:U:H5'	2.13	0.48
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.12	0.48
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.59	0.48
23:V:13:ILE:HG12	23:V:32:CYS:HB2	1.95	0.48
38:A:9264:HOH:O	14:M:41:HIS:HE1	1.96	0.48
12:K:107:ASN:C	12:K:107:ASN:HD22	2.17	0.48
7:F:86:THR:C	7:F:89:PRO:HD2	2.33	0.48
22:U:24:ARG:NH2	22:U:39:ASN:HD22	2.10	0.48
1:A:107:U:H2'	1:A:108:U:H5'	1.96	0.48
13:L:55:VAL:CG1	13:L:56:SER:N	2.77	0.48
1:A:1116:U:O2'	1:A:1118:A:C2	2.57	0.48
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.44	0.48
16:O:182:GLY:O	16:O:183:ASP:O	2.31	0.48
22:U:75:GLU:O	22:U:76:ASP:HB2	2.13	0.48
1:A:488:U:C2'	38:A:3497:HOH:O	2.57	0.48
1:A:1120:U:H5'	1:A:1121:G:OP2	2.13	0.48
6:E:54:LEU:HD21	6:E:87:ARG:HD2	1.95	0.48
1:A:1574:C:O5'	1:A:1574:C:H6	1.96	0.48
1:A:1503:U:H2'	1:A:1504:A:O4'	2.14	0.48
18:Q:3:LEU:HA	18:Q:6:GLN:OE1	2.13	0.48
1:A:2679:G:H2'	1:A:2681:A:OP2	2.13	0.48
38:A:7167:HOH:O	6:E:94:THR:HG21	2.14	0.48
15:N:38:VAL:C	15:N:63:VAL:HG13	2.34	0.48
5:D:320:GLN:HG3	5:D:321:PRO:CD	2.43	0.48
15:N:115:LEU:HD13	15:N:116:ASN:HB2	1.96	0.48
1:A:2720:C:O2	13:L:87:ARG:NH2	2.46	0.48
20:S:39:THR:O	20:S:40:ALA:C	2.50	0.48
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.42	0.48
5:D:156:LYS:HE3	38:D:8630:HOH:O	2.13	0.48
38:A:6862:HOH:O	22:U:2:LYS:HE2	2.13	0.48
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.29	0.48
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.49	0.48
6:E:19:PRO:HG2	6:E:22:PHE:CD1	2.49	0.48
1:A:221:G:H2'	1:A:222:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:6603:HOH:O	29:2:1:THR:HB	2.12	0.48
1:A:1687:C:O2	29:2:9:GLY:HA2	2.14	0.48
25:X:126:ASP:HB3	25:X:135:GLY:O	2.14	0.48
1:A:2428:G:C6	1:A:2464:C:H1'	2.48	0.48
11:J:139:ASP:H	11:J:140:PRO:HD3	1.73	0.48
3:5:75:C:N4	36:5:76:PPU:H102	2.28	0.48
16:O:67:ALA:HA	16:O:71:TRP:HB3	1.96	0.48
5:D:27:ASN:HB3	38:D:8628:HOH:O	2.12	0.48
12:K:107:ASN:HD22	12:K:109:TYR:H	1.59	0.48
1:A:2472:C:O2'	1:A:2634:G:H4'	2.12	0.48
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.44	0.48
1:A:1269:G:H2'	1:A:1270:U:C6	2.49	0.48
18:Q:7:LYS:CD	18:Q:21:VAL:CG2	2.92	0.48
1:A:2256:G:O2'	1:A:2257:G:H5'	2.13	0.48
1:A:1788:U:C2	1:A:1805:G:N2	2.81	0.48
1:A:420:U:H2'	1:A:421:C:C6	2.48	0.48
1:A:1211:G:O2'	1:A:1212:C:H5'	2.13	0.48
24:W:56:ILE:O	24:W:60:GLN:HG3	2.12	0.48
1:A:1434:A:H2'	1:A:1436:C:C5	2.49	0.48
1:A:1562:C:H2'	1:A:1562:C:O2	2.14	0.48
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.48
1:A:283:U:H5	1:A:284:C:N4	2.11	0.48
8:G:11:VAL:CG1	8:G:12:ASP:H	2.27	0.48
15:N:67:ILE:HG21	15:N:97:ILE:HG23	1.96	0.48
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.26	0.48
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.95	0.48
16:O:22:GLN:HG2	16:O:26:LEU:HD22	1.94	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.44	0.48
1:A:1819:G:H2'	1:A:1820:G:C4'	2.44	0.48
5:D:55:ASN:HB3	5:D:64:GLY:N	2.28	0.48
1:A:1543:G:N1	1:A:1641:A:OP2	2.36	0.48
1:A:60:A:C2	1:A:61:G:C8	3.02	0.48
13:L:18:ILE:HG22	13:L:93:ASN:HB2	1.96	0.48
1:A:1006:A:N1	1:A:2311:A:H1'	2.29	0.48
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.95	0.48
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.38	0.48
4:C:88:ILE:CD1	4:C:100:PRO:HD3	2.43	0.48
1:A:2768:A:O2'	1:A:2769:C:H5'	2.14	0.48
15:N:81:ARG:HB3	15:N:86:MET:HG2	1.96	0.48
1:A:128:A:C3'	1:A:128:A:C8	2.97	0.48
5:D:76:THR:N	5:D:77:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:25:VAL:HG23	17:P:26:TRP:H	1.79	0.48
1:A:1525:G:H5'	1:A:1526:A:OP2	2.14	0.48
1:A:422:G:C6	1:A:2446:G:C6	3.02	0.48
1:A:2729:C:O2'	1:A:2730:G:H5'	2.14	0.48
1:A:1308:A:O4'	6:E:226:GLY:HA3	2.14	0.48
26:Y:25:ARG:HG2	38:Y:5356:HOH:O	2.12	0.47
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.95	0.47
1:A:282:C:H2'	1:A:283:U:O4'	2.13	0.47
1:A:2281:C:O2'	1:A:2282:U:H5'	2.14	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.66	0.47
6:E:133:ARG:NH2	38:E:8431:HOH:O	2.46	0.47
8:G:18:LEU:HD13	8:G:34:TRP:CG	2.48	0.47
18:Q:18:LYS:O	18:Q:21:VAL:HG22	2.13	0.47
18:Q:27:ARG:HA	38:Q:177:HOH:O	2.13	0.47
1:A:2456:A:H5'	38:A:5164:HOH:O	2.13	0.47
38:A:8728:HOH:O	4:C:11:ARG:HD3	2.13	0.47
1:A:2120:U:H2'	1:A:2121:G:O4'	2.14	0.47
13:L:9:THR:O	13:L:10:GLN:C	2.52	0.47
25:X:64:THR:O	25:X:68:THR:HG22	2.14	0.47
1:A:1666:C:C2'	1:A:1667:A:C5'	2.92	0.47
23:V:17:THR:HG22	23:V:18:GLY:N	2.28	0.47
5:D:221:GLN:HE22	13:L:42:ASN:ND2	2.11	0.47
1:A:639:A:H2'	1:A:640:G:H8	1.77	0.47
20:S:113:HIS:O	20:S:145:LEU:HD12	2.13	0.47
38:A:9041:HOH:O	18:Q:81:LYS:HG2	2.13	0.47
1:A:2900:G:H2'	1:A:2901:C:O4'	2.14	0.47
5:D:54:VAL:HB	38:D:8613:HOH:O	2.14	0.47
6:E:61:PHE:HB3	38:E:8450:HOH:O	2.13	0.47
1:A:195:C:H2'	1:A:196:G:H5'	1.96	0.47
1:A:1205:U:C2'	1:A:1206:U:C5'	2.92	0.47
38:A:4446:HOH:O	11:J:57:ARG:HG3	2.14	0.47
4:C:192:VAL:O	4:C:192:VAL:CG1	2.62	0.47
6:E:162:VAL:CG1	6:E:162:VAL:O	2.61	0.47
1:A:1377:C:C6	1:A:1377:C:H5'	2.44	0.47
1:A:2300:A:H4'	1:A:2301:A:O5'	2.14	0.47
5:D:85:ARG:NH2	5:D:99:GLU:OE2	2.40	0.47
1:A:2445:U:H2'	1:A:2446:G:C8	2.49	0.47
16:O:24:LEU:O	16:O:28:LYS:HG2	2.14	0.47
8:G:107:PHE:CZ	8:G:108:LEU:HD13	2.49	0.47
1:A:240:C:O2	1:A:240:C:H2'	2.15	0.47
5:D:16:ARG:NE	38:D:8553:HOH:O	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:132:ASP:OD1	4:C:133:ARG:N	2.47	0.47
1:A:694:A:H2'	1:A:695:C:H5'	1.96	0.47
1:A:2243:C:HO2'	1:A:2244:A:H8	1.61	0.47
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.45	0.47
1:A:2715:G:O2'	5:D:262:ARG:HD2	2.14	0.47
38:A:9067:HOH:O	5:D:267:LYS:HD3	2.14	0.47
1:A:2748:G:C5'	38:A:6999:HOH:O	2.58	0.47
18:Q:10:ALA:O	18:Q:13:VAL:HG12	2.14	0.47
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.76	0.47
4:C:165:THR:O	4:C:165:THR:HG22	2.13	0.47
27:Z:203:VAL:HG12	27:Z:228:VAL:HG22	1.96	0.47
6:E:20:ASP:O	6:E:23:GLU:HB2	2.15	0.47
1:A:1515:A:H2'	1:A:1516:C:C6	2.49	0.47
1:A:432:G:O2'	1:A:433:C:H5'	2.13	0.47
1:A:39:G:N2	1:A:444:C:C2	2.83	0.47
2:B:3042:C:O2	7:F:76:ARG:NH1	2.47	0.47
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.30	0.47
1:A:2010:A:C2'	38:A:5418:HOH:O	2.63	0.47
1:A:169:A:HO2'	1:A:170:U:H6	1.62	0.47
1:A:816:G:C6	1:A:817:G:N1	2.82	0.47
1:A:2781:U:H2'	1:A:2782:G:C5'	2.45	0.47
1:A:1494:A:C4	1:A:1495:C:C5	3.03	0.47
1:A:398:U:H2'	1:A:399:C:C6	2.50	0.47
1:A:2894:C:O2'	1:A:2895:C:H5'	2.14	0.47
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.95	0.47
23:V:38:ASN:O	23:V:42:LEU:HG	2.15	0.47
28:1:47:LEU:HD13	28:1:64:ILE:HD11	1.97	0.47
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.97	0.47
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.29	0.47
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.30	0.47
15:N:69:LYS:O	15:N:73:ARG:CZ	2.62	0.47
9:H:60:VAL:O	9:H:61:MET:C	2.52	0.47
6:E:233:THR:CG2	6:E:234:VAL:N	2.78	0.47
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.49	0.47
6:E:25:PRO:HD2	38:E:8434:HOH:O	2.14	0.47
1:A:1072:G:OP2	27:Z:154:ARG:NH2	2.41	0.47
1:A:654:A:OP2	17:P:38:ARG:HD3	2.15	0.47
1:A:2407:G:O2'	1:A:2408:A:H5'	2.14	0.47
1:A:154:C:H2'	1:A:155:C:C6	2.49	0.47
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.47
18:Q:11:ALA:HB2	18:Q:18:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1565:C:O4'	1:A:2738:G:H1'	2.15	0.47
14:M:97:VAL:HG12	14:M:98:GLU:O	2.14	0.47
1:A:2697:A:H2'	1:A:2698:G:O4'	2.14	0.47
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.15	0.47
13:L:118:ALA:C	13:L:120:ARG:H	2.18	0.47
6:E:236:THR:C	38:E:8454:HOH:O	2.52	0.47
12:K:45:VAL:HG22	12:K:46:ILE:N	2.29	0.47
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.24	0.47
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.97	0.47
29:2:18:LYS:HB2	30:3:49:GLU:HG2	1.97	0.47
15:N:184:ARG:HB2	15:N:184:ARG:CZ	2.45	0.47
1:A:2271:G:H2'	1:A:2271:G:N3	2.29	0.47
23:V:47:ARG:CG	38:V:4381:HOH:O	2.56	0.47
1:A:1189:A:H1'	1:A:1209:C:H1'	1.97	0.47
1:A:926:A:H1'	14:M:38:HIS:O	2.14	0.47
16:O:73:ALA:HB1	16:O:74:PRO:HD2	1.96	0.47
1:A:2866:U:H4'	1:A:2867:G:H5'	1.97	0.47
9:H:21:GLU:HA	9:H:24:ARG:HE	1.79	0.47
5:D:63:GLU:HG3	5:D:63:GLU:O	2.14	0.47
15:N:46:LEU:HB2	38:N:8607:HOH:O	2.15	0.47
5:D:322:ARG:HB2	38:D:8608:HOH:O	2.14	0.47
21:T:29:ASP:OD1	21:T:31:ARG:NH1	2.47	0.47
1:A:12:U:H2'	1:A:13:G:H5'	1.97	0.47
1:A:474:C:O3'	6:E:73:LEU:HD21	2.14	0.47
18:Q:115:SER:C	18:Q:117:SER:H	2.18	0.47
1:A:1189:A:H1'	1:A:1209:C:O4'	2.15	0.47
1:A:331:A:C6	1:A:332:G:C4	3.02	0.47
29:2:21:ARG:HD3	29:2:45:ARG:NE	2.30	0.47
16:O:184:ILE:HG22	16:O:185:GLU:N	2.30	0.47
1:A:383:A:C6	1:A:407:A:C8	3.03	0.47
1:A:2016:U:H6	1:A:2016:U:O5'	1.97	0.47
20:S:119:VAL:CG2	20:S:142:ASP:HB2	2.44	0.47
1:A:929:A:O5'	1:A:929:A:H8	1.98	0.47
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.15	0.47
7:F:29:HIS:C	38:F:5858:HOH:O	2.53	0.47
1:A:1342:C:O2'	1:A:1343:C:H5'	2.15	0.47
11:J:162:SER:CB	11:J:163:PRO:CD	2.80	0.47
1:A:1119:G:N2	1:A:1246:A:H2	2.08	0.47
4:C:135:VAL:HG21	4:C:147:ARG:CZ	2.45	0.47
1:A:2346:C:H4'	7:F:52:THR:HG22	1.97	0.47
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2781:U:C2'	1:A:2782:G:H5'	2.45	0.47
1:A:392:U:O2'	15:N:182:LYS:HE2	2.14	0.47
1:A:84:G:O2'	1:A:85:C:H5'	2.15	0.47
6:E:35:VAL:HG21	6:E:227:GLY:HA2	1.95	0.47
1:A:2834:G:OP1	26:Y:39:LYS:HE2	2.15	0.47
6:E:7:ASP:OD1	6:E:11:ASN:O	2.33	0.47
1:A:2104:C:O2	1:A:2486:A:C2	2.68	0.47
1:A:731:U:H2'	1:A:732:C:C6	2.50	0.47
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.72	0.46
1:A:797:A:H4'	28:1:10:ARG:N	2.30	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.45	0.46
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.25	0.46
5:D:87:TYR:O	5:D:138:GLY:N	2.42	0.46
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.45	0.46
18:Q:143:ALA:HA	38:Q:197:HOH:O	2.15	0.46
15:N:47:ASP:CG	15:N:48:ARG:N	2.68	0.46
17:P:96:VAL:HG13	17:P:100:GLN:HB2	1.97	0.46
10:I:16:LYS:O	10:I:20:VAL:HG23	2.15	0.46
18:Q:37:ARG:O	18:Q:40:VAL:HB	2.15	0.46
6:E:65:ARG:HG3	6:E:67:GLN:HB2	1.98	0.46
4:C:9:ARG:HG2	4:C:16:PHE:CD2	2.50	0.46
9:H:37:THR:O	9:H:41:GLU:HG3	2.15	0.46
7:F:103:ASN:ND2	7:F:134:LEU:H	2.12	0.46
22:U:71:VAL:HG12	22:U:72:ILE:N	2.30	0.46
1:A:171:C:C2'	1:A:172:U:H5'	2.45	0.46
16:O:5:ARG:HG3	19:R:18:PRO:CB	2.45	0.46
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.16	0.46
4:C:211:LYS:HD3	38:C:8625:HOH:O	2.14	0.46
12:K:19:MET:HE1	12:K:132:LEU:CD1	2.45	0.46
2:B:3049:G:H2'	2:B:3050:G:O4'	2.15	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.50	0.46
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.45	0.46
31:4:74:CYS:SG	31:4:76:LYS:CG	3.03	0.46
8:G:22:VAL:O	8:G:28:SER:HA	2.15	0.46
1:A:1331:A:OP2	27:Z:142:SER:OG	2.25	0.46
1:A:1730:G:H4'	1:A:1731:C:O5'	2.15	0.46
1:A:383:A:C2	1:A:407:A:C4	3.03	0.46
1:A:1249:U:H2'	1:A:1250:C:C6	2.51	0.46
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.50	0.46
1:A:2279:G:OP1	38:A:4571:HOH:O	2.21	0.46
1:A:2247:C:H5"	38:A:6802:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:C:H5"	15:N:163:LEU:HD21	1.97	0.46
1:A:175:G:H2'	15:N:192:ALA:HB3	1.96	0.46
11:J:140:PRO:HA	11:J:142:VAL:HG12	1.98	0.46
1:A:1684:A:O2'	1:A:1685:A:H5"	2.15	0.46
2:B:3092:G:C6	2:B:3093:A:C6	3.04	0.46
1:A:407:A:H2'	1:A:408:A:C8	2.51	0.46
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.96	0.46
1:A:2451:G:O6	38:A:9891:HOH:O	2.19	0.46
1:A:1304:U:H2'	1:A:1305:C:C6	2.51	0.46
1:A:177:A:H2'	1:A:178:U:O4'	2.16	0.46
16:O:93:GLN:HG2	38:O:8554:HOH:O	2.13	0.46
1:A:2428:G:N7	38:A:3276:HOH:O	2.46	0.46
11:J:14:TYR:N	11:J:91:HIS:CE1	2.81	0.46
1:A:281:U:O2'	1:A:282:C:H5'	2.16	0.46
17:P:47:ARG:NH1	17:P:47:ARG:HG3	2.27	0.46
31:4:11:CYS:HB2	31:4:20:HIS:HE1	1.80	0.46
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.96	0.46
2:B:3064:C:H2'	2:B:3065:A:H5'	1.98	0.46
8:G:10:ASP:HA	38:G:3707:HOH:O	2.15	0.46
11:J:157:ILE:CG2	11:J:158:ASN:N	2.78	0.46
11:J:113:ALA:N	11:J:114:PRO:HD3	2.31	0.46
5:D:310:ARG:HD2	38:D:8648:HOH:O	2.15	0.46
1:A:952:G:OP1	19:R:42:LYS:HE2	2.15	0.46
29:2:29:THR:O	29:2:32:LYS:CE	2.64	0.46
1:A:1713:G:C1'	38:A:4547:HOH:O	2.60	0.46
1:A:317:A:H5"	22:U:52:ARG:HD2	1.97	0.46
1:A:1776:A:C8	1:A:1778:A:O4'	2.68	0.46
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.78	0.46
1:A:2265:U:H2'	1:A:2266:A:H8	1.81	0.46
1:A:1504:A:O2'	1:A:1506:U:OP2	2.31	0.46
1:A:1342:C:C2'	1:A:1343:C:H5'	2.46	0.46
7:F:99:ASP:HB3	7:F:103:ASN:H	1.80	0.46
1:A:2121:G:C2'	1:A:2122:C:H5'	2.44	0.46
1:A:1161:A:O5'	1:A:1161:A:H8	1.99	0.46
17:P:32:ARG:NE	38:P:3360:HOH:O	2.48	0.46
1:A:2840:A:OP1	5:D:211:THR:HG23	2.16	0.46
1:A:1850:U:H2'	1:A:1851:G:H8	1.80	0.46
7:F:169:THR:C	7:F:170:TYR:HD1	2.18	0.46
16:O:58:LEU:CD1	16:O:58:LEU:N	2.78	0.46
30:3:18:ASN:ND2	30:3:40:ARG:H	2.14	0.46
23:V:9:CYS:HG	23:V:11:THR:HG23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:39:THR:CB	20:S:42:GLU:HG3	2.42	0.46
1:A:1930:A:H2'	1:A:1931:A:C8	2.51	0.46
1:A:2769:C:O2'	1:A:2770:G:H5'	2.16	0.46
7:F:57:THR:HG23	7:F:63:ILE:CB	2.45	0.46
15:N:153:THR:O	15:N:156:ARG:HG3	2.15	0.46
1:A:95:A:H5"	1:A:97:G:O4'	2.16	0.46
11:J:157:ILE:HG22	11:J:158:ASN:N	2.30	0.46
11:J:43:PRO:HD2	11:J:137:ASN:HA	1.97	0.46
7:F:23:VAL:CG2	7:F:23:VAL:O	2.63	0.46
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.46	0.46
1:A:2432:C:H4'	31:4:36:ILE:HG12	1.97	0.46
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.51	0.46
1:A:660:A:H4'	1:A:661:G:O5'	2.16	0.46
1:A:169:A:C6	1:A:2469:A:C6	3.04	0.46
1:A:815:U:C4	1:A:816:G:C6	3.03	0.46
1:A:2028:U:H2'	1:A:2029:C:H6	1.79	0.46
1:A:2443:C:H3'	38:A:9970:HOH:O	2.16	0.46
38:A:5155:HOH:O	16:O:21:HIS:HE1	1.99	0.46
1:A:1754:A:H2'	1:A:1755:A:O4'	2.15	0.46
28:1:10:ARG:HA	38:1:8413:HOH:O	2.16	0.46
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.30	0.46
3:5:74:C:H2'	3:5:75:C:C5'	2.46	0.46
1:A:1306:U:OP1	6:E:184:ARG:HD2	2.16	0.46
5:D:42:ALA:HB3	5:D:79:MET:SD	2.56	0.46
7:F:86:THR:HG23	38:F:7477:HOH:O	2.15	0.46
1:A:2362:A:H2'	1:A:2363:G:C8	2.51	0.46
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.45	0.46
1:A:2672:C:O2'	1:A:2673:U:H5'	2.16	0.46
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.15	0.46
22:U:12:ARG:O	22:U:19:ARG:NH2	2.48	0.46
5:D:185:GLY:HA2	38:D:8633:HOH:O	2.16	0.46
1:A:2777:G:O2'	1:A:2778:A:H5'	2.15	0.46
6:E:34:ALA:HB3	6:E:220:THR:HG21	1.98	0.46
15:N:49:ALA:C	15:N:54:TYR:HB3	2.36	0.46
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.13	0.46
7:F:95:THR:C	7:F:97:GLN:N	2.67	0.46
10:I:12:ILE:O	10:I:13:PRO:C	2.53	0.46
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.81	0.46
1:A:392:U:H4'	15:N:193:LYS:HB3	1.98	0.46
1:A:941:G:O2'	1:A:942:U:H5'	2.16	0.46
27:Z:112:GLU:HA	27:Z:112:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.97	0.46
38:A:5700:HOH:O	4:C:22:ARG:HG2	2.16	0.46
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.45	0.45
2:B:3041:C:C6	7:F:50:VAL:HG21	2.51	0.45
30:3:40:ARG:NH1	30:3:40:ARG:HG2	2.30	0.45
6:E:218:VAL:HG12	38:E:8429:HOH:O	2.16	0.45
15:N:68:ARG:CD	15:N:68:ARG:O	2.63	0.45
13:L:6:ALA:HB3	13:L:116:GLU:HG2	1.98	0.45
25:X:121:PRO:HA	25:X:153:MET:HG2	1.98	0.45
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.51	0.45
8:G:20:ILE:HD12	8:G:33:LEU:HD12	1.95	0.45
22:U:96:VAL:CG1	22:U:97:ARG:N	2.79	0.45
1:A:407:A:H5'	38:A:5485:HOH:O	2.16	0.45
1:A:1634:G:H3'	38:A:3386:HOH:O	2.14	0.45
1:A:419:A:C2	1:A:2449:G:N3	2.84	0.45
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.40	0.45
