



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:14 am GMT

PDB ID : 1JJ2
Title : Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-07-03
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

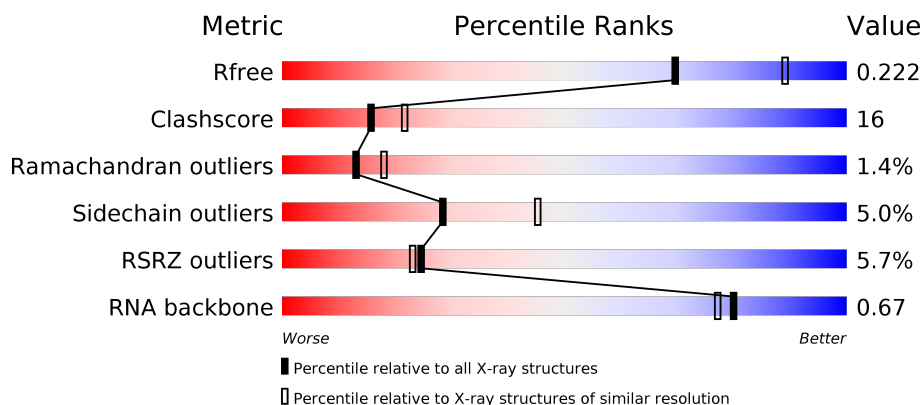
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>9%</div> <div>•</div> </div> </div>
3	A	239	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> <div>•</div> </div> </div>
4	B	337	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
30	2	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	0	8060	-	-	-	X
33	NA	0	8302	-	-	-	X
33	NA	0	8303	-	-	-	X
33	NA	0	8305	-	-	-	X
33	NA	0	8314	-	-	-	X
33	NA	0	8320	-	-	-	X
33	NA	0	8321	-	-	-	X
33	NA	0	8325	-	-	-	X
33	NA	0	8327	-	-	-	X
33	NA	0	8331	-	-	-	X
33	NA	0	8340	-	-	-	X
33	NA	0	8350	-	-	-	X
33	NA	0	8361	-	-	-	X
33	NA	0	8362	-	-	-	X
33	NA	0	8364	-	-	-	X
33	NA	0	8366	-	-	-	X
33	NA	0	8371	-	-	-	X
33	NA	0	8372	-	-	-	X
33	NA	0	8374	-	-	-	X
33	NA	0	8376	-	-	-	X
33	NA	K	8380	-	-	-	X
33	NA	Q	8386	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98543 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	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
1	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	109	Total Mg 109 109	0	0
31	J	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	A	2	Total Mg 2 2	0	0
31	X	1	Total Mg 1 1	0	0
31	2	1	Total Mg 1 1	0	0
31	9	1	Total Mg 1 1	0	0
31	S	1	Total Mg 1 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	2	Total K 2 2	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	72	Total Na 72 72	0	0
33	P	1	Total Na 1 1	0	0
33	Q	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	H	2	Total Na 2 2	0	0
33	I	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	A	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	2	Total 2	Na 2	0	0
33	L	1	Total 1	Na 1	0	0
33	S	1	Total 1	Na 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	10	Total 10	Cl 10	0	0
34	Q	1	Total 1	Cl 1	0	0
34	K	1	Total 1	Cl 1	0	0
34	B	1	Total 1	Cl 1	0	0
34	I	3	Total 3	Cl 3	0	0
34	A	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	2	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total 1	Cd 1	0	0
35	Y	1	Total 1	Cd 1	0	0
35	T	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	2	1	Total	Cd	0	0
			1	1		
35	N	1	Total	Cd	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	5938	Total	O	0	0
			5938	5938		
36	9	135	Total	O	0	0
			135	135		
36	A	126	Total	O	0	0
			126	126		
36	B	150	Total	O	0	0
			150	150		
36	C	172	Total	O	0	0
			172	172		
36	D	53	Total	O	0	0
			53	53		
36	E	46	Total	O	0	0
			46	46		
36	F	28	Total	O	0	0
			28	28		
36	G	21	Total	O	0	0
			21	21		
36	H	74	Total	O	0	0
			74	74		
36	I	56	Total	O	0	0
			56	56		
36	J	62	Total	O	0	0
			62	62		
36	K	80	Total	O	0	0
			80	80		
36	L	127	Total	O	0	0
			127	127		
36	M	70	Total	O	0	0
			70	70		
36	N	43	Total	O	0	0
			43	43		
36	O	68	Total	O	0	0
			68	68		