13:L:130:MET:SD	23:V:25:ASP:O	2.73	0.45
21:T:73:ASP:OD1	21:T:75:GLN:HB2	2.16	0.45
1:A:1644:C:H2'	1:A:1645:U:H6	1.81	0.45
1:A:1592:G:O2'	1:A:1593:C:O5'	2.34	0.45
1:A:1246:A:O2'	1:A:1247:A:H3'	2.16	0.45
26:Y:25:ARG:NH1	38:Y:3861:HOH:O	2.49	0.45
1:A:541:C:O2'	1:A:542:A:H5"	2.16	0.45
1:A:677:C:H4'	6:E:246:ARG:NH2	2.32	0.45
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.97	0.45
1:A:1667:A:H5'	1:A:1667:A:C8	2.48	0.45
5:D:254:GLN:HG2	5:D:255:GLY:N	2.31	0.45
4:C:101:GLU:HG2	4:C:131:HIS:ND1	2.31	0.45
14:M:104:ASP:HB2	38:M:8580:HOH:O	2.16	0.45
27:Z:115:ARG:HG3	35:Z:8517:CL:CL	2.53	0.45
1:A:2266:A:P	38:A:5323:HOH:O	2.73	0.45
1:A:1200:A:C4'	38:A:6798:HOH:O	2.64	0.45
4:C:217:ARG:CG	4:C:217:ARG:HH11	2.29	0.45
1:A:2785:C:H4'	1:A:2786:G:OP2	2.17	0.45
19:R:28:ARG:NH1	38:R:6206:HOH:O	2.43	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
13:L:99:ASP:OD1	13:L:101:ASN:N	2.49	0.45
4:C:112:PRO:HD3	4:C:152:CYS:SG	2.56	0.45
25:X:75:GLY:HA3	38:X:5763:HOH:O	2.17	0.45
38:A:4393:HOH:O	15:N:14:ARG:HB3	2.16	0.45
5:D:7:ARG:CD	5:D:9:GLY:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:178:GLN:C	6:E:180:SER:N	2.67	0.45
12:K:70:PHE:O	12:K:70:PHE:CD2	2.69	0.45
18:Q:28:GLN:N	38:Q:203:HOH:O	2.50	0.45
27:Z:136:LYS:HE2	27:Z:138:ARG:NH1	2.31	0.45
15:N:37:VAL:CG2	15:N:108:LYS:HG3	2.45	0.45
23:V:9:CYS:SG	23:V:11:THR:N	2.83	0.45
7:F:173:GLU:O	7:F:174:VAL:C	2.54	0.45
15:N:59:GLY:C	15:N:141:ILE:HD11	2.37	0.45
7:F:84:LEU:C	7:F:86:THR:H	2.19	0.45
1:A:603:A:H4'	1:A:604:G:O5'	2.16	0.45
1:A:380:A:H5"	15:N:48:ARG:NH2	2.31	0.45
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.39	0.45
7:F:58:VAL:CG1	7:F:59:GLY:N	2.78	0.45
1:A:790:A:H2'	1:A:791:A:O4'	2.16	0.45
1:A:1609:C:H2'	1:A:1610:G:H8	1.81	0.45
1:A:1336:U:C2	1:A:1337:A:C8	3.04	0.45
1:A:1440:U:P	38:A:3954:HOH:O	2.73	0.45
1:A:451:C:O2'	1:A:452:G:H5'	2.16	0.45
1:A:466:A:H2'	1:A:467:G:O4'	2.16	0.45
1:A:1384:C:H5'	26:Y:30:MET:HG2	1.99	0.45
1:A:590:A:H2'	1:A:591:A:H5'	1.99	0.45
28:1:59:HIS:HA	38:1:8439:HOH:O	2.15	0.45
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.80	0.45
7:F:25:MET:SD	7:F:40:ILE:HD11	2.56	0.45
1:A:291:C:H2'	1:A:292:G:O4'	2.16	0.45
15:N:184:ARG:HB2	15:N:184:ARG:NH1	2.32	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
25:X:146:ILE:HG23	25:X:150:LEU:CD1	2.47	0.45
5:D:162:MET:HE2	5:D:310:ARG:HD3	1.98	0.45
7:F:67:ASP:O	7:F:69:ILE:HG13	2.16	0.45
4:C:153:ARG:CB	4:C:153:ARG:HH11	2.29	0.45
1:A:2314:G:O2'	1:A:2315:C:H5'	2.16	0.45
1:A:2044:G:OP1	26:Y:23:HIS:HE1	2.00	0.45
27:Z:186:ARG:NH1	27:Z:186:ARG:HG2	2.31	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
10:I:73:ASP:C	38:I:2994:HOH:O	2.54	0.45
8:G:157:LYS:NZ	38:G:2401:HOH:O	2.49	0.45
1:A:628:A:C8	1:A:2071:C:N4	2.85	0.45
1:A:1279:U:H5"	38:A:9093:HOH:O	2.16	0.45
1:A:2819:C:O4'	5:D:96:PRO:HB2	2.16	0.45
1:A:382:U:C5	1:A:406:G:N2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:A:O2'	28:1:13:ARG:HD3	2.16	0.45
12:K:130:VAL:CG1	12:K:131:THR:N	2.79	0.45
4:C:8:ARG:NH1	38:C:8558:HOH:O	2.42	0.45
13:L:27:ARG:CD	38:L:4747:HOH:O	2.61	0.45
5:D:248:ARG:O	5:D:251:VAL:HG13	2.17	0.45
10:I:64:ASN:N	10:I:64:ASN:ND2	2.64	0.45
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.97	0.45
1:A:1805:G:H2'	1:A:1806:G:H8	1.81	0.45
1:A:1225:C:H4'	38:A:8903:HOH:O	2.16	0.45
29:2:25:LYS:CG	30:3:49:GLU:H	2.29	0.45
16:O:25:ARG:HA	16:O:28:LYS:HG3	1.97	0.45
1:A:2050:G:H5"	20:S:80:TYR:O	2.17	0.45
1:A:2385:G:H2'	1:A:2386:U:C6	2.51	0.45
1:A:247:A:C8	1:A:262:A:N6	2.85	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.45
11:J:86:ARG:NH1	11:J:130:HIS:CD2	2.85	0.45
2:B:3055:U:H4'	2:B:3056:A:C8	2.52	0.45
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.50	0.45
1:A:2116:U:C4	1:A:2271:G:C6	3.05	0.45
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.16	0.45
14:M:38:HIS:CD2	14:M:39:GLU:HG3	2.51	0.45
9:H:28:ALA:CB	9:H:99:THR:HG23	2.46	0.45
25:X:38:THR:HG22	25:X:39:ASP:N	2.32	0.45
1:A:1878:G:C1'	38:A:5581:HOH:O	2.63	0.45
16:O:19:ASP:N	38:O:8525:HOH:O	2.15	0.45
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.52	0.45
11:J:6:TYR:HE2	11:J:94:ARG:O	2.00	0.45
1:A:222:A:H2'	1:A:223:G:O4'	2.16	0.45
38:E:8358:HOH:O	17:P:3:THR:HG21	2.17	0.45
1:A:2299:G:O6	19:R:1:PRO:HA	2.16	0.45
11:J:163:PRO:HG2	38:J:8339:HOH:O	2.16	0.45
28:1:22:ILE:HG22	28:1:23:ARG:N	2.32	0.45
1:A:2468:A:C8	31:4:54:LYS:HE2	2.51	0.45
13:L:87:ARG:CZ	38:L:4854:HOH:O	2.65	0.45
1:A:2591:C:H2'	1:A:2592:G:O4'	2.17	0.45
1:A:2432:C:H2'	1:A:2433:A:C8	2.51	0.45
2:B:3008:G:O6	16:O:11:ARG:NH1	2.48	0.45
17:P:39:THR:HB	38:P:3360:HOH:O	2.16	0.45
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.17	0.45
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.47	0.45
14:M:140:VAL:CG2	38:M:8562:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3034:A:H1'	16:O:153:GLN:HE22	1.82	0.45
15:N:49:ALA:HB1	15:N:54:TYR:CB	2.47	0.45
8:G:16:ASP:O	8:G:17:HIS:HB2	2.17	0.45
1:A:2656:G:O2'	1:A:2657:G:H5'	2.17	0.45
1:A:758:A:H2'	1:A:759:C:O4'	2.17	0.45
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.35	0.45
15:N:69:LYS:HD3	15:N:125:ARG:HA	1.98	0.45
6:E:192:ILE:CG2	6:E:234:VAL:HG12	2.48	0.45
25:X:139:GLY:O	25:X:141:HIS:CD2	2.70	0.45
8:G:116:THR:CG2	8:G:151:LEU:HD22	2.47	0.45
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.51	0.45
4:C:199:HIS:CE1	4:C:225:VAL:HG11	2.52	0.45
16:O:141:ARG:N	38:O:8566:HOH:O	2.50	0.45
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.82	0.45
1:A:553:G:H5'	38:A:9994:HOH:O	2.15	0.45
5:D:101:TRP:HB2	5:D:119:HIS:CD2	2.52	0.45
1:A:92:G:H4'	24:W:44:GLY:HA3	1.98	0.45
1:A:1014:A:H2'	1:A:1015:C:H5'	1.99	0.45
1:A:392:U:C5'	15:N:193:LYS:HB3	2.47	0.45
1:A:496:G:C6	1:A:498:A:C6	3.05	0.45
17:P:21:SER:OG	17:P:106:PRO:HB2	2.17	0.45
1:A:1427:A:N6	38:A:6184:HOH:O	2.40	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	1.98	0.45
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.51	0.45
21:T:11:THR:H	21:T:14:ALA:HB3	1.81	0.45
5:D:8:LYS:HG3	5:D:220:VAL:HG12	1.98	0.45
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.99	0.45
1:A:831:U:O2	38:A:3936:HOH:O	2.21	0.45
14:M:7:GLN:HB3	14:M:13:HIS:CE1	2.52	0.45
1:A:101:C:H2'	1:A:102:A:H8	1.82	0.45
28:1:57:CYS:O	28:1:61:GLY:HA2	2.17	0.44
15:N:35:PRO:CG	15:N:38:VAL:CG2	2.87	0.44
1:A:1886:A:C2'	38:A:4297:HOH:O	2.65	0.44
38:A:6880:HOH:O	22:U:9:LYS:HD2	2.17	0.44
1:A:2435:U:OP1	31:4:28:GLY:HA3	2.16	0.44
7:F:173:GLU:HG3	7:F:174:VAL:N	2.32	0.44
16:O:163:PHE:O	16:O:164:ASP:O	2.34	0.44
5:D:238:ASN:ND2	5:D:240:GLY:H	2.14	0.44
1:A:821:U:H5"	38:A:9546:HOH:O	2.16	0.44
1:A:2356:A:H2'	1:A:2357:G:O4'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:52:VAL:O	5:D:53:LEU:HD12	2.16	0.44
1:A:696:C:C2'	1:A:697:G:H5'	2.48	0.44
6:E:237:GLU:N	38:E:8454:HOH:O	2.50	0.44
1:A:2122:C:H3'	38:A:4762:HOH:O	2.17	0.44
11:J:149:ALA:C	11:J:151:MET:H	2.20	0.44
11:J:150:LYS:HE2	38:J:8379:HOH:O	2.16	0.44
16:O:67:ALA:C	16:O:69:TYR:N	2.70	0.44
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.48	0.44
27:Z:144:ARG:NE	38:Z:8616:HOH:O	2.49	0.44
1:A:2547:C:H2'	1:A:2548:C:H6	1.81	0.44
1:A:553:G:H2'	1:A:554:G:H5'	1.98	0.44
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.46	0.44
1:A:876:A:H2'	1:A:876:A:N3	2.32	0.44
4:C:66:ARG:HH11	4:C:66:ARG:HB2	1.80	0.44
16:O:38:LYS:HB2	16:O:38:LYS:HE3	1.76	0.44
11:J:45:GLN:NE2	11:J:135:TRP:HE1	2.16	0.44
5:D:258:GLY:N	5:D:260:HIS:CE1	2.78	0.44
25:X:121:PRO:CA	25:X:153:MET:HG2	2.48	0.44
5:D:280:VAL:CG1	5:D:281:ASP:N	2.80	0.44
29:2:29:THR:O	29:2:32:LYS:HE2	2.18	0.44
16:O:108:SER:HA	16:O:109:PRO:HD3	1.81	0.44
31:4:7:PHE:HE2	31:4:22:VAL:CG2	2.30	0.44
31:4:7:PHE:CE1	31:4:9:THR:HB	2.52	0.44
1:A:1523:G:C6	1:A:1524:U:O4	2.70	0.44
1:A:1921:A:C6	1:A:1922:A:C2	3.06	0.44
28:1:77:LYS:HA	28:1:80:MET:HE2	1.98	0.44
20:S:125:ARG:HG2	38:S:8541:HOH:O	2.16	0.44
1:A:584:U:H3'	38:A:5555:HOH:O	2.17	0.44
1:A:1970:G:C5'	38:A:6529:HOH:O	2.65	0.44
23:V:49:LEU:O	23:V:55:ALA:CB	2.65	0.44
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.52	0.44
1:A:1827:G:H2'	1:A:1828:G:C8	2.52	0.44
1:A:1461:U:H2'	1:A:1462:C:C6	2.51	0.44
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.38	0.44
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.47	0.44
1:A:2766:A:O2'	5:D:265:LEU:O	2.30	0.44
1:A:1189:A:N3	38:A:7139:HOH:O	2.50	0.44
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.47	0.44
25:X:149:LEU:HG	25:X:153:MET:HE1	1.99	0.44
1:A:2055:A:H5'	20:S:134:SER:HB2	2.00	0.44
16:O:143:ARG:HH12	16:O:173:ASP:CG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:G:C4	1:A:686:A:C2	3.06	0.44
1:A:407:A:C2	1:A:408:A:C4	3.05	0.44
22:U:38:ARG:HG3	22:U:38:ARG:HH11	1.81	0.44
8:G:9:GLU:HG3	8:G:10:ASP:N	2.33	0.44
7:F:81:GLU:O	7:F:85:GLN:HG3	2.17	0.44
1:A:602:A:O2'	1:A:605:C:H4'	2.17	0.44
20:S:129:ALA:O	20:S:130:MET:HB2	2.17	0.44
1:A:1134:G:C4'	11:J:151:MET:HE1	2.28	0.44
16:O:67:ALA:HA	16:O:71:TRP:H	1.81	0.44
25:X:4:LEU:HA	25:X:4:LEU:HD23	1.82	0.44
5:D:17:LYS:O	5:D:260:HIS:HD2	2.01	0.44
16:O:104:ILE:O	16:O:107:ASN:HB2	2.17	0.44
14:M:142:LEU:HG	14:M:146:GLY:HA3	2.00	0.44
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.46	0.44
1:A:1423:C:O2'	1:A:1424:A:H5'	2.18	0.44
10:I:71:LEU:C	10:I:73:ASP:H	2.21	0.44
1:A:696:C:HO2'	1:A:697:G:H5'	1.82	0.44
19:R:75:ILE:CD1	19:R:84:ILE:HD11	2.48	0.44
1:A:2466:G:P	38:A:3142:HOH:O	2.73	0.44
1:A:1829:A:H61	28:1:18:TYR:CA	2.26	0.44
27:Z:213:LYS:O	27:Z:217:ILE:HG13	2.18	0.44
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	2.18	0.44
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.52	0.44
16:O:161:GLY:O	16:O:162:ASP:C	2.55	0.44
2:B:3092:G:H22	11:J:52:LYS:NZ	2.15	0.44
1:A:2635:A:C2'	1:A:2636:C:H5'	2.46	0.44
1:A:1462:C:H2'	1:A:1463:A:C8	2.53	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.18	0.44
15:N:123:ASP:C	15:N:123:ASP:OD1	2.55	0.44
1:A:1859:A:H8	1:A:1859:A:O5'	2.01	0.44
1:A:1313:A:H5'	27:Z:208:LYS:O	2.17	0.44
1:A:1041:U:H2'	1:A:1042:U:H5'	2.00	0.44
38:A:4009:HOH:O	15:N:94:LYS:HE3	2.18	0.44
1:A:716:G:H2'	1:A:717:C:O5'	2.18	0.44
38:A:3472:HOH:O	31:4:57:GLY:HA2	2.17	0.44
11:J:165:GLY:C	11:J:166:ASN:HD22	2.21	0.44
12:K:46:ILE:HG12	12:K:53:ILE:HD13	1.99	0.44
16:O:71:TRP:N	38:O:8539:HOH:O	2.50	0.44
1:A:1189:A:C4	38:A:7139:HOH:O	2.56	0.44
12:K:39:VAL:HG11	12:K:107:ASN:CB	2.48	0.44
16:O:152:GLU:C	16:O:154:LEU:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:94:LEU:N	4:C:94:LEU:CD2	2.81	0.44
1:A:1299:G:N7	14:M:6:ARG:NH1	2.65	0.44
1:A:1644:C:O2'	1:A:1645:U:H5'	2.17	0.44
28:1:48:LYS:HG2	38:1:8429:HOH:O	2.18	0.44
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.99	0.44
1:A:2387:U:H2'	1:A:2388:C:C6	2.53	0.44
1:A:40:C:H4'	38:A:6462:HOH:O	2.17	0.44
1:A:2873:C:N4	1:A:2874:G:C6	2.86	0.44
19:R:88:ALA:O	19:R:90:HIS:N	2.51	0.44
1:A:2620:U:O4	36:5:76:PPU:O	2.36	0.44
31:4:60:LYS:HD2	31:4:61:PRO:HD2	1.99	0.44
12:K:39:VAL:CG1	12:K:40:ASN:N	2.81	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.83	0.44
1:A:1008:C:H2'	1:A:1009:U:C6	2.53	0.44
6:E:7:ASP:OD2	6:E:9:ASP:HB2	2.18	0.44
8:G:162:PHE:CD1	8:G:162:PHE:N	2.85	0.44
13:L:80:ILE:HG13	13:L:80:ILE:O	2.17	0.44
1:A:1135:G:H5'	38:A:5388:HOH:O	2.17	0.44
17:P:44:ASN:HA	17:P:65:LEU:O	2.18	0.44
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.99	0.44
28:1:40:PRO:CD	28:1:47:LEU:HD11	2.29	0.44
1:A:2123:A:OP1	15:N:89:ASN:ND2	2.51	0.44
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.16	0.44
13:L:45:PRO:HB2	38:L:7169:HOH:O	2.17	0.44
11:J:26:LYS:HG3	11:J:58:HIS:HB2	2.00	0.44
29:2:8:GLN:NE2	29:2:11:LYS:HZ2	2.02	0.44
1:A:1874:U:OP1	4:C:51:ARG:HD2	2.18	0.44
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.53	0.44
1:A:1637:A:H2'	1:A:1638:U:C6	2.53	0.44
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.17	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.66	0.44
27:Z:197:ASP:C	27:Z:197:ASP:OD1	2.55	0.44
28:1:38:LYS:HD3	38:1:8423:HOH:O	2.17	0.43
28:1:57:CYS:O	28:1:61:GLY:CA	2.65	0.43
11:J:151:MET:HA	11:J:151:MET:CE	2.48	0.43
28:1:10:ARG:CG	28:1:11:THR:N	2.81	0.43
2:B:3057:A:H2'	2:B:3058:G:H5'	2.00	0.43
16:O:86:LEU:HD12	16:O:125:ALA:CB	2.40	0.43
6:E:218:VAL:CG1	38:E:8429:HOH:O	2.66	0.43
5:D:248:ARG:O	5:D:251:VAL:HG12	2.18	0.43
22:U:96:VAL:HG13	22:U:97:ARG:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:G:H2'	1:A:657:G:H8	1.83	0.43
8:G:36:PRO:HD3	12:K:127:ILE:HD12	2.00	0.43
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.82	0.43
17:P:26:TRP:N	38:P:3062:HOH:O	2.49	0.43
1:A:883:U:O2	1:A:883:U:H2'	2.17	0.43
1:A:1391:G:H2'	1:A:1392:A:H5'	2.00	0.43
5:D:274:GLU:HA	5:D:292:GLY:O	2.18	0.43
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.99	0.43
1:A:1711:A:O2'	1:A:1712:A:H5'	2.18	0.43
13:L:98:VAL:HG22	13:L:102:GLU:C	2.38	0.43
1:A:1825:U:O2'	1:A:1826:C:H5'	2.18	0.43
16:O:34:LEU:HA	16:O:47:LEU:CD2	2.48	0.43
38:A:6486:HOH:O	4:C:211:LYS:HG2	2.17	0.43
12:K:77:GLY:O	12:K:78:ILE:C	2.57	0.43
1:A:2779:G:O2'	1:A:2780:C:H5'	2.18	0.43
3:5:74:C:H2'	3:5:75:C:H5'	2.01	0.43
16:O:116:PHE:CB	38:O:8556:HOH:O	2.66	0.43
7:F:19:GLU:HG3	38:F:6165:HOH:O	2.18	0.43
26:Y:76:ARG:NH1	26:Y:76:ARG:CG	2.80	0.43
1:A:1730:G:C5'	1:A:1731:C:H6	2.31	0.43
1:A:2438:G:H2'	1:A:2439:C:O4'	2.18	0.43
1:A:2255:A:C6	1:A:2256:G:C5	3.06	0.43
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.48	0.43
6:E:7:ASP:C	6:E:9:ASP:H	2.22	0.43
5:D:88:GLU:HG3	5:D:88:GLU:O	2.18	0.43
9:H:26:THR:HB	9:H:102:GLY:HA3	1.99	0.43
24:W:5:VAL:HG23	38:W:2271:HOH:O	2.18	0.43
2:B:3107:C:H5	38:B:8437:HOH:O	2.00	0.43
1:A:1265:G:H1'	38:A:4475:HOH:O	2.17	0.43
1:A:24:G:N2	1:A:518:G:H1'	2.33	0.43
1:A:860:U:H2'	1:A:861:A:C8	2.53	0.43
6:E:84:VAL:O	6:E:85:LYS:HB2	2.18	0.43
1:A:1471:A:H2'	1:A:1472:C:C6	2.53	0.43
1:A:1385:G:O3'	26:Y:49:ARG:NH1	2.52	0.43
1:A:2123:A:H5'	15:N:89:ASN:ND2	2.34	0.43
1:A:1119:G:H8	12:K:52:GLN:NE2	2.15	0.43
25:X:122:ARG:NH1	25:X:152:ALA:O	2.51	0.43
4:C:223:ARG:CG	38:C:8616:HOH:O	2.48	0.43
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.18	0.43
1:A:1329:A:C2	38:A:4165:HOH:O	2.57	0.43
27:Z:234:VAL:HG12	27:Z:235:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:170:TYR:N	7:F:170:TYR:CD1	2.87	0.43
1:A:567:U:C5'	38:A:5862:HOH:O	2.65	0.43
1:A:886:A:OP2	1:A:2113:G:H5'	2.19	0.43
31:4:73:GLU:HB2	38:4:8525:HOH:O	2.18	0.43
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.88	0.43
25:X:85:ALA:HB2	25:X:91:ASP:O	2.18	0.43
1:A:2621:U:H5	38:A:9479:HOH:O	2.01	0.43
1:A:1624:A:H4'	1:A:1626:A:H5"	2.01	0.43
21:T:10:VAL:O	21:T:10:VAL:HG22	2.19	0.43
20:S:33:ARG:NH1	38:S:8542:HOH:O	2.51	0.43
18:Q:83:LYS:O	18:Q:86:ALA:HB3	2.18	0.43
1:A:1925:G:O2'	1:A:1926:G:H5'	2.19	0.43
1:A:295:C:H2'	1:A:296:G:O4'	2.18	0.43
28:1:46:LYS:CB	28:1:57:CYS:HG	2.24	0.43
7:F:99:ASP:O	7:F:159:PRO:HG3	2.18	0.43
1:A:171:C:OP2	15:N:84:LYS:HG3	2.18	0.43
1:A:2461:U:O2	1:A:2466:G:H1'	2.18	0.43
18:Q:115:SER:C	18:Q:117:SER:N	2.71	0.43
13:L:37:TYR:HD2	38:L:7169:HOH:O	1.92	0.43
9:H:61:MET:SD	15:N:23:LEU:HD11	2.58	0.43
11:J:112:ARG:O	11:J:113:ALA:C	2.57	0.43
1:A:401:C:H2'	1:A:402:U:H6	1.81	0.43
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.48	0.43
31:4:22:VAL:HG12	31:4:90:PHE:HE2	1.83	0.43
18:Q:16:VAL:HG13	18:Q:20:ARG:NH1	2.33	0.43
16:O:82:TYR:C	16:O:82:TYR:CD2	2.91	0.43
26:Y:70:ILE:HG23	26:Y:70:ILE:O	2.17	0.43
7:F:151:ILE:HA	7:F:152:PRO:HD3	1.80	0.43
4:C:195:ASN:O	4:C:196:ALA:C	2.56	0.43
28:1:40:PRO:HG2	28:1:64:ILE:HD13	2.01	0.43
6:E:5:ILE:HG12	38:E:8436:HOH:O	2.19	0.43
11:J:163:PRO:O	11:J:164:ALA:HB2	2.18	0.43
38:A:9957:HOH:O	12:K:46:ILE:HD12	2.18	0.43
1:A:2780:C:C1'	8:G:143:GLN:NE2	2.81	0.43
3:5:74:C:H2'	3:5:75:C:O4'	2.17	0.43
29:2:45:ARG:HB3	38:2:988:HOH:O	2.18	0.43
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.18	0.43
1:A:2321:A:O2'	1:A:2322:U:H3'	2.18	0.43
1:A:160:A:C4	1:A:177:A:C2	3.06	0.43
28:1:13:ARG:NH1	38:1:8419:HOH:O	2.50	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1624:A:H5'	1:A:1626:A:O4'	2.19	0.43
1:A:482:G:H4'	1:A:508:A:N1	2.34	0.43
7:F:15:GLU:HA	7:F:16:PRO:HD3	1.85	0.43
1:A:536:A:H3'	38:A:4525:HOH:O	2.17	0.43
2:B:3045:A:C8	2:B:3046:C:C5	3.07	0.43
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.47	0.43
21:T:57:THR:HG21	21:T:59:ASP:HB2	2.01	0.43
1:A:962:C:H5'	38:A:6424:HOH:O	2.19	0.43
16:O:90:LEU:CB	16:O:186:LEU:HD22	2.49	0.43
27:Z:187:VAL:HG12	27:Z:205:ILE:HA	2.00	0.43
1:A:1058:A:H2'	1:A:1060:C:C5'	2.42	0.43
1:A:1159:G:H1	1:A:1208:C:H42	1.67	0.43
38:A:3911:HOH:O	31:4:34:LYS:HD3	2.18	0.43
1:A:1572:A:H2'	1:A:1573:A:C8	2.53	0.43
1:A:97:G:C2	22:U:107:LYS:HD2	2.53	0.43
1:A:913:A:N3	1:A:1042:U:O2'	2.44	0.43
1:A:2450:C:O5'	1:A:2450:C:H6	2.02	0.43
1:A:1311:G:C2	1:A:1312:G:C8	3.07	0.43
15:N:96:ASN:ND2	38:N:8541:HOH:O	2.49	0.43
20:S:15:LYS:HE3	38:S:8577:HOH:O	2.18	0.43
13:L:40:THR:O	13:L:41:LYS:C	2.57	0.43
1:A:812:A:H2'	1:A:813:C:O4'	2.19	0.43
1:A:844:A:C6	1:A:882:A:C5	3.06	0.43
16:O:47:LEU:HD13	16:O:97:VAL:HG11	2.01	0.43
1:A:1164:U:C1'	1:A:1165:G:OP1	2.67	0.43
27:Z:187:VAL:O	27:Z:187:VAL:HG13	2.17	0.43
1:A:559:U:C6	1:A:559:U:H5'	2.42	0.43
20:S:40:ALA:O	20:S:44:VAL:HG23	2.18	0.43
17:P:39:THR:CB	38:P:3360:HOH:O	2.66	0.43
8:G:7:ILE:HA	8:G:8:PRO:HD3	1.92	0.43
1:A:2851:G:C2'	1:A:2852:A:H5'	2.49	0.43
2:B:3003:A:N6	2:B:3022:G:H1'	2.33	0.43
15:N:39:ARG:NH2	38:N:8624:HOH:O	2.51	0.43
1:A:2106:C:H2'	1:A:2107:U:C6	2.53	0.43
22:U:38:ARG:HG3	22:U:38:ARG:NH1	2.33	0.43
1:A:2247:C:C5'	38:A:6802:HOH:O	2.67	0.43
2:B:3065:A:O2'	2:B:3066:G:P	2.75	0.43
1:A:1644:C:C2	1:A:1645:U:C6	3.07	0.43
1:A:1592:G:H2'	1:A:1593:C:C6	2.54	0.43
1:A:860:U:H2'	38:A:5151:HOH:O	2.19	0.43
1:A:675:U:H2'	1:A:676:C:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:83:PHE:CD1	11:J:134:ALA:HB2	2.54	0.43
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.43
16:O:47:LEU:HD12	16:O:92:ALA:HB1	2.00	0.43
2:B:3039:U:H3'	2:B:3040:C:H5"	1.99	0.43
25:X:26:ILE:HB	38:X:5420:HOH:O	2.17	0.43
7:F:19:GLU:O	7:F:133:ASN:HB3	2.19	0.43
1:A:290:C:O2'	1:A:291:C:H5'	2.18	0.43
4:C:36:ASP:O	4:C:37:VAL:C	2.56	0.43
5:D:71:VAL:CG1	5:D:296:LEU:HB3	2.46	0.43
25:X:38:THR:CB	38:X:5390:HOH:O	2.66	0.43
5:D:204:GLY:CA	38:D:8653:HOH:O	2.61	0.43
1:A:1167:G:O2'	1:A:1168:C:H5'	2.19	0.43
1:A:661:G:C6	1:A:686:A:C2	3.06	0.43
1:A:1422:U:H2'	1:A:1423:C:H6	1.80	0.43
25:X:41:TYR:CD2	25:X:44:MET:HE3	2.54	0.43
1:A:885:G:H5"	1:A:886:A:H5'	1.99	0.43
1:A:731:U:O2'	1:A:732:C:H5'	2.18	0.43
1:A:326:G:O2'	1:A:327:A:H5'	2.18	0.43
1:A:2563:U:H2'	1:A:2565:C:O5'	2.19	0.43
1:A:955:A:C2	1:A:1013:A:C4	3.06	0.43
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.49	0.43
21:T:57:THR:HG22	21:T:59:ASP:HB2	2.01	0.43
11:J:62:GLU:HA	38:J:8385:HOH:O	2.18	0.43
21:T:33:SER:O	21:T:37:VAL:HG23	2.18	0.43
1:A:1269:G:H2'	1:A:1270:U:H6	1.84	0.43
1:A:2113:G:C6	1:A:2114:C:C4	3.06	0.43
7:F:60:GLU:C	7:F:62:ASP:N	2.72	0.43
1:A:696:C:O2'	1:A:697:G:H5'	2.19	0.43
1:A:1714:C:O2'	1:A:1715:C:H5'	2.18	0.43
1:A:2577:A:H5'	38:A:7211:HOH:O	2.19	0.43
7:F:76:ARG:O	7:F:77:ASP:HB2	2.19	0.43
6:E:1:MET:HG2	6:E:2:GLN:N	2.32	0.43
1:A:588:G:O6	25:X:154:ARG:NH1	2.52	0.43
16:O:67:ALA:C	16:O:69:TYR:H	2.22	0.43
1:A:319:A:H4'	1:A:338:C:C5	2.53	0.43
18:Q:59:ARG:HH22	18:Q:66:GLN:NE2	2.17	0.43
25:X:65:VAL:HA	25:X:68:THR:CG2	2.49	0.43
4:C:135:VAL:HG11	4:C:147:ARG:NH2	2.34	0.43
1:A:952:G:N3	1:A:2302:A:H2'	2.33	0.43
2:B:3003:A:H2'	38:B:8421:HOH:O	2.19	0.43
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.48	0.43
1:A:1051:C:H2'	1:A:1052:G:O4'	2.19	0.43
2:B:3031:C:H2'	2:B:3032:G:O4'	2.19	0.43
38:A:6363:HOH:O	8:G:157:LYS:HD3	2.18	0.43
1:A:818:A:H5"	38:A:6050:HOH:O	2.19	0.43
1:A:2604:A:H5'	38:A:5256:HOH:O	2.18	0.43
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.43
1:A:440:C:H2'	1:A:441:A:C8	2.54	0.43
1:A:2502:C:H2'	1:A:2503:A:C5'	2.46	0.42
25:X:110:GLN:HA	25:X:110:GLN:HE21	1.83	0.42
6:E:246:ARG:NE	38:E:8429:HOH:O	2.51	0.42
14:M:146:GLY:C	14:M:148:GLU:H	2.22	0.42
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	2.01	0.42
5:D:11:LEU:C	38:D:8617:HOH:O	2.57	0.42
1:A:854:G:N7	38:A:3800:HOH:O	2.36	0.42
1:A:2359:G:H3'	38:A:5160:HOH:O	2.19	0.42
1:A:622:G:P	27:Z:148:GLY:HA3	2.59	0.42
17:P:24:ALA:N	38:P:3062:HOH:O	2.52	0.42
5:D:215:VAL:O	5:D:219:GLY:HA2	2.18	0.42
1:A:968:G:O2'	1:A:969:G:H5'	2.19	0.42
1:A:1236:A:H2'	1:A:1237:U:O4'	2.19	0.42
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.91	0.42
12:K:104:TYR:HA	38:K:2238:HOH:O	2.19	0.42
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.49	0.42
15:N:38:VAL:HG12	15:N:38:VAL:O	2.17	0.42
1:A:1771:U:O2'	28:1:23:ARG:NH2	2.50	0.42
26:Y:74:ALA:HB2	26:Y:85:VAL:HG13	2.00	0.42
7:F:77:ASP:HB3	7:F:78:GLU:H	1.57	0.42
6:E:107:ARG:CB	6:E:107:ARG:NH1	2.73	0.42
5:D:212:GLN:HB2	5:D:257:THR:CG2	2.38	0.42
1:A:1182:C:H1'	1:A:1192:A:C8	2.51	0.42
16:O:110:THR:HA	16:O:111:PRO:HD3	1.90	0.42
38:A:3159:HOH:O	15:N:79:LYS:HD2	2.18	0.42
1:A:1667:A:H2'	1:A:1668:U:C6	2.54	0.42
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.54	0.42
1:A:2673:U:C2'	1:A:2674:G:H5'	2.49	0.42
1:A:128:A:O2'	1:A:129:A:H5'	2.18	0.42
18:Q:58:SER:CB	38:Q:186:HOH:O	2.66	0.42
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.19	0.42
5:D:132:HIS:CE1	5:D:171:VAL:CG2	3.02	0.42
6:E:129:HIS:HD2	6:E:165:ASP:OD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:133:LEU:N	15:N:133:LEU:HD12	2.33	0.42
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.42
1:A:2735:U:H2'	1:A:2736:U:C6	2.54	0.42
14:M:24:ALA:HB2	14:M:30:ARG:HD2	2.00	0.42
2:B:3025:G:C8	2:B:3026:C:H5'	2.55	0.42
4:C:36:ASP:HB2	4:C:85:ASP:H	1.84	0.42
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.34	0.42
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.81	0.42
1:A:1681:G:H5"	1:A:1682:A:OP1	2.19	0.42
1:A:1298:U:H2'	1:A:1299:G:C8	2.54	0.42
1:A:1730:G:C5'	1:A:1731:C:C6	3.03	0.42
17:P:96:VAL:HG12	17:P:97:SER:O	2.18	0.42
1:A:2453:G:H3'	38:A:5380:HOH:O	2.18	0.42
1:A:2247:C:O2'	1:A:2248:C:H5'	2.20	0.42
13:L:130:MET:SD	23:V:26:GLY:HA3	2.59	0.42
5:D:53:LEU:HD21	5:D:270:ILE:HD12	2.00	0.42
1:A:1389:G:H1'	1:A:1435:U:O2	2.19	0.42
1:A:1907:U:C4	1:A:1908:G:C5	3.07	0.42
25:X:119:HIS:HD2	25:X:120:PRO:O	2.02	0.42
1:A:2122:C:P	38:A:6038:HOH:O	2.67	0.42
25:X:80:ASP:O	25:X:84:VAL:HG23	2.18	0.42
15:N:38:VAL:O	15:N:63:VAL:HG13	2.20	0.42
26:Y:71:ARG:HD3	38:Y:2171:HOH:O	2.18	0.42
7:F:94:ALA:HB3	7:F:174:VAL:HA	2.01	0.42
1:A:332:G:H4'	22:U:2:LYS:O	2.19	0.42
1:A:951:A:H2'	1:A:952:G:H5'	2.01	0.42
13:L:28:GLU:HB3	13:L:59:LYS:HB2	2.01	0.42
1:A:553:G:C2'	1:A:554:G:H5'	2.49	0.42
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.37	0.42
22:U:19:ARG:NH1	22:U:68:ASP:O	2.52	0.42
1:A:2911:C:H2'	1:A:2912:C:H6	1.84	0.42
9:H:34:ASN:O	9:H:38:LYS:HG3	2.19	0.42
1:A:1494:A:C2	1:A:1495:C:C4	3.07	0.42
21:T:29:ASP:CG	21:T:31:ARG:NH1	2.73	0.42
1:A:1871:U:O4'	1:A:1873:G:C8	2.73	0.42
2:B:3045:A:C5	2:B:3046:C:C4	3.07	0.42
2:B:3045:A:C5	2:B:3046:C:C5	3.07	0.42
5:D:277:GLU:N	5:D:278:PRO:CD	2.82	0.42
1:A:321:A:O2'	1:A:322:G:H5'	2.19	0.42
1:A:1896:G:C6	1:A:1897:U:C4	3.07	0.42
1:A:2573:G:N3	38:A:6756:HOH:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:U:O2'	1:A:36:C:H5'	2.20	0.42
15:N:25:TRP:HE3	15:N:26:HIS:HD2	1.66	0.42
1:A:1657:A:H2'	1:A:1658:A:C8	2.54	0.42
1:A:1134:G:H4'	11:J:151:MET:CE	2.29	0.42
11:J:49:VAL:O	11:J:157:ILE:HG23	2.20	0.42
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.32	0.42
15:N:84:LYS:O	15:N:87:MET:HG2	2.20	0.42
16:O:86:LEU:O	16:O:90:LEU:HG	2.19	0.42
11:J:57:ARG:C	11:J:59:ASN:N	2.70	0.42
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.34	0.42
1:A:1701:A:H5"	1:A:1702:U:H3'	2.02	0.42
4:C:200:PRO:HG2	4:C:225:VAL:HG21	2.01	0.42
5:D:7:ARG:NH2	5:D:250:THR:O	2.53	0.42
1:A:2634:G:O2'	1:A:2635:A:H5'	2.19	0.42
2:B:3003:A:H2	2:B:3021:G:N3	2.17	0.42
22:U:55:PHE:HB2	38:U:6384:HOH:O	2.20	0.42
1:A:2530:C:O2'	1:A:2531:U:H5'	2.20	0.42
9:H:22:VAL:HG21	9:H:104:ALA:HB2	2.01	0.42
6:E:212:VAL:HG23	6:E:212:VAL:O	2.20	0.42
18:Q:16:VAL:HG12	18:Q:20:ARG:HB2	2.00	0.42
18:Q:7:LYS:HD3	18:Q:21:VAL:CG2	2.49	0.42
1:A:1324:G:C2	1:A:1334:C:O2	2.73	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
1:A:2112:A:H2'	1:A:2113:G:H8	1.84	0.42
1:A:1314:U:H5"	1:A:1316:G:O4'	2.18	0.42
5:D:275:GLY:O	5:D:291:ASP:HA	2.19	0.42
1:A:2637:A:H5'	38:A:8784:HOH:O	2.20	0.42
1:A:1869:A:H2'	1:A:1870:C:O4'	2.20	0.42
1:A:1566:C:H2'	1:A:1567:A:H8	1.85	0.42
28:1:38:LYS:HG2	38:1:8408:HOH:O	2.20	0.42
6:E:236:THR:O	6:E:239:ALA:N	2.53	0.42
11:J:84:ARG:CZ	11:J:135:TRP:CH2	3.02	0.42
15:N:63:VAL:O	15:N:130:GLU:HA	2.19	0.42
16:O:47:LEU:HD23	16:O:47:LEU:HA	1.72	0.42
1:A:1943:C:O4'	4:C:212:PRO:HA	2.19	0.42
12:K:79:PHE:O	12:K:79:PHE:HD2	2.01	0.42
1:A:960:G:N3	1:A:960:G:C2'	2.82	0.42
6:E:184:ARG:NE	38:E:8415:HOH:O	2.43	0.42
25:X:65:VAL:HG12	25:X:116:LEU:HD13	2.01	0.42
1:A:1010:C:H4'	16:O:4:PRO:HB2	2.02	0.42
1:A:877:G:C5'	1:A:878:G:OP1	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:G:O2'	1:A:951:A:H5'	2.18	0.42
5:D:7:ARG:HD3	5:D:9:GLY:O	2.20	0.42
11:J:53:PRO:HA	11:J:125:VAL:O	2.20	0.42
8:G:15:GLN:NE2	8:G:40:VAL:O	2.53	0.42
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.83	0.42
4:C:173:GLY:O	4:C:177:HIS:CD2	2.72	0.42
1:A:1044:C:H5"	38:A:8542:HOH:O	2.19	0.42
1:A:2252:A:C5	1:A:2253:G:H1'	2.54	0.42
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.19	0.42
1:A:23:G:O2'	1:A:24:G:H5'	2.19	0.42
4:C:110:SER:N	4:C:114:ASP:OD2	2.52	0.42
19:R:53:HIS:O	19:R:55:ARG:N	2.53	0.42
14:M:55:GLN:HA	14:M:58:GLN:NE2	2.33	0.42
1:A:171:C:O2'	1:A:172:U:H5'	2.20	0.42
2:B:3055:U:H4'	2:B:3056:A:H8	1.83	0.42
23:V:9:CYS:SG	38:V:6796:HOH:O	2.62	0.42
15:N:185:PRO:CG	15:N:189:VAL:HG11	2.48	0.42
16:O:107:ASN:OD1	35:O:8507:CL:CL	2.75	0.42
8:G:101:GLU:OE2	8:G:115:ARG:HD3	2.19	0.42
1:A:2004:U:H5"	1:A:2005:G:C8	2.54	0.42
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.54	0.42
22:U:28:SER:O	22:U:32:ARG:HG3	2.18	0.42
7:F:59:GLY:C	7:F:61:PHE:H	2.23	0.42
4:C:125:ASN:HB3	4:C:158:VAL:HG12	2.02	0.42
25:X:73:LEU:HD12	25:X:73:LEU:HA	1.88	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.78	0.42
1:A:2335:C:C2	1:A:2350:G:C2	3.07	0.42
20:S:4:TYR:N	38:S:8546:HOH:O	2.52	0.42
4:C:169:PHE:O	4:C:170:VAL:HB	2.20	0.42
31:4:54:LYS:NZ	38:4:8526:HOH:O	2.52	0.42
26:Y:85:VAL:HG12	26:Y:86:GLU:H	1.85	0.42
1:A:1603:A:H4'	1:A:1605:G:C8	2.55	0.42
1:A:2346:C:H4'	7:F:52:THR:CG2	2.48	0.42
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.27	0.42
1:A:67:A:H5"	1:A:69:A:C8	2.55	0.42
1:A:1743:G:H1'	38:A:4365:HOH:O	2.19	0.42
1:A:553:G:P	27:Z:204:ARG:NH2	2.92	0.42
1:A:1855:G:H8	4:C:144:GLU:OE2	2.03	0.42
1:A:949:U:O2'	19:R:40:HIS:HE1	2.03	0.42
1:A:1268:C:H2'	1:A:1269:G:C8	2.54	0.42
17:P:26:TRP:HB2	38:P:3062:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:A:H1'	1:A:1921:A:C2	2.55	0.42
1:A:251:C:O2'	1:A:252:C:H5'	2.19	0.42
38:A:5000:HOH:O	15:N:58:GLN:HG3	2.19	0.42
29:2:12:ASN:HB3	38:2:5389:HOH:O	2.19	0.42
9:H:4:VAL:HG13	9:H:76:PHE:CE1	2.54	0.42
38:A:3626:HOH:O	26:Y:59:TRP:HB2	2.19	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.52	0.42
25:X:28:HIS:HD2	25:X:31:HIS:CE1	2.38	0.42
16:O:116:PHE:HB2	38:O:8556:HOH:O	2.18	0.42
25:X:76:ASP:O	25:X:77:ALA:C	2.59	0.42
16:O:162:ASP:HB3	16:O:163:PHE:H	1.61	0.42
1:A:2909:G:O2'	1:A:2910:A:H5'	2.20	0.42
8:G:64:THR:HG22	8:G:68:HIS:CD2	2.55	0.42
1:A:303:C:H2'	1:A:304:G:O4'	2.20	0.42
5:D:132:HIS:HB2	5:D:137:LEU:HD22	2.02	0.42
13:L:121:PHE:HB3	38:L:2659:HOH:O	2.19	0.42
1:A:2311:A:H5"	11:J:115:PHE:CD2	2.54	0.42
1:A:2456:A:H2'	1:A:2457:U:C6	2.55	0.42
4:C:128:LEU:HG	38:C:8583:HOH:O	2.19	0.42
5:D:277:GLU:N	5:D:278:PRO:HD2	2.34	0.42
19:R:16:ASN:HA	19:R:16:ASN:HD22	1.59	0.42
15:N:40:ILE:HG13	15:N:40:ILE:O	2.20	0.42
1:A:2607:U:C4	5:D:242:TRP:CZ2	3.07	0.42
1:A:1501:A:C6	1:A:1502:A:C6	3.07	0.42
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.50	0.42
1:A:2452:G:OP2	38:A:6202:HOH:O	2.21	0.42
24:W:45:ARG:C	24:W:47:LYS:N	2.73	0.42
1:A:10:U:HO2'	1:A:11:A:P	2.43	0.42
12:K:4:ALA:O	12:K:5:GLU:O	2.38	0.42
8:G:24:GLY:HA3	8:G:76:VAL:HB	2.02	0.42
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.90	0.42
1:A:1242:A:H5'	12:K:82:THR:CG2	2.39	0.42
1:A:319:A:H4'	1:A:338:C:C4	2.55	0.42
1:A:111:C:O2'	1:A:112:G:H5'	2.20	0.42
7:F:55:LYS:O	7:F:56:ARG:HB2	2.20	0.42
11:J:71:TYR:O	11:J:73:GLN:N	2.53	0.42
1:A:449:A:C8	6:E:43:LYS:HG2	2.54	0.42
8:G:69:ILE:HA	8:G:72:MET:HE2	2.01	0.42
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.35	0.42
1:A:221:G:C6	1:A:222:A:C6	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2655:U:C4	1:A:2656:G:N7	2.88	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.42
38:A:8592:HOH:O	5:D:214:PRO:HD2	2.20	0.42
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.35	0.41
16:O:91:ARG:HG3	16:O:186:LEU:CD2	2.48	0.41
30:3:49:GLU:CD	38:3:719:HOH:O	2.58	0.41
5:D:146:THR:O	5:D:159:PRO:HB3	2.19	0.41
4:C:103:VAL:HA	4:C:104:PRO:HD3	1.80	0.41
5:D:190:MET:HE2	5:D:194:PHE:HD1	1.83	0.41
13:L:115:ARG:CG	13:L:116:GLU:N	2.79	0.41
1:A:2430:A:H2'	1:A:2431:C:C6	2.54	0.41
20:S:25:PHE:N	38:S:8508:HOH:O	2.51	0.41
1:A:155:C:OP2	15:N:188:ARG:HD3	2.20	0.41
8:G:35:TYR:HA	12:K:127:ILE:HD12	2.02	0.41
18:Q:11:ALA:HB1	18:Q:16:VAL:O	2.20	0.41
14:M:73:VAL:HG21	14:M:116:HIS:CD2	2.55	0.41
1:A:512:G:O3'	1:A:513:A:H8	2.03	0.41
1:A:1384:C:O5'	1:A:1384:C:H6	2.03	0.41
1:A:758:A:OP1	14:M:31:GLY:N	2.50	0.41
1:A:876:A:C2'	1:A:876:A:N3	2.83	0.41
9:H:109:GLU:O	9:H:112:ALA:HB3	2.21	0.41
1:A:795:G:HO2'	1:A:796:A:P	2.43	0.41
4:C:43:VAL:O	4:C:44:ASP:HB2	2.20	0.41
5:D:224:LYS:HD3	5:D:224:LYS:HA	1.75	0.41
18:Q:121:ASP:HB2	38:Q:201:HOH:O	2.19	0.41
3:5:74:C:C4	3:5:75:C:C2	3.08	0.41
1:A:1192:A:O2'	1:A:1193:A:OP1	2.29	0.41
16:O:69:TYR:HE2	16:O:183:ASP:OD2	2.03	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.78	0.41
25:X:146:ILE:HG23	25:X:150:LEU:HD12	2.02	0.41
5:D:205:VAL:O	5:D:307:ARG:CD	2.68	0.41
1:A:1930:A:H1'	1:A:2128:G:H5'	2.02	0.41
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	2.01	0.41
1:A:1973:A:H5'	1:A:1973:A:H8	1.84	0.41
1:A:2865:G:HO2'	1:A:2866:U:H5	1.67	0.41
1:A:1562:C:H42	1:A:2738:G:H1	1.67	0.41
1:A:2385:G:H2'	1:A:2386:U:H6	1.85	0.41
9:H:26:THR:HB	9:H:102:GLY:C	2.41	0.41
15:N:133:LEU:O	15:N:134:ILE:HD13	2.21	0.41
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.20	0.41
1:A:699:C:C2	1:A:744:G:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:36:ARG:NH1	38:E:8400:HOH:O	2.53	0.41
12:K:135:ILE:O	12:K:139:LEU:HG	2.20	0.41
11:J:65:ARG:CZ	38:J:8385:HOH:O	2.68	0.41
16:O:67:ALA:O	16:O:69:TYR:N	2.54	0.41
1:A:1448:A:C6	1:A:1451:C:C2	3.09	0.41
1:A:183:A:C5'	15:N:157:LEU:HD12	2.50	0.41