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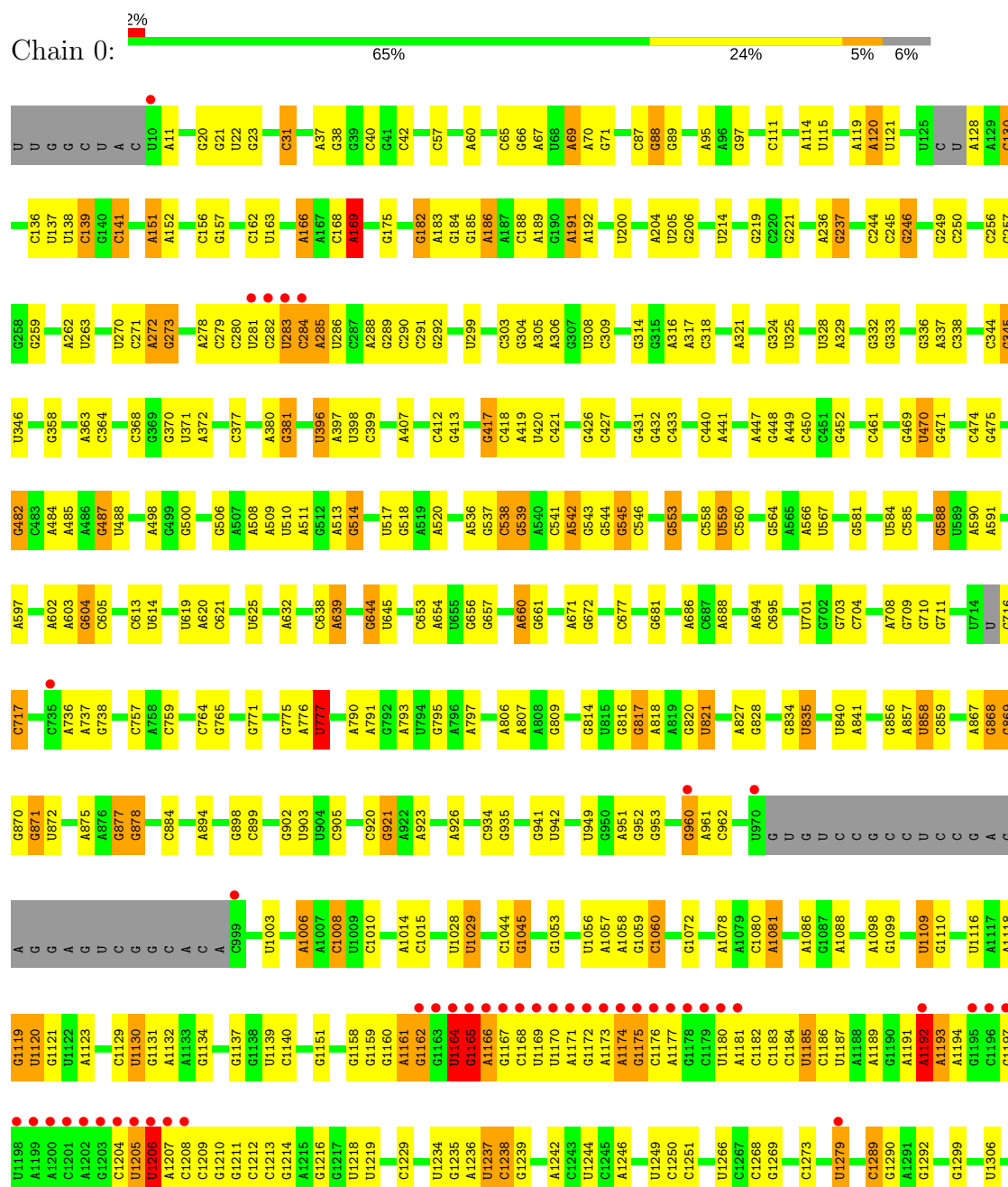
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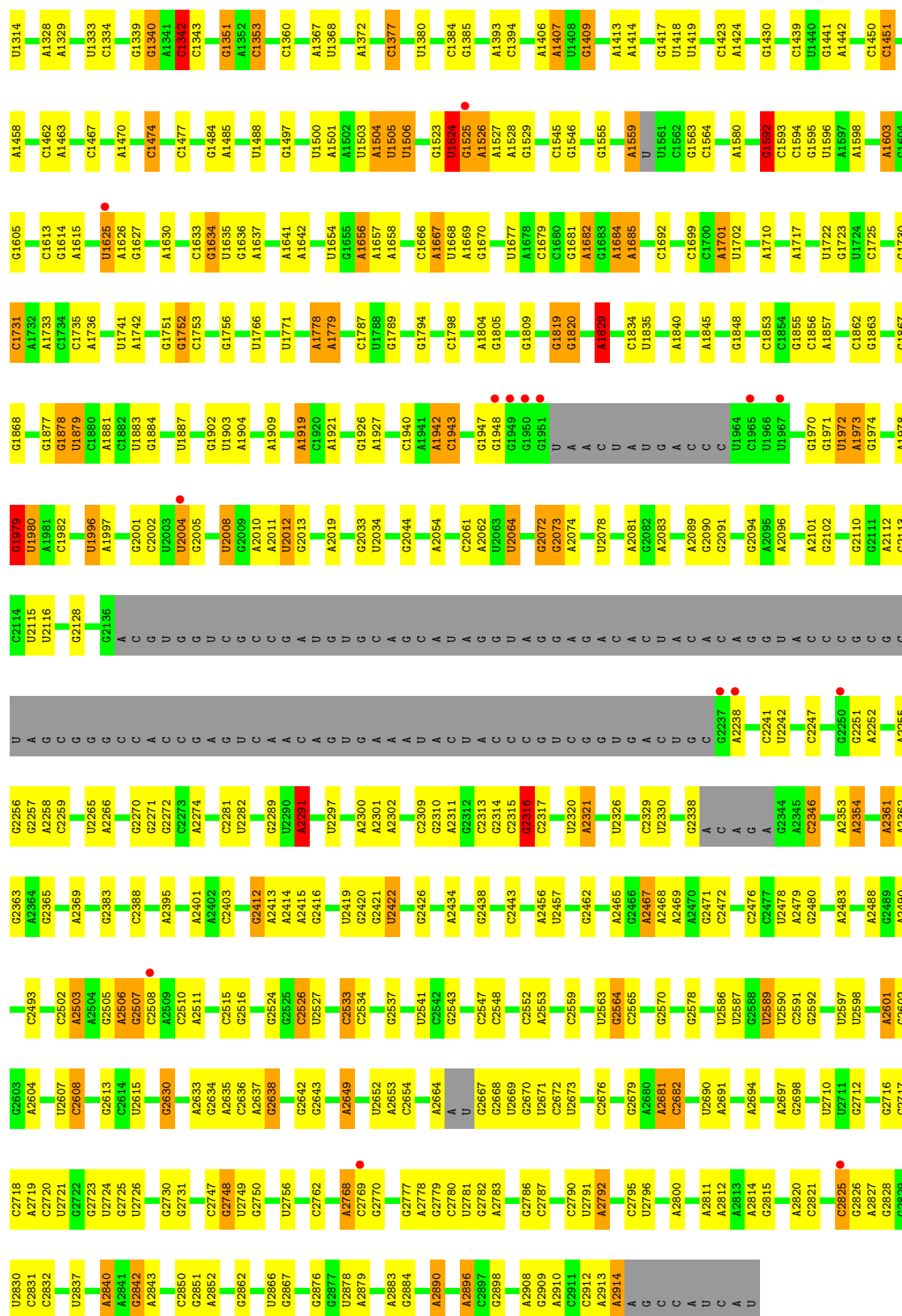
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	53	Total 53	O 53	0	0
36	Q	81	Total 81	O 81	0	0
36	R	32	Total 32	O 32	0	0
36	S	39	Total 39	O 39	0	0
36	T	25	Total 25	O 25	0	0
36	U	15	Total 15	O 15	0	0
36	V	67	Total 67	O 67	0	0
36	W	29	Total 29	O 29	0	0
36	X	99	Total 99	O 99	0	0
36	Y	39	Total 39	O 39	0	0
36	Z	53	Total 53	O 53	0	0
36	1	40	Total 40	O 40	0	0
36	2	72	Total 72	O 72	0	0