1:A:182:G:C4'	15:N:157:LEU:HD13	2.47	0.41
6:E:191:SER:OG	6:E:192:ILE:N	2.53	0.41
11:J:111:MET:O	11:J:114:PRO:HD3	2.20	0.41
24:W:39:ALA:C	24:W:41:GLU:N	2.73	0.41
1:A:2769:C:H2'	1:A:2770:G:C5'	2.50	0.41
5:D:279:THR:HG22	5:D:280:VAL:O	2.21	0.41
1:A:2108:A:C2	1:A:2110:G:C8	3.08	0.41
15:N:155:HIS:ND1	15:N:158:ARG:NE	2.55	0.41
1:A:1851:G:O2'	1:A:1852:A:H5'	2.20	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.41
1:A:2388:C:O2'	1:A:2389:U:H5'	2.20	0.41
15:N:93:ARG:HG2	15:N:93:ARG:H	1.54	0.41
1:A:209:G:C6	1:A:210:U:N3	2.89	0.41
5:D:69:VAL:HA	5:D:70:PRO:HD3	1.95	0.41
8:G:172:PRO:HB3	38:G:6931:HOH:O	2.20	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.20	0.41
16:O:37:ARG:HD3	16:O:37:ARG:HA	1.84	0.41
1:A:596:C:H2'	1:A:597:A:C8	2.55	0.41
4:C:36:ASP:CB	4:C:85:ASP:H	2.32	0.41
4:C:42:VAL:HG11	4:C:75:GLY:O	2.21	0.41
38:A:3268:HOH:O	23:V:17:THR:CG2	2.69	0.41
5:D:238:ASN:HD22	5:D:240:GLY:N	2.14	0.41
1:A:638:C:H2'	1:A:639:A:H8	1.85	0.41
1:A:1513:C:O2'	1:A:1514:C:H5'	2.19	0.41
1:A:710:G:OP1	17:P:24:ALA:HB3	2.20	0.41
26:Y:12:ILE:HG23	26:Y:36:HIS:CG	2.55	0.41
1:A:1217:G:H2'	1:A:1218:U:C6	2.55	0.41
1:A:1506:U:H6	1:A:1506:U:H5'	1.86	0.41
14:M:93:VAL:HG12	14:M:97:VAL:HG23	2.03	0.41
13:L:118:ALA:O	13:L:120:ARG:N	2.54	0.41
1:A:590:A:C2'	1:A:591:A:H5'	2.51	0.41
17:P:80:ASP:OD1	17:P:81:PHE:N	2.53	0.41
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.88	0.41
22:U:71:VAL:CG1	22:U:72:ILE:N	2.83	0.41
15:N:74:ARG:HD3	15:N:88:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:87:MET:HE1	38:N:8531:HOH:O	2.21	0.41
1:A:292:G:N2	38:A:5231:HOH:O	2.30	0.41
1:A:2346:C:O3'	7:F:52:THR:HG23	2.20	0.41
12:K:6:PHE:O	12:K:8:ALA:N	2.53	0.41
16:O:164:ASP:OD1	16:O:164:ASP:C	2.58	0.41
7:F:101:THR:HG22	7:F:101:THR:O	2.20	0.41
5:D:280:VAL:HG11	5:D:335:ASN:H	1.86	0.41
5:D:280:VAL:HG13	5:D:333:GLU:O	2.20	0.41
1:A:2547:C:H2'	1:A:2548:C:C6	2.56	0.41
1:A:736:A:H2'	1:A:737:A:O4'	2.20	0.41
1:A:920:C:H5'	1:A:921:G:C4	2.55	0.41
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.41
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.56	0.41
1:A:1600:G:H8	1:A:1600:G:OP2	2.03	0.41
25:X:29:VAL:O	25:X:30:ASN:HB2	2.21	0.41
1:A:1749:U:O2	1:A:1751:G:C8	2.74	0.41
7:F:163:VAL:HA	38:F:6326:HOH:O	2.20	0.41
1:A:1161:A:O5'	1:A:1161:A:C8	2.73	0.41
11:J:26:LYS:CD	11:J:28:ILE:HB	2.51	0.41
1:A:2460:A:OP1	31:4:60:LYS:HB2	2.21	0.41
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.85	0.41
24:W:27:LEU:HA	24:W:49:LEU:HD13	2.02	0.41
10:I:65:THR:O	10:I:69:ARG:HB2	2.20	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
7:F:60:GLU:O	7:F:62:ASP:N	2.53	0.41
9:H:4:VAL:HG13	9:H:76:PHE:CD1	2.55	0.41
1:A:2880:A:H2'	1:A:2881:C:O4'	2.20	0.41
1:A:1023:C:O2'	1:A:1024:G:H5'	2.21	0.41
1:A:1795:G:H2'	1:A:1796:A:O4'	2.21	0.41
1:A:1059:G:C8	1:A:2491:G:H4'	2.55	0.41
8:G:158:ASP:OD1	8:G:160:ARG:HB2	2.20	0.41
1:A:840:U:C2	1:A:2648:U:O4	2.73	0.41
6:E:40:ALA:CB	6:E:100:LEU:HD12	2.51	0.41
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.56	0.41
6:E:114:ALA:HB1	6:E:223:LEU:HB3	2.02	0.41
7:F:35:ALA:C	7:F:37:ALA:N	2.74	0.41
5:D:144:THR:CG2	5:D:145:HIS:N	2.83	0.41
7:F:94:ALA:O	7:F:95:THR:O	2.38	0.41
30:3:36:ASN:HB3	30:3:39:ARG:NE	2.36	0.41
1:A:2651:C:H2'	1:A:2652:U:O4'	2.20	0.41
5:D:168:GLY:H	5:D:174:ARG:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:U:O2'	29:2:16:HIS:CD2	2.73	0.41
29:2:5:THR:N	29:2:6:PRO:HD2	2.35	0.41
1:A:1616:A:H5"	1:A:1617:C:OP1	2.20	0.41
14:M:72:ASN:OD1	14:M:75:LEU:HD12	2.21	0.41
1:A:1767:A:O2'	1:A:1768:C:H5'	2.21	0.41
1:A:2445:U:H2'	1:A:2446:G:H8	1.84	0.41
1:A:731:U:OP2	38:A:3515:HOH:O	2.22	0.41
1:A:1383:U:H2'	1:A:1384:C:C6	2.56	0.41
1:A:697:G:H4'	1:A:730:G:O3'	2.21	0.41
8:G:149:GLU:OE1	8:G:168:ILE:HG12	2.21	0.41
25:X:130:HIS:O	25:X:136:GLY:HA3	2.20	0.41
27:Z:109:LEU:HA	38:Z:8576:HOH:O	2.21	0.41
1:A:333:G:O2'	1:A:334:G:H5'	2.21	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
1:A:1352:A:N1	6:E:48:SER:HB3	2.35	0.41
1:A:328:U:O4'	6:E:202:THR:HG22	2.20	0.41
1:A:1916:C:C2	1:A:1924:A:C2	3.08	0.41
1:A:2134:G:C6	1:A:2258:A:C8	3.09	0.41
11:J:132:PHE:O	11:J:133:ILE:HD13	2.20	0.41
28:1:39:CYS:SG	28:1:47:LEU:CD2	2.85	0.41
24:W:12:THR:HG23	24:W:14:ALA:H	1.85	0.41
18:Q:115:SER:HG	18:Q:118:GLN:HG3	1.83	0.41
26:Y:78:GLU:CG	26:Y:79:GLU:N	2.72	0.41
25:X:154:ARG:HE	25:X:154:ARG:HB3	1.64	0.41
1:A:1603:A:H5'	1:A:1605:G:C4'	2.49	0.41
16:O:110:THR:HB	16:O:113:SER:OG	2.20	0.41
11:J:1:LYS:HA	11:J:2:PRO:HD3	1.81	0.41
7:F:146:LYS:HE2	16:O:107:ASN:ND2	2.36	0.41
1:A:1477:C:H5'	1:A:1868:G:C5'	2.50	0.41
29:2:29:THR:O	29:2:32:LYS:NZ	2.53	0.41
29:2:31:LYS:O	29:2:32:LYS:HB2	2.21	0.41
1:A:316:A:N3	1:A:336:G:O2'	2.49	0.41
1:A:1855:G:O6	4:C:141:PRO:HG2	2.21	0.41
1:A:920:C:H4'	1:A:921:G:N2	2.35	0.41
22:U:40:VAL:HA	22:U:119:ALA:O	2.21	0.41
1:A:688:A:H62	14:M:111:ALA:HB2	1.85	0.41
1:A:397:A:P	38:A:3833:HOH:O	2.78	0.41
27:Z:116:LEU:HD23	27:Z:116:LEU:HA	1.82	0.41
1:A:1880:C:C2	1:A:1881:A:C8	3.09	0.41
15:N:43:PRO:HG3	15:N:62:VAL:HG21	2.03	0.41
28:1:46:LYS:O	28:1:57:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.21	0.41
7:F:99:ASP:HB2	7:F:103:ASN:H	1.86	0.41
13:L:37:TYR:CE2	13:L:45:PRO:HA	2.55	0.41
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.50	0.41
25:X:122:ARG:HG2	25:X:122:ARG:NH1	2.27	0.41
25:X:122:ARG:CG	25:X:122:ARG:NH1	2.83	0.41
1:A:1166:A:H2'	1:A:1166:A:N3	2.35	0.41
1:A:2506:A:H1'	38:A:5515:HOH:O	2.21	0.41
1:A:951:A:O2'	1:A:952:G:H5'	2.21	0.41
31:4:42:ARG:HH11	31:4:42:ARG:CG	2.33	0.41
7:F:57:THR:HA	7:F:63:ILE:HA	2.01	0.41
1:A:1162:G:N3	1:A:1162:G:H2'	2.36	0.41
1:A:154:C:O2'	1:A:155:C:H5'	2.20	0.41
4:C:217:ARG:NH1	4:C:217:ARG:CG	2.84	0.41
1:A:2257:G:H4'	1:A:2259:C:C2	2.56	0.41
1:A:1218:U:H2'	1:A:1219:U:H6	1.85	0.41
1:A:1706:G:C6	1:A:1707:G:C6	3.08	0.41
4:C:165:THR:CG2	4:C:165:THR:O	2.69	0.41
1:A:2834:G:C4	1:A:2847:G:N2	2.89	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.86	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:1969:A:N7	1:A:1970:G:C6	2.88	0.41
1:A:1463:A:H2'	1:A:1464:U:C6	2.56	0.41
1:A:861:A:H2'	1:A:862:U:C6	2.55	0.41
1:A:1566:C:O2'	1:A:1567:A:H5'	2.21	0.41
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.41
1:A:2839:C:O5'	1:A:2839:C:H6	2.04	0.41
1:A:151:A:C2	1:A:442:A:C8	3.09	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.20	0.41
4:C:231:LYS:O	4:C:232:ARG:HB3	2.21	0.41
1:A:2501:G:H1'	38:A:4029:HOH:O	2.20	0.41
5:D:14:GLY:HA3	38:D:8609:HOH:O	2.20	0.41
11:J:129:ASN:HD22	11:J:129:ASN:N	2.18	0.41
9:H:115:VAL:O	9:H:118:LEU:N	2.54	0.41
8:G:154:ILE:HG13	8:G:156:ASP:OD1	2.21	0.41
1:A:2398:A:H2'	1:A:2399:G:O4'	2.21	0.41
1:A:123:U:O2'	1:A:124:C:H5'	2.21	0.41
1:A:1003:U:O2	11:J:90:PHE:CZ	2.73	0.41
6:E:118:THR:HG22	6:E:137:PRO:HB3	2.03	0.41
1:A:21:G:H5"	20:S:1:GLY:O	2.21	0.41
38:A:9692:HOH:O	14:M:4:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B:8386:HOH:O	19:R:25:PRO:HB3	2.20	0.41
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.86	0.41
1:A:2462:G:O6	31:4:61:PRO:HG3	2.20	0.41
38:B:8525:HOH:O	16:O:107:ASN:HB3	2.21	0.41
17:P:35:LYS:HD3	38:P:3360:HOH:O	2.20	0.41
4:C:179:MET:HG2	4:C:186:TRP:CG	2.56	0.41
15:N:169:ARG:NH1	38:N:8576:HOH:O	2.54	0.41
7:F:67:ASP:N	7:F:67:ASP:OD1	2.54	0.41
1:A:1121:G:H21	1:A:1248:A:C4'	2.34	0.41
14:M:125:PHE:CE1	14:M:140:VAL:HG13	2.56	0.41
19:R:40:HIS:CE1	19:R:94:GLN:HA	2.56	0.41
1:A:2786:G:O2'	1:A:2787:C:H5'	2.21	0.41
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.54	0.41
21:T:10:VAL:HG11	24:W:36:ALA:HA	2.02	0.41
1:A:1656:A:H2'	1:A:1657:A:O4'	2.21	0.41
1:A:1345:A:H2'	1:A:1346:U:C6	2.56	0.41
1:A:453:A:H4'	1:A:455:A:N7	2.36	0.41
22:U:14:ALA:HA	22:U:15:PRO:HD3	1.93	0.41
1:A:658:C:O2'	1:A:662:U:OP1	2.34	0.41
6:E:127:ARG:NH2	6:E:225:PRO:O	2.53	0.40
20:S:106:GLY:HA2	20:S:109:MET:CE	2.48	0.40
1:A:506:G:N2	1:A:509:A:C5'	2.71	0.40
11:J:26:LYS:HD2	11:J:28:ILE:HB	2.03	0.40
11:J:62:GLU:OE2	11:J:66:VAL:CG2	2.69	0.40
5:D:60:SER:C	5:D:62:ARG:H	2.23	0.40
1:A:1191:A:N1	1:A:1206:U:O4	2.54	0.40
5:D:265:LEU:CD2	5:D:316:ARG:HD3	2.51	0.40
11:J:113:ALA:N	11:J:114:PRO:CD	2.84	0.40
15:N:97:ILE:CD1	15:N:127:LYS:HD2	2.51	0.40
22:U:55:PHE:O	22:U:56:ALA:C	2.59	0.40
1:A:2090:G:H2'	1:A:2091:G:C8	2.56	0.40
1:A:2588:G:H2'	1:A:2589:U:H4'	2.03	0.40
8:G:132:THR:HB	38:G:2227:HOH:O	2.21	0.40
1:A:78:G:C6	1:A:79:G:C6	3.09	0.40
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.52	0.40
7:F:168:SER:OG	7:F:168:SER:O	2.35	0.40
6:E:120:ASP:OD1	6:E:120:ASP:C	2.60	0.40
1:A:1861:C:H4'	4:C:6:GLY:O	2.21	0.40
17:P:49:GLU:HB2	17:P:70:LEU:HD12	2.03	0.40
1:A:1611:G:O2'	1:A:1612:A:H5'	2.22	0.40
1:A:164:G:C6	1:A:165:A:C5	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2846:C:OP1	5:D:158:LYS:HD3	2.21	0.40
1:A:724:G:O2'	1:A:725:C:H5'	2.21	0.40
1:A:243:A:H61	1:A:269:G:H1'	1.86	0.40
5:D:222:LYS:HE2	38:D:8547:HOH:O	2.21	0.40
1:A:2047:C:H5'	38:A:9316:HOH:O	2.21	0.40
1:A:593:A:N7	38:A:3887:HOH:O	2.53	0.40
1:A:1886:A:C5'	38:1:8405:HOH:O	2.69	0.40
25:X:151:GLU:O	25:X:154:ARG:HB3	2.20	0.40
2:B:3050:G:OP1	16:O:147:ILE:CD1	2.68	0.40
11:J:14:TYR:HB2	38:J:8353:HOH:O	2.21	0.40
1:A:2620:U:O4	36:5:76:PPU:CA	2.69	0.40
5:D:265:LEU:HD21	5:D:316:ARG:HD3	2.02	0.40
1:A:2590:U:H2'	1:A:2591:C:H5'	2.03	0.40
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.83	0.40
1:A:2004:U:H2'	1:A:2005:G:OP1	2.21	0.40
1:A:1594:C:C2	1:A:1601:G:C2	3.09	0.40
1:A:1850:U:H2'	1:A:1851:G:C8	2.56	0.40
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.51	0.40
26:Y:14:LEU:HD12	26:Y:67:PRO:O	2.21	0.40
1:A:329:A:C5	1:A:347:A:C2	3.10	0.40
1:A:88:G:H2'	1:A:89:G:C8	2.55	0.40
38:A:8866:HOH:O	29:2:1:THR:HA	2.20	0.40
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.85	0.40
1:A:585:C:H6	38:A:5555:HOH:O	2.04	0.40
6:E:85:LYS:CE	38:E:8328:HOH:O	2.67	0.40
2:B:3078:G:O2'	2:B:3079:U:OP2	2.39	0.40
1:A:587:A:H5"	38:A:6745:HOH:O	2.19	0.40
1:A:1498:G:O2'	1:A:1499:U:H5'	2.21	0.40
9:H:66:LEU:HD12	9:H:66:LEU:HA	1.85	0.40
1:A:2649:A:H5'	1:A:2649:A:H8	1.86	0.40
1:A:2364:A:H5"	19:R:15:LYS:HD3	2.03	0.40
15:N:137:ASP:HA	15:N:142:LYS:HE3	2.03	0.40
1:A:958:G:O2'	1:A:959:C:H5'	2.21	0.40
1:A:2868:C:H2'	1:A:2869:G:O4'	2.21	0.40
11:J:31:PHE:HE2	11:J:87:LYS:O	2.04	0.40
7:F:48:MET:HA	7:F:49:PRO:HD3	1.81	0.40
15:N:69:LYS:HD3	15:N:124:GLY:O	2.21	0.40
11:J:35:ASN:ND2	11:J:79:ALA:O	2.54	0.40
27:Z:144:ARG:NH1	38:Z:8581:HOH:O	2.51	0.40
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.40
18:Q:143:ALA:CA	38:Q:197:HOH:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:U:OP2	1:A:139:C:H5	2.04	0.40
2:B:3034:A:H2'	2:B:3035:C:O4'	2.21	0.40
1:A:1815:A:H4'	1:A:2751:C:O4'	2.22	0.40
1:A:2541:U:O2'	1:A:2542:C:H5'	2.21	0.40
38:A:3897:HOH:O	4:C:11:ARG:CZ	2.70	0.40
1:A:39:G:C2	1:A:444:C:C2	3.10	0.40
1:A:590:A:H2'	1:A:591:A:O4'	2.21	0.40
1:A:2355:G:H5"	1:A:2356:A:OP2	2.22	0.40
1:A:860:U:C2'	38:A:5151:HOH:O	2.69	0.40
22:U:101:LEU:HD13	22:U:112:LEU:HD11	2.03	0.40
1:A:1309:U:OP2	6:E:189:PRO:HA	2.21	0.40
14:M:107:LYS:HD2	14:M:124:ASP:OD2	2.21	0.40
7:F:128:LEU:N	38:F:5495:HOH:O	2.54	0.40
16:O:5:ARG:HG3	19:R:18:PRO:HB3	2.02	0.40
16:O:37:ARG:CZ	38:O:8534:HOH:O	2.69	0.40
1:A:2533:C:O2'	1:A:2534:C:H5'	2.21	0.40
27:Z:189:ASN:ND2	27:Z:189:ASN:C	2.70	0.40
29:2:25:LYS:CD	30:3:49:GLU:H	2.33	0.40
5:D:16:ARG:NH1	38:D:8617:HOH:O	2.53	0.40
5:D:279:THR:OG1	5:D:290:VAL:HB	2.22	0.40
1:A:1972:U:H2'	1:A:1973:A:C5'	2.49	0.40
1:A:220:C:C4'	38:A:5208:HOH:O	2.69	0.40
1:A:2011:A:H4'	1:A:2012:U:O5'	2.22	0.40
17:P:59:VAL:CG2	17:P:111:VAL:HG23	2.52	0.40
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.56	0.40
1:A:2255:A:H2'	1:A:2256:G:O4'	2.21	0.40
5:D:224:LYS:O	5:D:227:HIS:HB2	2.22	0.40
17:P:63:LYS:HG3	17:P:80:ASP:O	2.22	0.40
1:A:269:G:C2	1:A:270:U:O4	2.73	0.40
6:E:123:LEU:HA	6:E:123:LEU:HD23	1.92	0.40
13:L:66:ARG:HG2	13:L:66:ARG:HH11	1.86	0.40
1:A:690:G:H4'	1:A:741:C:O2	2.22	0.40
1:A:2821:C:H4'	5:D:116:PRO:HB3	2.03	0.40
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.51	0.40
1:A:1816:C:H2'	1:A:1817:U:O4'	2.21	0.40
1:A:2481:G:C3'	1:A:2482:G:H5"	2.51	0.40
6:E:80:VAL:HA	6:E:81:PRO:HD3	1.94	0.40
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.40
6:E:3:ALA:N	6:E:16:VAL:O	2.53	0.40
1:A:2123:A:P	15:N:89:ASN:ND2	2.95	0.40
2:B:3058:G:H3'	2:B:3059:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:51:ARG:HA	38:F:7636:HOH:O	2.22	0.40
10:I:23:ILE:CD1	10:I:67:LEU:HD23	2.41	0.40
1:A:2269:C:C2'	1:A:2270:G:H5'	2.51	0.40
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.40
31:4:70:ARG:HD3	38:4:8537:HOH:O	2.21	0.40
8:G:108:LEU:HD11	8:G:164:ASP:HB2	2.04	0.40
1:A:299:U:C5'	38:A:6794:HOH:O	2.60	0.40
16:O:167:ASP:O	16:O:168:LEU:HD23	2.22	0.40
1:A:2348:C:C5'	7:F:22:VAL:HG21	2.51	0.40
11:J:73:GLN:OE1	11:J:73:GLN:CA	2.69	0.40
1:A:853:C:H2'	1:A:854:G:O4'	2.21	0.40
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.85	0.40
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.85	0.40
14:M:72:ASN:HB2	38:M:8585:HOH:O	2.21	0.40
15:N:77:PHE:O	15:N:77:PHE:CD1	2.75	0.40
6:E:7:ASP:O	6:E:9:ASP:N	2.55	0.40
1:A:382:U:C5	1:A:406:G:C2	3.09	0.40
5:D:215:VAL:HA	5:D:220:VAL:HG22	2.02	0.40
1:A:101:C:O2'	1:A:102:A:H5'	2.21	0.40
1:A:2554:U:C6	1:A:2577:A:N6	2.90	0.40
1:A:1316:G:H1'	1:A:1340:G:N2	2.37	0.40
38:L:1387:HOH:O	23:V:20:MET:HE1	2.22	0.40
16:O:114:LYS:O	16:O:117:ALA:HB3	2.21	0.40
1:A:1252:A:H2'	1:A:1253:C:O4'	2.21	0.40
1:A:1215:A:O3'	1:A:1216:G:C4'	2.69	0.40
1:A:953:G:H2'	38:A:7145:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	C	235/239 (98%)	202 (86%)	29 (12%)	4 (2%)	11 44
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	7 34
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	39 79
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	1 4
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	30 71
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	7 32
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4 19
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	5 24
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	4 22
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	13 48
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	26 68
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	34 75
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	3 18
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100 100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	26 68
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	5 25
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	26 68
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100 100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100 100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100 100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5 25
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	15 52
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	4 20
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100 100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	6 29
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
30	3	42/48 (88%)	42 (100%)	0	0	100 100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	8 36
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	10 41