3 Residue-property plots

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

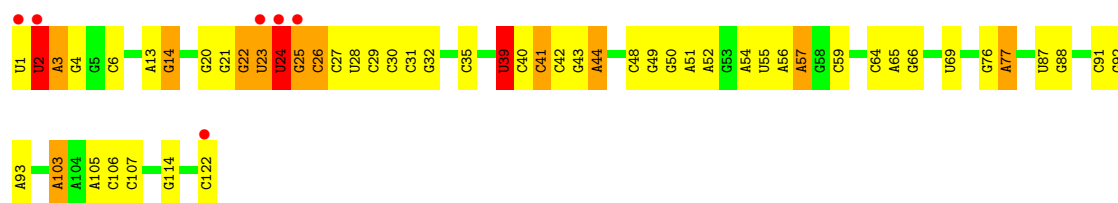
• Molecule 1: 23S rRNA



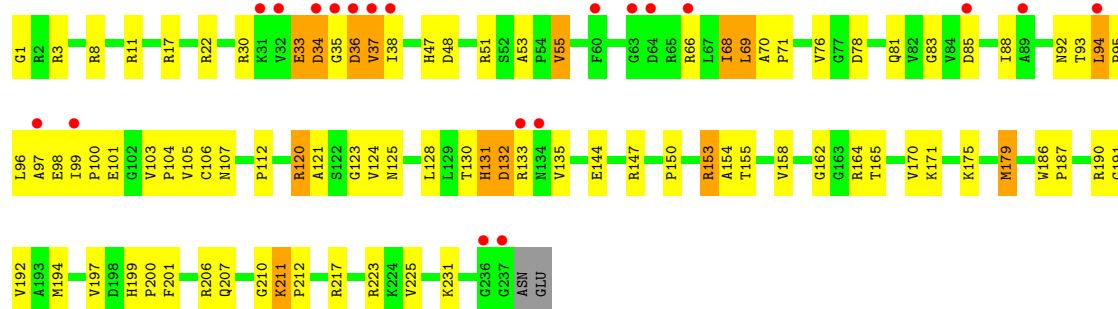


• Molecule 2: 5S rRNA

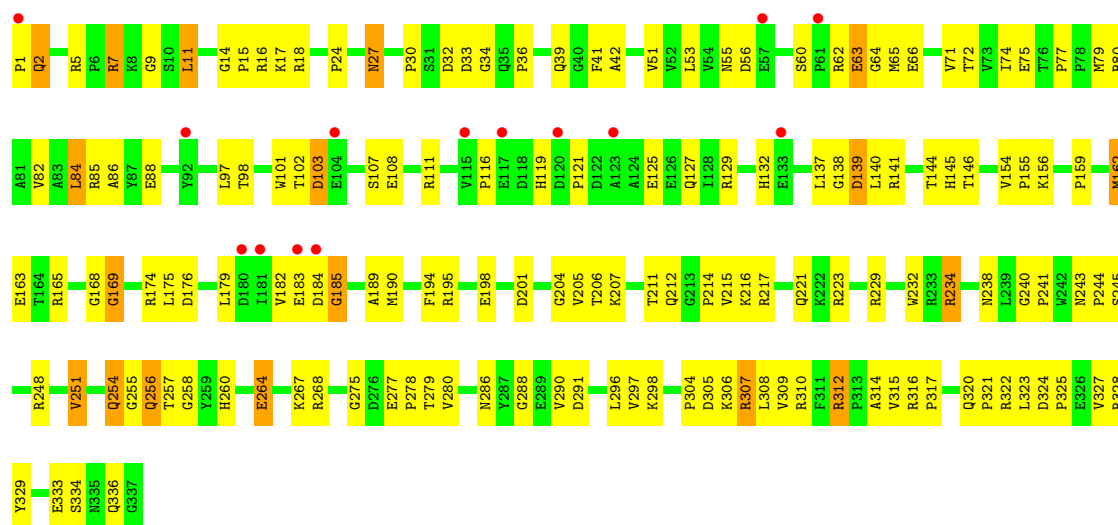




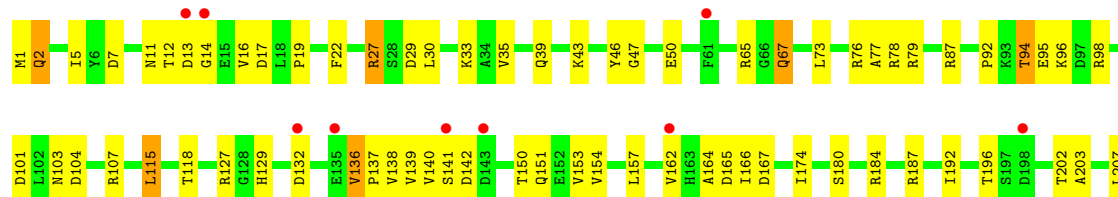
• Molecule 3: RIBOSOMAL PROTEIN L2



• Molecule 4: RIBOSOMAL PROTEIN L3