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
7	F	173	GLU
9	H	101	ALA
11	J	162	SER
14	M	80	ASP
16	O	154	LEU
16	O	162	ASP
16	O	164	ASP
16	O	183	ASP
26	Y	87	ALA
4	C	34	ASP
5	D	34	GLY
5	D	169	GLY
6	E	8	LEU
7	F	36	ASN
11	J	138	PRO
11	J	164	ALA
12	K	5	GLU
12	K	143	LYS
13	L	119	GLN
16	O	167	ASP
18	Q	116	SER
19	R	89	ALA
24	W	43	PRO
25	X	77	ALA
28	1	81	LYS
31	4	57	GLY
4	C	132	ASP
5	D	184	ASP
7	F	16	PRO
7	F	20	LYS
7	F	61	PHE
7	F	171	ASP
8	G	44	GLY
11	J	40	PRO
12	K	76	ASP
15	N	140	ALA
16	O	181	ASP
25	X	49	ASN
26	Y	77	PHE

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Mol	Chain	Res	Type
31	4	56	PRO
4	C	62	ASP
5	D	107	SER
7	F	11	HIS
7	F	96	SER
7	F	170	TYR
10	I	72	ASP
13	L	126	SER
26	Y	78	GLU
5	D	2	GLN
5	D	185	GLY
9	H	64	PRO
12	K	7	ASP
12	K	50	GLU
16	O	68	GLU
16	O	155	GLU
4	C	37	VAL
9	H	61	MET
19	R	18	PRO
19	R	54	PRO
24	W	40	PRO
11	J	72	VAL
20	S	106	GLY
28	1	41	VAL
5	D	5	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	C	179/181 (99%)	167 (93%)	12 (7%)	20 56
5	D	282/282 (100%)	264 (94%)	18 (6%)	22 58
6	E	193/193 (100%)	176 (91%)	17 (9%)	12 41
7	F	117/147 (80%)	107 (92%)	10 (8%)	13 43
8	G	152/155 (98%)	148 (97%)	4 (3%)	54 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	H	92/92 (100%)	91 (99%)	1 (1%)	80 94
10	I	27/283 (10%)	27 (100%)	0	100 100
11	J	122/122 (100%)	110 (90%)	12 (10%)	10 35
12	K	118/121 (98%)	107 (91%)	11 (9%)	11 38
13	L	106/106 (100%)	103 (97%)	3 (3%)	51 83
14	M	112/126 (89%)	108 (96%)	4 (4%)	42 78
15	N	166/166 (100%)	157 (95%)	9 (5%)	27 65
16	O	149/149 (100%)	143 (96%)	6 (4%)	38 75
17	P	93/93 (100%)	89 (96%)	4 (4%)	35 74
18	Q	113/116 (97%)	110 (97%)	3 (3%)	52 84
19	R	79/79 (100%)	75 (95%)	4 (5%)	29 67
20	S	117/121 (97%)	113 (97%)	4 (3%)	44 80
21	T	71/73 (97%)	70 (99%)	1 (1%)	74 92
22	U	105/105 (100%)	102 (97%)	3 (3%)	50 83
23	V	44/52 (85%)	42 (96%)	2 (4%)	34 72
24	W	51/56 (91%)	49 (96%)	2 (4%)	39 76
25	X	130/130 (100%)	121 (93%)	9 (7%)	19 55
26	Y	66/73 (90%)	61 (92%)	5 (8%)	16 49
27	Z	120/195 (62%)	112 (93%)	8 (7%)	20 56
28	1	56/56 (100%)	50 (89%)	6 (11%)	8 29
29	2	46/46 (100%)	46 (100%)	0	100 100
30	3	42/44 (96%)	41 (98%)	1 (2%)	57 86
31	4	79/79 (100%)	73 (92%)	6 (8%)	16 49
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	27 64

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU

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Mol	Chain	Res	Type
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	195	ARG
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	264	GLU
5	D	304	PRO
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	67	GLN
6	E	76	ARG
6	E	91	PRO
6	E	94	THR
6	E	101	ASP
6	E	115	LEU
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU
6	E	246	ARG
7	F	24	HIS

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Mol	Chain	Res	Type
7	F	50	VAL
7	F	61	PHE
7	F	99	ASP
7	F	100	ASP
7	F	131	THR
7	F	133	ASN
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	54	ASP
8	G	102	VAL
8	G	164	ASP
9	H	12	LEU
11	J	1	LYS
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	85	ILE
11	J	86	ARG
11	J	94	ARG
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	52	GLN
12	K	74	ARG
12	K	76	ASP
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	125	SER
12	K	127	ILE
12	K	131	THR
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	30	ARG
14	M	35	ARG

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Mol	Chain	Res	Type
14	M	80	ASP
14	M	117	GLU
15	N	38	VAL
15	N	46	LEU
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	136	PRO
15	N	164	THR
16	O	26	LEU
16	O	47	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	28	ASP
17	P	98	LEU
17	P	111	VAL
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
20	S	132	ARG
21	T	10	VAL
22	U	39	ASN
22	U	48	VAL
22	U	73	HIS
23	V	9	CYS
23	V	32	CYS
24	W	43	PRO
24	W	65	ASP
25	X	4	LEU
25	X	35	VAL

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Mol	Chain	Res	Type
25	X	52	VAL
25	X	73	LEU
25	X	120	PRO
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	44	ASP
26	Y	52	PRO
26	Y	72	VAL
27	Z	154	ARG
27	Z	163	THR
27	Z	172	THR
27	Z	186	ARG
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
27	Z	235	GLU
28	1	11	THR
28	1	32	LYS
28	1	42	CYS
28	1	60	CYS
28	1	64	ILE
28	1	68	CYS
30	3	18	ASN
31	4	3	MET
31	4	14	CYS
31	4	42	ARG
31	4	56	PRO
31	4	65	THR
31	4	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	47	HIS
4	C	92	ASN
4	C	127	GLN
4	C	199	HIS
5	D	27	ASN

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Mol	Chain	Res	Type
5	D	145	HIS
5	D	221	GLN
5	D	238	ASN
5	D	256	GLN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	129	HIS
7	F	85	GLN
7	F	103	ASN
7	F	133	ASN
8	G	106	ASN
8	G	143	GLN
10	I	17	GLN
10	I	64	ASN
11	J	35	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	166	ASN
12	K	52	GLN
12	K	107	ASN
13	L	10	GLN
14	M	18	HIS
14	M	41	HIS
14	M	58	GLN
14	M	116	HIS
15	N	26	HIS
15	N	58	GLN
15	N	89	ASN
15	N	176	GLN
16	O	93	GLN
16	O	107	ASN
16	O	119	GLN
16	O	140	GLN
16	O	153	GLN

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Mol	Chain	Res	Type
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	123	GLN
21	T	53	ASN
22	U	39	ASN
22	U	73	HIS
23	V	39	ASN
23	V	48	ASN
24	W	60	GLN
25	X	27	HIS
25	X	28	HIS
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	18	ASN
30	3	37	HIS
30	3	41	HIS
30	3	45	ASN
31	4	30	GLN
31	4	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	36 (1%)
2	B	121/122 (99%)	18 (14%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	266 (9%)	41 (1%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A

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Mol	Chain	Res	Type
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G

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Mol	Chain	Res	Type
1	A	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C

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Mol	Chain	Res	Type
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1380	U
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A

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Mol	Chain	Res	Type
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2006	C
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A

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Mol	Chain	Res	Type
1	A	2422	U
1	A	2462	G
1	A	2466	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2590	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G

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Mol	Chain	Res	Type
1	A	2890	A
1	A	2896	A
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1237	U

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Mol	Chain	Res	Type
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1685	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2466	G
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3023	U
2	B	3024	U
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	PPU	5	76	3	30,40,41	2.25	12 (40%)	37,57,60	1.81	9 (24%)

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
36	PPU	5	76	3	-	0/21/43/44	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	C10-N6	-3.82	1.36	1.45
36	5	76	PPU	CE2-CD2	-3.79	1.31	1.38
36	5	76	PPU	CD1-CG	-3.54	1.31	1.38
36	5	76	PPU	C9-N6	-3.37	1.37	1.45
36	5	76	PPU	CE1-CD1	-3.04	1.33	1.38
36	5	76	PPU	O2'-C2'	-2.36	1.37	1.43
36	5	76	PPU	CA-N	2.25	1.61	1.49
36	5	76	PPU	C2-N1	2.26	1.38	1.33
36	5	76	PPU	CE1-CZ	2.40	1.43	1.38
36	5	76	PPU	O-C	3.62	1.30	1.23
36	5	76	PPU	C-N3'	4.20	1.43	1.34
36	5	76	PPU	CB-CG	4.69	1.62	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	76	PPU	C3'-N3'-C	-3.87	117.09	123.18
36	5	76	PPU	CG-CB-CA	-3.54	105.98	114.31
36	5	76	PPU	C2'-C1'-N9	-2.37	110.67	114.29
36	5	76	PPU	CE2-CZ-CE1	-2.05	116.86	120.20
36	5	76	PPU	CA-C-N3'	-2.01	110.28	115.94
36	5	76	PPU	CM-OC-CZ	2.96	124.45	117.51
36	5	76	PPU	C2-N1-C6	3.30	118.45	111.43
36	5	76	PPU	C2'-C3'-N3'	3.75	122.82	113.18
36	5	76	PPU	C2'-C3'-C4'	3.81	106.99	102.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	A	2754/2922 (94%)	0.12	75 (2%) 58 35	19, 45, 94, 144	0
2	B	122/122 (100%)	0.47	5 (4%) 41 22	33, 67, 97, 147	0
3	5	2/2 (100%)	2.18	1 (50%) 0 0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.61	26 (10%) 7 4	30, 62, 97, 109	0
5	D	337/337 (100%)	0.20	8 (2%) 62 39	22, 50, 77, 89	0
6	E	246/246 (100%)	0.07	5 (2%) 68 46	20, 44, 69, 78	0
7	F	140/176 (79%)	2.20	68 (48%) 0 0	65, 101, 122, 128	0
8	G	172/177 (97%)	0.97	21 (12%) 5 3	38, 62, 84, 89	0
9	H	119/119 (100%)	0.98	25 (21%) 1 1	51, 76, 99, 107	0
10	I	29/348 (8%)	2.42	18 (62%) 0 0	66, 87, 95, 99	0
11	J	156/167 (93%)	0.78	18 (11%) 6 3	35, 59, 82, 89	0
12	K	142/145 (97%)	0.09	2 (1%) 78 57	32, 44, 67, 78	0
13	L	132/132 (100%)	0.28	2 (1%) 76 56	33, 49, 75, 82	0
14	M	145/164 (88%)	1.32	40 (27%) 1 0	26, 79, 106, 111	0
15	N	194/194 (100%)	0.65	22 (11%) 7 3	28, 47, 106, 118	0
16	O	186/186 (100%)	1.13	34 (18%) 2 1	46, 73, 112, 125	0
17	P	115/115 (100%)	0.27	1 (0%) 85 69	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.58	9 (6%) 23 11	34, 53, 76, 85	0
19	R	95/95 (100%)	0.22	3 (3%) 51 30	36, 47, 63, 82	0
20	S	150/154 (97%)	0.01	0 100 100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.54	4 (4%) 33 18	44, 62, 82, 88	0
22	U	119/119 (100%)	0.85	15 (12%) 5 2	40, 55, 84, 104	0
23	V	53/66 (80%)	2.41	29 (54%) 0 0	77, 92, 100, 108	0
24	W	65/70 (92%)	1.46	21 (32%) 1 0	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	154/154 (100%)	0.09	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.73	10 (12%) 5 3	37, 53, 77, 91	0
27	Z	142/240 (59%)	0.19	7 (4%) 33 18	25, 41, 64, 82	0
28	1	73/73 (100%)	5.68	53 (72%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.23	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.90	7 (15%) 3 1	34, 63, 96, 105	0
31	4	92/92 (100%)	9.00	92 (100%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.59	621 (9%) 11 5	19, 52, 105, 147	0

All (621) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	29.1
28	1	11	THR	20.4
31	4	37	ASP	19.4
31	4	83	TRP	19.1
31	4	62	THR	18.4
28	1	26	VAL	16.1
31	4	11	CYS	15.6
31	4	1	MET	15.4
28	1	20	LEU	14.0
31	4	14	CYS	13.4
31	4	10	TYR	13.4
31	4	31	THR	13.4
28	1	15	GLY	13.3
31	4	91	GLN	13.2
31	4	20	HIS	13.2
31	4	38	ARG	13.1
28	1	12	GLY	13.0
31	4	39	GLN	12.9
31	4	71	CYS	12.7
31	4	76	LYS	12.5
31	4	33	MET	12.5
31	4	35	TRP	12.4
28	1	30	GLU	12.2
15	N	71	SER	12.2
31	4	36	ILE	12.0
24	W	1	THR	11.9
28	1	19	GLY	11.8
28	1	34	LYS	11.8

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Mol	Chain	Res	Type	RSRZ
31	4	78	HIS	11.6
31	4	44	SER	11.4
31	4	34	LYS	11.3
31	4	41	GLU	11.1
31	4	22	VAL	11.1
28	1	14	PHE	11.1
28	1	16	PRO	11.0
31	4	4	PRO	11.0
28	1	31	ILE	10.7
28	1	23	ARG	10.6
31	4	9	THR	10.6
31	4	85	ALA	10.6
31	4	59	ASP	10.6
31	4	65	THR	10.5
31	4	15	ASN	10.3
28	1	22	ILE	10.3
31	4	16	GLU	10.3
31	4	18	GLN	10.3
28	1	39	CYS	10.2
31	4	67	LEU	10.2
31	4	84	ARG	9.8
31	4	23	GLU	9.8
31	4	27	SER	9.8
31	4	86	GLY	9.7
28	1	35	LYS	9.7
15	N	89	ASN	9.7
31	4	74	CYS	9.7
31	4	68	LYS	9.7
28	1	28	ASP	9.7
31	4	17	HIS	9.7
28	1	44	PHE	9.5
31	4	3	MET	9.4
31	4	13	HIS	9.2
28	1	45	LYS	9.2
31	4	60	LYS	9.0
31	4	8	ASN	8.9
31	4	77	ALA	8.9
31	4	2	GLN	8.7
31	4	88	LEU	8.7
31	4	42	ARG	8.6
31	4	32	GLY	8.6
28	1	33	HIS	8.6