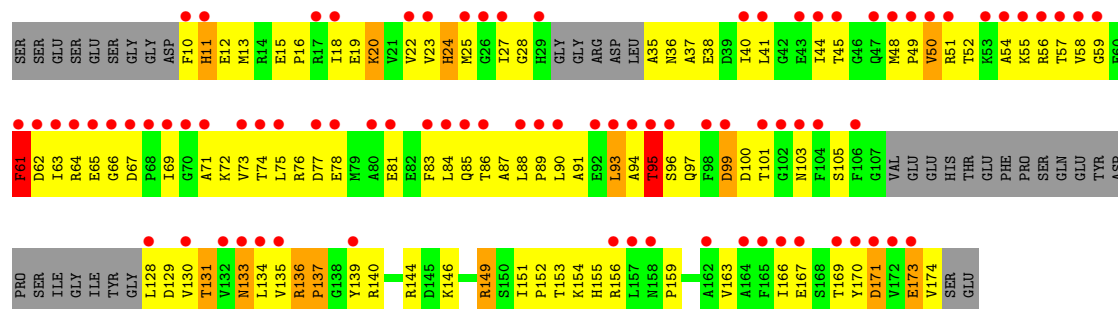


• Molecule 5: RIBOSOMAL PROTEIN L4

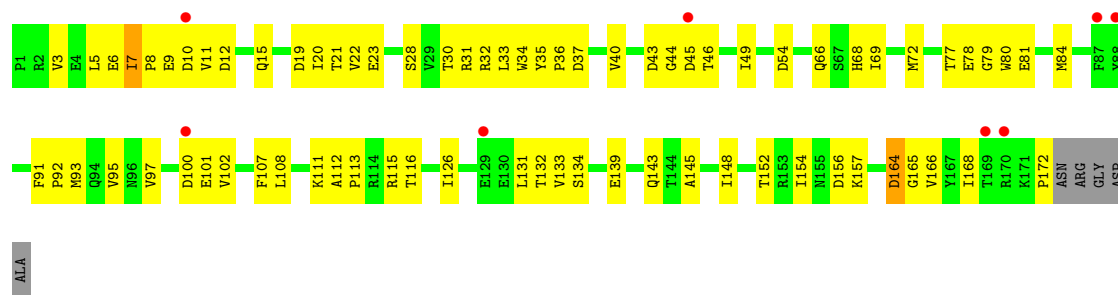




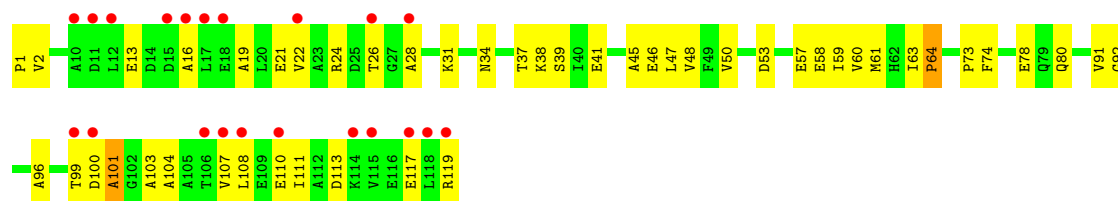
• Molecule 6: RIBOSOMAL PROTEIN L5



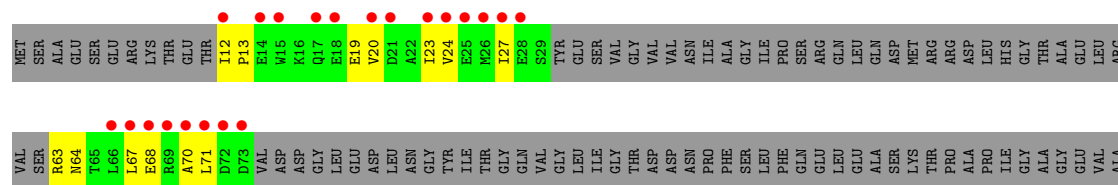
• Molecule 7: RIBOSOMAL PROTEIN L6

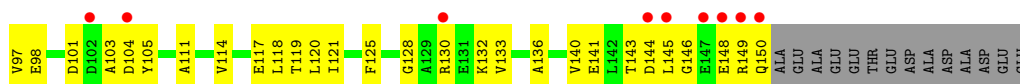


• Molecule 8: RIBOSOMAL PROTEIN L7AE