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Mol	Chain	Res	Type	RSRZ
31	4	21	GLU	8.3
31	4	61	PRO	8.3
28	1	24	VAL	8.2
31	4	81	GLU	8.2
7	F	69	ILE	8.1
7	F	57	THR	8.1
15	N	80	GLY	8.0
31	4	43	ASN	7.9
31	4	56	PRO	7.9
28	1	32	LYS	7.8
28	1	25	ARG	7.8
31	4	51	LYS	7.8
28	1	18	TYR	7.7
7	F	63	ILE	7.6
31	4	47	GLY	7.5
15	N	78	ASN	7.4
28	1	42	CYS	7.4
28	1	57	CYS	7.3
31	4	12	PRO	7.2
31	4	30	GLN	7.2
31	4	75	GLY	7.1
28	1	27	ALA	7.0
31	4	69	TYR	6.9
28	1	29	VAL	6.9
31	4	63	LYS	6.9
31	4	80	ARG	6.8
28	1	21	LYS	6.8
31	4	19	GLU	6.8
15	N	70	GLY	6.7
31	4	53	SER	6.7
31	4	6	ARG	6.7
28	1	10	ARG	6.6
10	I	27	ILE	6.6
31	4	45	GLY	6.5
28	1	43	GLY	6.5
1	A	735	C	6.4
2	B	3001	U	6.2
31	4	90	PHE	6.1
31	4	58	GLY	6.1
31	4	52	PHE	6.0
16	O	179	LEU	6.0
31	4	46	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
31	4	92	GLU	6.0
31	4	72	GLY	5.9
31	4	48	ASN	5.9
28	1	41	VAL	5.9
28	1	13	ARG	5.8
14	M	44	GLU	5.8
7	F	10	PHE	5.8
14	M	36	ASP	5.8
7	F	56	ARG	5.7
7	F	66	GLY	5.7
23	V	52	THR	5.7
14	M	60	GLU	5.7
15	N	83	SER	5.6
31	4	40	ARG	5.6
31	4	70	ARG	5.6
15	N	77	PHE	5.5
16	O	162	ASP	5.5
31	4	66	ASP	5.5
14	M	42	ASN	5.5
31	4	26	ARG	5.4
16	O	186	LEU	5.4
16	O	138	ASP	5.4
28	1	40	PRO	5.3
28	1	38	LYS	5.3
15	N	81	ARG	5.3
23	V	48	ASN	5.3
2	B	3025	G	5.3
23	V	54	THR	5.2
28	1	17	ARG	5.2
31	4	55	VAL	5.2
30	3	36	ASN	5.1
16	O	160	SER	5.1
11	J	83	PHE	5.1
31	4	89	GLU	5.1
16	O	184	ILE	5.1
22	U	119	ALA	5.0
28	1	37	HIS	5.0
10	I	23	ILE	5.0
15	N	90	ARG	5.0
7	F	88	LEU	4.9
7	F	27	ILE	4.9
7	F	87	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
24	W	39	ALA	4.9
31	4	87	ARG	4.8
31	4	49	ASP	4.8
23	V	51	TRP	4.8
14	M	133	VAL	4.8
23	V	9	CYS	4.8
30	3	39	ARG	4.8
15	N	72	SER	4.8
23	V	55	ALA	4.8
1	A	1173	A	4.8
31	4	28	GLY	4.7
31	4	64	LYS	4.7
7	F	64	ARG	4.7
15	N	88	VAL	4.7
7	F	25	MET	4.7
31	4	29	ARG	4.6
28	1	79	VAL	4.6
15	N	75	THR	4.5
16	O	163	PHE	4.5
14	M	80	ASP	4.5
26	Y	88	GLU	4.5
14	M	46	LEU	4.5
1	A	1177	A	4.5
31	4	24	LYS	4.5
14	M	34	GLY	4.5
1	A	1171	A	4.5
15	N	74	ARG	4.4
31	4	73	GLU	4.4
7	F	75	LEU	4.4
16	O	167	ASP	4.4
28	1	53	GLY	4.4
28	1	47	LEU	4.4
31	4	5	ARG	4.4
28	1	58	GLY	4.4
7	F	90	LEU	4.4
15	N	82	ARG	4.3
31	4	79	LEU	4.3
1	A	1951	G	4.3
7	F	166	ILE	4.3
11	J	135	TRP	4.2
9	H	106	THR	4.2
8	G	45	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
7	F	61	PHE	4.2
28	1	55	TRP	4.2
23	V	53	ASP	4.2
16	O	147	ILE	4.2
28	1	36	LYS	4.2
14	M	47	GLY	4.2
14	M	45	PRO	4.1
15	N	73	ARG	4.1
31	4	50	GLY	4.1
4	C	37	VAL	4.1
21	T	81	ILE	4.1
1	A	1198	U	4.1
28	1	46	LYS	4.1
1	A	2237	G	4.1
16	O	159	TYR	4.0
31	4	7	PHE	4.0
7	F	47	GLN	4.0
7	F	86	THR	4.0
23	V	46	ALA	4.0
7	F	96	SER	4.0
19	R	95	GLU	4.0
23	V	6	CYS	4.0
1	A	1199	A	3.9
28	1	82	ALA	3.9
23	V	11	THR	3.9
7	F	134	LEU	3.9
10	I	26	MET	3.9
7	F	26	GLY	3.9
7	F	44	ILE	3.9
16	O	185	GLU	3.9
28	1	80	MET	3.9
28	1	59	HIS	3.9
1	A	1172	G	3.9
23	V	47	ARG	3.8
16	O	80	SER	3.8
7	F	18	ILE	3.8
16	O	78	MET	3.8
7	F	58	VAL	3.8
31	4	57	GLY	3.8
7	F	92	GLU	3.8
1	A	282	C	3.7
14	M	124	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
7	F	83	PHE	3.7
14	M	130	ARG	3.7
24	W	40	PRO	3.7
10	I	15	TRP	3.7
18	Q	110	ASP	3.7
18	Q	137	LEU	3.7
7	F	93	LEU	3.6
14	M	104	ASP	3.6
16	O	172	PHE	3.6
7	F	49	PRO	3.6
8	G	100	ASP	3.6
9	H	107	VAL	3.6
14	M	73	VAL	3.6
10	I	20	VAL	3.6
1	A	1175	G	3.6
7	F	171	ASP	3.5
23	V	39	ASN	3.5
15	N	87	MET	3.5
24	W	61	GLY	3.5
10	I	65	THR	3.5
3	5	74	C	3.5
4	C	82	VAL	3.5
4	C	36	ASP	3.5
9	H	19	ALA	3.5
2	B	3122	C	3.5
14	M	105	TYR	3.5
28	1	60	CYS	3.4
9	H	17	LEU	3.4
24	W	8	ILE	3.4
4	C	60	PHE	3.4
10	I	67	LEU	3.4
5	D	1	PRO	3.4
14	M	106	VAL	3.4
9	H	16	ALA	3.4
14	M	59	GLU	3.4
4	C	91	GLY	3.4
7	F	11	HIS	3.4
23	V	49	LEU	3.4
7	F	130	VAL	3.4
14	M	38	HIS	3.4
16	O	139	TRP	3.3
6	E	135	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
8	G	108	LEU	3.3
1	A	1181	A	3.3
4	C	38	ILE	3.3
7	F	170	TYR	3.3
23	V	43	GLY	3.3
24	W	37	GLY	3.3
11	J	139	ASP	3.3
11	J	146	TRP	3.3
23	V	50	GLU	3.3
10	I	71	LEU	3.3
28	1	56	MET	3.3
14	M	123	ASP	3.3
14	M	43	HIS	3.3
15	N	79	LYS	3.3
24	W	38	GLY	3.3
7	F	62	ASP	3.2
4	C	85	ASP	3.2
14	M	81	VAL	3.2
23	V	40	ALA	3.2
1	A	1947	G	3.2
7	F	84	LEU	3.2
22	U	116	ASP	3.2
27	Z	108	ASP	3.2
7	F	24	HIS	3.2
22	U	112	LEU	3.2
16	O	75	THR	3.2
7	F	65	GLU	3.2
1	A	1163	G	3.2
16	O	74	PRO	3.2
1	A	1182	C	3.2
10	I	66	LEU	3.1
24	W	3	LEU	3.1
9	H	44	SER	3.1
9	H	22	VAL	3.1
1	A	1948	G	3.1
9	H	26	THR	3.1
14	M	41	HIS	3.1
1	A	1190	G	3.1
4	C	237	GLY	3.1
7	F	68	PRO	3.1
11	J	36	ASN	3.1
16	O	158	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
16	O	127	LEU	3.0
1	A	1168	C	3.0
7	F	54	ALA	3.0
24	W	52	ALA	3.0
18	Q	116	SER	3.0
23	V	13	ILE	3.0
4	C	96	LEU	3.0
9	H	119	ARG	3.0
1	A	736	A	3.0
4	C	31	LYS	3.0
23	V	12	ASP	3.0
9	H	20	LEU	3.0
1	A	2344	G	3.0
8	G	22	VAL	3.0
14	M	140	VAL	3.0
1	A	2345	A	3.0
14	M	48	LYS	3.0
26	Y	82	GLU	3.0
23	V	36	CYS	3.0
22	U	37	GLN	3.0
26	Y	7	GLU	3.0
14	M	118	LEU	3.0
23	V	56	ARG	3.0
7	F	50	VAL	2.9
9	H	102	GLY	2.9
11	J	35	ASN	2.9
15	N	86	MET	2.9
30	3	35	ARG	2.9
1	A	1162	G	2.9
7	F	23	VAL	2.9
4	C	133	ARG	2.9
14	M	102	ASP	2.9
7	F	22	VAL	2.9
7	F	85	GLN	2.9
2	B	3002	U	2.9
1	A	2239	C	2.9
1	A	960	G	2.9
7	F	43	GLU	2.9
14	M	89	PHE	2.9
7	F	28	GLY	2.9
21	T	77	VAL	2.9
16	O	175	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
11	J	81	TYR	2.8
9	H	15	ASP	2.8
26	Y	80	GLU	2.8
4	C	84	VAL	2.8
8	G	131	LEU	2.8
7	F	45	THR	2.8
9	H	98	VAL	2.8
24	W	62	GLU	2.8
7	F	128	LEU	2.8
7	F	159	PRO	2.8
15	N	68	ARG	2.8
1	A	1525	G	2.8
7	F	67	ASP	2.8
31	4	25	VAL	2.8
26	Y	10	VAL	2.8
1	A	1000	C	2.7
10	I	68	GLU	2.7
23	V	29	THR	2.7
16	O	155	GLU	2.7
7	F	51	ARG	2.7
22	U	27	LEU	2.7
1	A	1202	A	2.7
4	C	80	LEU	2.7
24	W	2	VAL	2.7
1	A	280	C	2.7
1	A	2508	C	2.7
9	H	18	GLU	2.7
7	F	42	GLY	2.7
10	I	24	VAL	2.7
11	J	70	ARG	2.7
1	A	1929	G	2.7
1	A	1950	G	2.7
22	U	42	VAL	2.7
9	H	101	ALA	2.7
16	O	142	THR	2.6
30	3	37	HIS	2.6
1	A	1913	C	2.6
1	A	1200	A	2.6
7	F	17	ARG	2.6
15	N	76	ARG	2.6
16	O	178	THR	2.6
8	G	129	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
23	V	45	GLU	2.6
22	U	99	THR	2.6
27	Z	235	GLU	2.6
14	M	37	LYS	2.6
24	W	11	MET	2.6
4	C	62	ASP	2.6
24	W	41	GLU	2.6
4	C	64	ASP	2.6
30	3	48	ASP	2.6
18	Q	1	THR	2.6
9	H	90	GLU	2.6
11	J	32	ASP	2.6
1	A	1925	G	2.6
1	A	2250	G	2.6
14	M	69	ILE	2.5
28	1	62	TYR	2.5
1	A	2637	A	2.5
1	A	1167	G	2.5
1	A	2249	G	2.5
7	F	55	LYS	2.5
1	A	368	C	2.5
9	H	103	ALA	2.5
27	Z	98	GLN	2.5
23	V	33	SER	2.5
8	G	6	GLU	2.5
5	D	329	TYR	2.5
4	C	58	VAL	2.5
1	A	1165	G	2.5
1	A	1192	A	2.5
16	O	68	GLU	2.5
23	V	4	ARG	2.5
24	W	63	GLU	2.5
8	G	1	PRO	2.5
1	A	2238	A	2.5
7	F	71	ALA	2.5
22	U	80	GLU	2.5
24	W	59	ILE	2.5
22	U	117	ASP	2.5
23	V	22	VAL	2.5
7	F	80	ALA	2.4
16	O	81	ALA	2.4
1	A	130	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1204	C	2.4
8	G	43	ASP	2.4
27	Z	234	VAL	2.4
4	C	128	LEU	2.4
9	H	75	ILE	2.4
1	A	2433	A	2.4
9	H	49	PHE	2.4
22	U	40	VAL	2.4
5	D	117	GLU	2.4
11	J	114	PRO	2.4
11	J	142	VAL	2.4
21	T	49	VAL	2.4
31	4	54	LYS	2.4
14	M	120	LEU	2.4
4	C	112	PRO	2.4
7	F	89	PRO	2.4
16	O	157	PRO	2.4
10	I	69	ARG	2.4
1	A	806	A	2.4
7	F	73	VAL	2.4
1	A	1949	G	2.4
13	L	119	GLN	2.4
7	F	158	ASN	2.4
10	I	64	ASN	2.4
14	M	39	GLU	2.4
30	3	49	GLU	2.4
14	M	108	VAL	2.4
10	I	63	ARG	2.4
10	I	13	PRO	2.4
24	W	6	GLN	2.4
8	G	85	GLU	2.4
26	Y	85	VAL	2.4
7	F	70	GLY	2.3
7	F	102	GLY	2.3
23	V	44	ARG	2.3
18	Q	141	ILE	2.3
14	M	101	ASP	2.3
22	U	118	SER	2.3
1	A	2507	G	2.3
5	D	169	GLY	2.3
14	M	40	PHE	2.3
1	A	284	C	2.3

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Mol	Chain	Res	Type	RSRZ
8	G	95	VAL	2.3
4	C	129	LEU	2.3
7	F	81	GLU	2.3
9	H	100	ASP	2.3
1	A	1665	G	2.3
1	A	1971	G	2.3
4	C	99	ILE	2.3
1	A	999	C	2.3
16	O	83	LEU	2.3
26	Y	74	ALA	2.3
4	C	88	ILE	2.3
8	G	20	ILE	2.3
11	J	85	ILE	2.3
16	O	71	TRP	2.3
4	C	135	VAL	2.3
8	G	10	ASP	2.3
30	3	44	ARG	2.3
1	A	970	U	2.3
1	A	1166	A	2.3
23	V	41	ASP	2.3
21	T	45	TYR	2.3
19	R	75	ILE	2.3
1	A	1626	A	2.3
5	D	104	GLU	2.3
9	H	47	LEU	2.3
11	J	163	PRO	2.3
28	1	51	GLY	2.3
1	A	805	G	2.3
1	A	1195	G	2.3
17	P	51	TYR	2.3
23	V	8	TYR	2.2
24	W	4	HIS	2.2
24	W	45	ARG	2.2
16	O	115	VAL	2.2
23	V	10	GLY	2.2
8	G	87	PHE	2.2
24	W	7	GLU	2.2
27	Z	226	ILE	2.2
1	A	601	G	2.2
9	H	71	GLY	2.2
28	1	61	GLY	2.2
14	M	99	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
18	Q	120	ARG	2.2
9	H	28	ALA	2.2
24	W	46	ILE	2.2
28	1	54	ILE	2.2
1	A	2432	C	2.2
1	A	285	A	2.2
6	E	132	ASP	2.2
16	O	150	TYR	2.2
7	F	15	GLU	2.2
14	M	129	ALA	2.2
6	E	245	GLU	2.2
15	N	165	SER	2.2
6	E	101	ASP	2.2
11	J	84	ARG	2.2
24	W	9	ARG	2.2
8	G	118	ILE	2.2
26	Y	72	VAL	2.2
18	Q	77	ALA	2.2
4	C	34	ASP	2.2
4	C	65	ARG	2.2
18	Q	114	LEU	2.2
1	A	1184	C	2.1
1	A	1527	A	2.1
2	B	3023	U	2.1
16	O	151	ASP	2.1
26	Y	77	PHE	2.1
8	G	46	THR	2.1
1	A	1169	U	2.1
16	O	180	LEU	2.1
8	G	73	PHE	2.1
16	O	152	GLU	2.1
7	F	16	PRO	2.1
7	F	13	MET	2.1
6	E	244	ALA	2.1
1	A	370	G	2.1
1	A	2004	U	2.1
14	M	150	GLN	2.1
7	F	153	THR	2.1
12	K	8	ALA	2.1
7	F	104	PHE	2.1
4	C	110	SER	2.1
1	A	1170	U	2.1

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Mol	Chain	Res	Type	RSRZ
19	R	81	GLU	2.1
12	K	39	VAL	2.1
13	L	21	ALA	2.1
7	F	52	THR	2.1
10	I	28	GLU	2.1
18	Q	66	GLN	2.1
27	Z	97	LEU	2.1
1	A	579	G	2.1
8	G	39	ASP	2.1
10	I	72	ASP	2.1
15	N	152	ARG	2.1
4	C	111	SER	2.1
1	A	2252	A	2.1
7	F	79	MET	2.1
7	F	156	ARG	2.1
7	F	39	ASP	2.1
14	M	79	ASP	2.1
5	D	183	GLU	2.1
16	O	143	ARG	2.1
11	J	34	GLY	2.0
1	A	219	G	2.0
1	A	1197	G	2.0
22	U	115	GLU	2.0
9	H	99	THR	2.0
22	U	35	TYR	2.0
1	A	1189	A	2.0
1	A	1919	A	2.0
5	D	116	PRO	2.0
1	A	1914	C	2.0
8	G	98	GLU	2.0
22	U	33	GLU	2.0
22	U	49	GLU	2.0
10	I	12	ILE	2.0
11	J	59	ASN	2.0
14	M	35	ARG	2.0
28	1	49	ARG	2.0
8	G	124	VAL	2.0
11	J	79	ALA	2.0
5	D	181	ILE	2.0
27	Z	233	TYR	2.0
9	H	12	LEU	2.0
14	M	114	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	2253	G	2.0
1	A	804	C	2.0
8	G	5	LEU	2.0
11	J	69	ASN	2.0
26	Y	41	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	A	8332	1/1	0.80	0.45	111.27	68,68,68,68	0
34	NA	A	8371	1/1	0.53	0.60	32.79	54,54,54,54	0
34	NA	B	8383	1/1	0.69	0.94	27.54	77,77,77,77	0
34	NA	A	8303	1/1	0.84	0.36	27.43	51,51,51,51	0
34	NA	A	8356	1/1	0.85	0.81	27.34	57,57,57,57	0
34	NA	A	8364	1/1	0.89	0.33	25.97	54,54,54,54	0
34	NA	A	8382	1/1	0.48	0.52	21.69	79,79,79,79	0
34	NA	A	8374	1/1	0.82	0.66	20.98	60,60,60,60	0
34	NA	A	8378	1/1	0.84	0.55	19.39	52,52,52,52	0
34	NA	A	8335	1/1	0.90	0.26	14.67	57,57,57,57	0
34	NA	A	8365	1/1	0.55	0.56	14.66	46,46,46,46	0
34	NA	A	8372	1/1	0.66	0.54	14.24	80,80,80,80	0
34	NA	A	8321	1/1	0.94	0.42	14.01	48,48,48,48	0
34	NA	A	8361	1/1	0.94	0.46	11.79	62,62,62,62	0
34	NA	S	8386	1/1	0.62	0.53	11.25	70,70,70,70	0
34	NA	A	8325	1/1	0.95	0.25	11.01	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	A	8323	1/1	0.94	0.22	9.06	45,45,45,45	0
34	NA	A	8366	1/1	0.90	0.43	8.50	47,47,47,47	0
35	CL	A	8515	1/1	0.91	0.31	8.31	68,68,68,68	0
34	NA	A	8326	1/1	0.76	0.65	8.26	60,60,60,60	0
34	NA	A	8379	1/1	0.96	0.23	7.88	48,48,48,48	0
35	CL	D	8519	1/1	0.81	0.40	7.14	70,70,70,70	0
32	MG	A	8064	1/1	0.88	0.24	6.36	24,24,24,24	0
34	NA	A	8368	1/1	0.79	0.24	6.34	56,56,56,56	0
35	CL	M	8510	1/1	0.41	0.43	5.86	97,97,97,97	0
34	NA	A	8327	1/1	0.77	0.20	5.37	40,40,40,40	0
34	NA	A	8320	1/1	0.95	0.23	5.34	42,42,42,42	0
33	K	A	8201	1/1	0.97	0.24	5.07	71,71,71,71	0
35	CL	A	8505	1/1	0.85	0.26	4.19	74,74,74,74	0
34	NA	A	8362	1/1	0.92	0.20	3.52	74,74,74,74	0
34	NA	A	8373	1/1	0.70	0.27	3.50	54,54,54,54	0
32	MG	A	8060	1/1	0.95	0.18	3.29	44,44,44,44	0
32	MG	A	8053	1/1	0.91	0.19	3.28	41,41,41,41	0
32	MG	A	8112	1/1	0.90	0.20	3.10	57,57,57,57	0
34	NA	A	8353	1/1	0.88	0.22	2.56	53,53,53,53	0
36	PPU	5	76	37/38	0.91	0.27	2.22	60,64,69,71	0
34	NA	A	8350	1/1	0.94	0.16	1.96	37,37,37,37	0
35	CL	K	8521	1/1	0.93	0.24	1.72	60,60,60,60	0
34	NA	S	8337	1/1	0.65	0.26	1.61	52,52,52,52	0
35	CL	P	8508	1/1	0.98	0.31	1.23	82,82,82,82	0
34	NA	A	8376	1/1	0.98	0.17	0.99	79,79,79,79	0
34	NA	A	8324	1/1	0.92	0.25	0.92	51,51,51,51	0
32	MG	1	8105	1/1	0.59	0.73	0.90	58,58,58,58	0
32	MG	A	8044	1/1	0.95	0.15	0.30	54,54,54,54	0
34	NA	A	8381	1/1	0.73	0.16	0.21	46,46,46,46	0
34	NA	J	8309	1/1	0.92	0.18	-0.09	42,42,42,42	0
34	NA	R	8348	1/1	0.69	0.21	-0.14	57,57,57,57	0
34	NA	K	8346	1/1	0.86	0.19	-0.29	37,37,37,37	0
32	MG	Z	8109	1/1	0.89	0.15	-0.34	38,38,38,38	0
33	K	A	8202	1/1	0.93	0.15	-0.37	89,89,89,89	0
34	NA	A	8331	1/1	0.92	0.15	-0.43	76,76,76,76	0
32	MG	A	8047	1/1	0.91	0.16	-0.64	31,31,31,31	0
35	CL	N	8518	1/1	0.90	0.18	-0.66	46,46,46,46	0
32	MG	A	8057	1/1	0.94	0.17	-0.86	46,46,46,46	0
34	NA	M	8380	1/1	0.93	0.17	-0.93	65,65,65,65	0
32	MG	A	8086	1/1	0.99	0.09	-1.14	49,49,49,49	0
32	MG	D	8055	1/1	0.82	0.15	-1.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8056	1/1	0.94	0.15	-1.28	56,56,56,56	0
34	NA	E	8304	1/1	0.91	0.14	-1.35	25,25,25,25	0
35	CL	A	8512	1/1	0.97	0.11	-1.48	31,31,31,31	0
32	MG	4	8078	1/1	0.93	0.19	-1.53	74,74,74,74	0
32	MG	C	8065	1/1	0.96	0.12	-1.57	68,68,68,68	0
32	MG	A	8062	1/1	0.94	0.14	-1.70	49,49,49,49	0
32	MG	U	8073	1/1	0.84	0.21	-1.73	48,48,48,48	0
37	CD	1	8403	1/1	0.73	0.31	-1.78	203,203,203,203	0
34	NA	A	8317	1/1	0.95	0.06	-2.06	32,32,32,32	0
34	NA	C	8345	1/1	0.95	0.12	-2.11	35,35,35,35	0
32	MG	A	8008	1/1	0.94	0.08	-2.18	42,42,42,42	0
34	NA	U	8343	1/1	0.95	0.09	-2.21	27,27,27,27	0
32	MG	A	8091	1/1	0.96	0.10	-2.30	67,67,67,67	0
34	NA	A	8314	1/1	0.95	0.10	-2.42	43,43,43,43	0
34	NA	N	8347	1/1	0.90	0.12	-2.47	24,24,24,24	0
37	CD	2	8402	1/1	0.99	0.07	-2.74	57,57,57,57	0
34	NA	A	8333	1/1	0.93	0.08	-3.04	33,33,33,33	0
32	MG	A	8107	1/1	0.98	0.06	-3.10	36,36,36,36	0
32	MG	A	8033	1/1	0.97	0.12	-3.11	25,25,25,25	0
32	MG	A	8027	1/1	0.93	0.05	-3.34	54,54,54,54	0
32	MG	A	8032	1/1	0.97	0.06	-3.43	34,34,34,34	0
34	NA	A	8344	1/1	0.94	0.07	-3.51	27,27,27,27	0
37	CD	V	8401	1/1	0.96	0.15	-3.52	129,129,129,129	0
32	MG	A	8074	1/1	0.97	0.05	-3.52	42,42,42,42	0
32	MG	A	8012	1/1	0.97	0.10	-3.53	44,44,44,44	0
34	NA	A	8338	1/1	0.96	0.09	-3.86	44,44,44,44	0
32	MG	A	8067	1/1	0.96	0.14	-3.97	41,41,41,41	0
32	MG	A	8077	1/1	0.94	0.06	-4.24	32,32,32,32	0
32	MG	A	8010	1/1	0.94	0.05	-4.24	30,30,30,30	0
32	MG	A	8059	1/1	0.93	0.10	-4.29	47,47,47,47	0
32	MG	A	8058	1/1	0.96	0.08	-4.48	39,39,39,39	0
37	CD	4	8404	1/1	0.74	0.42	-4.66	203,203,203,203	0
32	MG	A	8021	1/1	0.97	0.11	-4.68	32,32,32,32	0
34	NA	A	8305	1/1	0.98	0.09	-4.81	27,27,27,27	0
34	NA	A	8339	1/1	0.95	0.09	-5.19	30,30,30,30	0
32	MG	A	8006	1/1	0.97	0.09	-5.23	57,57,57,57	0
32	MG	A	8108	1/1	0.92	0.06	-5.30	53,53,53,53	0
32	MG	A	8004	1/1	0.95	0.07	-5.59	53,53,53,53	0
32	MG	A	8071	1/1	0.90	0.07	-5.70	93,93,93,93	0
32	MG	A	8013	1/1	0.94	0.12	-6.15	42,42,42,42	0
32	MG	A	8052	1/1	0.95	0.08	-6.15	51,51,51,51	0
32	MG	A	8080	1/1	0.99	0.06	-6.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8028	1/1	0.96	0.07	-6.35	37,37,37,37	0
32	MG	A	8017	1/1	0.97	0.05	-6.40	35,35,35,35	0
32	MG	A	8001	1/1	0.97	0.09	-6.75	33,33,33,33	0
32	MG	A	8038	1/1	0.97	0.05	-6.85	33,33,33,33	0
32	MG	A	8039	1/1	0.95	0.05	-7.08	51,51,51,51	0
32	MG	A	8015	1/1	0.98	0.05	-7.94	50,50,50,50	0
32	MG	A	8084	1/1	0.98	0.05	-8.13	50,50,50,50	0
32	MG	A	8019	1/1	0.99	0.07	-8.87	30,30,30,30	0
32	MG	A	8018	1/1	0.95	0.08	-9.06	42,42,42,42	0
32	MG	A	8035	1/1	0.94	0.06	-9.25	48,48,48,48	0
32	MG	A	8002	1/1	0.97	0.05	-9.46	36,36,36,36	0
32	MG	A	8020	1/1	0.98	0.05	-9.53	46,46,46,46	0
32	MG	A	8110	1/1	0.97	0.07	-10.71	30,30,30,30	0
32	MG	A	8003	1/1	0.97	0.07	-11.38	23,23,23,23	0
32	MG	A	8034	1/1	0.95	0.05	-12.24	36,36,36,36	0
32	MG	A	8054	1/1	0.97	0.06	-12.45	33,33,33,33	0
32	MG	A	8007	1/1	0.97	0.03	-12.53	28,28,28,28	0
32	MG	A	8096	1/1	0.93	0.07	-13.19	51,51,51,51	0
32	MG	A	8014	1/1	0.97	0.07	-34.59	20,20,20,20	0
34	NA	A	8355	1/1	0.82	0.62	-	64,64,64,64	0
34	NA	A	8306	1/1	0.92	0.61	-	44,44,44,44	0
32	MG	A	8016	1/1	0.92	0.13	-	36,36,36,36	0
32	MG	A	8075	1/1	0.94	0.12	-	45,45,45,45	0
32	MG	A	8100	1/1	0.94	0.13	-	79,79,79,79	0
35	CL	A	8514	1/1	0.94	0.27	-	50,50,50,50	0
32	MG	A	8011	1/1	0.99	0.13	-	24,24,24,24	0
35	CL	A	8503	1/1	0.90	0.24	-	57,57,57,57	0
32	MG	A	8092	1/1	0.73	0.47	-	91,91,91,91	0
34	NA	A	8341	1/1	0.87	0.17	-	55,55,55,55	0
34	NA	A	8310	1/1	0.76	0.54	-	40,40,40,40	0
32	MG	A	8090	1/1	0.93	0.19	-	70,70,70,70	0
32	MG	A	8025	1/1	0.99	0.06	-	40,40,40,40	0
32	MG	A	8043	1/1	0.94	0.09	-	32,32,32,32	0
32	MG	A	8099	1/1	0.88	0.24	-	68,68,68,68	0
32	MG	A	8042	1/1	0.94	0.17	-	34,34,34,34	0
32	MG	A	8087	1/1	0.95	0.09	-	49,49,49,49	0
35	CL	K	8516	1/1	0.87	0.27	-	61,61,61,61	0
32	MG	A	8040	1/1	0.96	0.13	-	100,100,100,100	0
34	NA	A	8308	1/1	0.90	0.15	-	63,63,63,63	0
35	CL	R	8511	1/1	0.83	0.38	-	67,67,67,67	0
34	NA	4	8369	1/1	0.79	0.33	-	66,66,66,66	0
32	MG	A	8045	1/1	0.82	0.13	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8089	1/1	0.84	0.22	-	82,82,82,82	0
32	MG	A	8111	1/1	0.98	0.07	-	61,61,61,61	0
32	MG	A	8114	1/1	0.70	1.02	-	124,124,124,124	0
34	NA	A	8316	1/1	0.88	0.21	-	45,45,45,45	0
32	MG	A	8093	1/1	0.80	0.23	-	44,44,44,44	0
34	NA	A	8358	1/1	0.89	0.45	-	105,105,105,105	0
32	MG	A	8116	1/1	0.91	0.16	-	55,55,55,55	0
34	NA	A	8330	1/1	0.94	0.20	-	35,35,35,35	0
35	CL	A	8522	1/1	0.79	0.62	-	83,83,83,83	0
32	MG	A	8022	1/1	0.97	0.05	-	32,32,32,32	0
35	CL	K	8501	1/1	0.91	0.17	-	58,58,58,58	0
32	MG	A	8061	1/1	0.95	0.06	-	45,45,45,45	0
35	CL	4	8504	1/1	0.39	0.37	-	101,101,101,101	0
32	MG	A	8104	1/1	0.92	0.20	-	52,52,52,52	0
32	MG	A	8097	1/1	0.95	0.20	-	32,32,32,32	0
34	NA	A	8311	1/1	0.91	0.13	-	31,31,31,31	0
32	MG	A	8030	1/1	0.95	0.12	-	34,34,34,34	0
34	NA	A	8359	1/1	0.94	0.45	-	60,60,60,60	0
32	MG	A	8072	1/1	0.96	0.07	-	53,53,53,53	0
32	MG	A	8024	1/1	0.37	0.60	-	110,110,110,110	0
35	CL	Z	8517	1/1	0.96	0.31	-	61,61,61,61	0
34	NA	A	8352	1/1	0.78	0.33	-	39,39,39,39	0
32	MG	A	8063	1/1	0.93	0.11	-	85,85,85,85	0
34	NA	A	8363	1/1	0.57	0.78	-	48,48,48,48	0
34	NA	A	8307	1/1	0.77	0.64	-	58,58,58,58	0
34	NA	J	8322	1/1	0.84	0.37	-	72,72,72,72	0
32	MG	A	8037	1/1	0.97	0.09	-	43,43,43,43	0
32	MG	A	8117	1/1	0.97	0.08	-	33,33,33,33	0
34	NA	A	8336	1/1	0.93	0.10	-	49,49,49,49	0
32	MG	A	8048	1/1	0.97	0.07	-	33,33,33,33	0
34	NA	A	8357	1/1	0.76	0.10	-	49,49,49,49	0
37	CD	P	8405	1/1	0.94	0.07	-	89,89,89,89	0
32	MG	A	8026	1/1	0.99	0.05	-	33,33,33,33	0
32	MG	A	8102	1/1	0.62	1.13	-	135,135,135,135	0
34	NA	A	8377	1/1	0.85	0.33	-	86,86,86,86	0
35	CL	C	8509	1/1	0.83	0.32	-	86,86,86,86	0
32	MG	A	8101	1/1	0.87	0.10	-	50,50,50,50	0
35	CL	S	8506	1/1	0.91	0.20	-	60,60,60,60	0
32	MG	B	8095	1/1	0.83	0.08	-	72,72,72,72	0
34	NA	A	8328	1/1	0.70	0.57	-	47,47,47,47	0
32	MG	A	8070	1/1	0.95	0.78	-	69,69,69,69	0
32	MG	A	8051	1/1	0.90	0.10	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	A	8375	1/1	0.90	0.25	-	55,55,55,55	0
32	MG	A	8041	1/1	0.92	0.17	-	55,55,55,55	0
34	NA	A	8342	1/1	0.94	0.14	-	28,28,28,28	0
32	MG	A	8023	1/1	0.96	0.12	-	45,45,45,45	0
32	MG	A	8094	1/1	0.93	0.17	-	65,65,65,65	0
34	NA	A	8367	1/1	0.96	0.14	-	43,43,43,43	0
32	MG	A	8031	1/1	0.98	0.04	-	32,32,32,32	0
32	MG	A	8103	1/1	0.89	0.23	-	45,45,45,45	0
32	MG	A	8106	1/1	0.93	0.21	-	76,76,76,76	0
34	NA	A	8315	1/1	0.98	0.16	-	43,43,43,43	0
34	NA	T	8312	1/1	0.39	0.57	-	80,80,80,80	0
32	MG	L	8069	1/1	0.98	0.09	-	81,81,81,81	0
34	NA	A	8385	1/1	0.71	0.34	-	46,46,46,46	0
35	CL	Z	8520	1/1	0.92	0.15	-	35,35,35,35	0
35	CL	K	8502	1/1	0.80	0.19	-	71,71,71,71	0
34	NA	A	8349	1/1	0.93	0.23	-	67,67,67,67	0
34	NA	A	8360	1/1	0.96	0.74	-	61,61,61,61	0
34	NA	A	8370	1/1	0.91	0.32	-	52,52,52,52	0
34	NA	A	8334	1/1	0.94	0.09	-	46,46,46,46	0
34	NA	A	8354	1/1	0.86	0.39	-	51,51,51,51	0
32	MG	A	8082	1/1	0.93	0.16	-	56,56,56,56	0
32	MG	A	8009	1/1	0.98	0.06	-	32,32,32,32	0
34	NA	A	8319	1/1	0.79	0.15	-	44,44,44,44	0
32	MG	A	8076	1/1	0.34	0.17	-	79,79,79,79	0
34	NA	A	8329	1/1	0.53	0.34	-	61,61,61,61	0
32	MG	A	8098	1/1	0.98	0.17	-	33,33,33,33	0
32	MG	A	8113	1/1	0.76	0.32	-	54,54,54,54	0
32	MG	A	8005	1/1	0.99	0.07	-	38,38,38,38	0
32	MG	A	8088	1/1	0.85	0.15	-	65,65,65,65	0
34	NA	B	8351	1/1	0.56	0.39	-	75,75,75,75	0
32	MG	A	8068	1/1	0.95	0.11	-	46,46,46,46	0
35	CL	A	8513	1/1	0.96	0.12	-	56,56,56,56	0
32	MG	A	8085	1/1	0.85	0.16	-	95,95,95,95	0
34	NA	A	8318	1/1	0.97	0.27	-	43,43,43,43	0
32	MG	A	8115	1/1	0.85	0.09	-	59,59,59,59	0
32	MG	A	8046	1/1	0.83	0.10	-	53,53,53,53	0
32	MG	A	8083	1/1	0.97	0.08	-	37,37,37,37	0
34	NA	A	8313	1/1	0.94	0.10	-	74,74,74,74	0
32	MG	A	8036	1/1	0.98	0.06	-	38,38,38,38	0
32	MG	A	8049	1/1	0.33	0.69	-	95,95,95,95	0
32	MG	A	8050	1/1	0.95	0.10	-	52,52,52,52	0
34	NA	A	8302	1/1	0.90	0.20	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8079	1/1	0.94	0.07	-	48,48,48,48	0
34	NA	A	8301	1/1	0.82	0.14	-	31,31,31,31	0
35	CL	O	8507	1/1	0.87	0.23	-	65,65,65,65	0
34	NA	A	8340	1/1	0.52	0.59	-	58,58,58,58	0
32	MG	A	8081	1/1	0.95	0.08	-	39,39,39,39	0
32	MG	A	8066	1/1	0.94	0.16	-	65,65,65,65	0
32	MG	A	8029	1/1	0.95	0.10	-	38,38,38,38	0
34	NA	A	8384	1/1	0.12	0.76	-	82,82,82,82	0

6.5 Other polymers

There are no such residues in this entry.