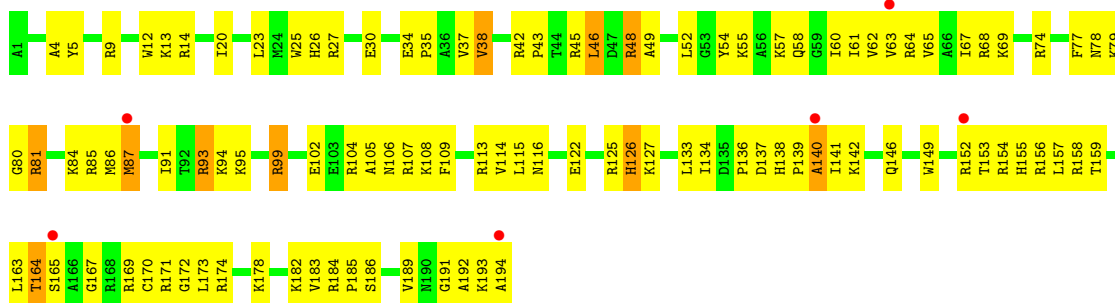


• Molecule 9: RIBOSOMAL PROTEIN L10

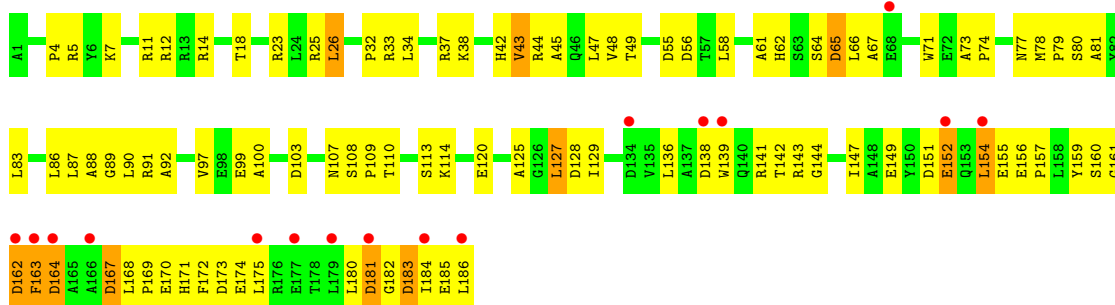




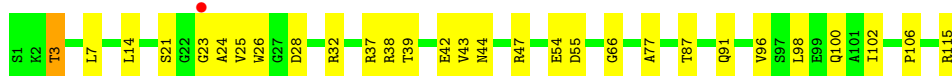
• Molecule 14: RIBOSOMAL PROTEIN L15E



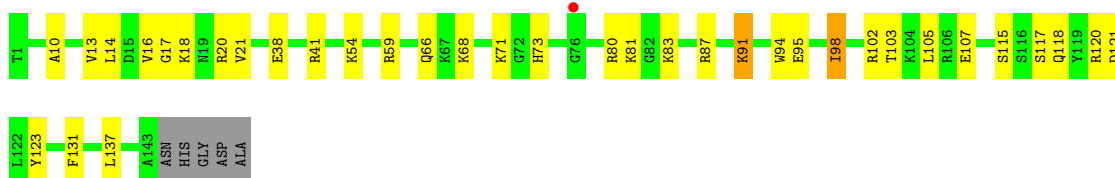
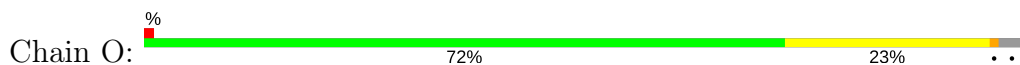
• Molecule 15: RIBOSOMAL PROTEIN L18



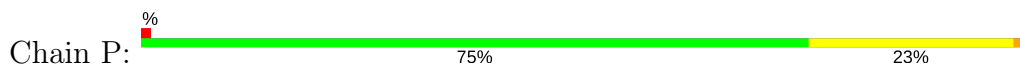
• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E



• Molecule 18: RIBOSOMAL PROTEIN L21E

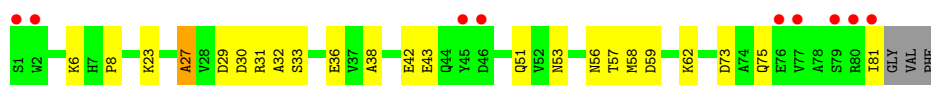




• Molecule 19: RIBOSOMAL PROTEIN L22



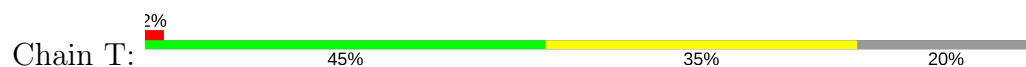
• Molecule 20: RIBOSOMAL PROTEIN L23



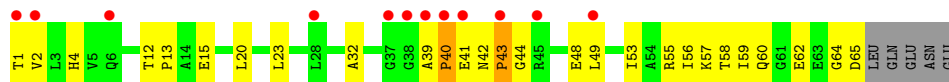
• Molecule 21: RIBOSOMAL PROTEIN L24



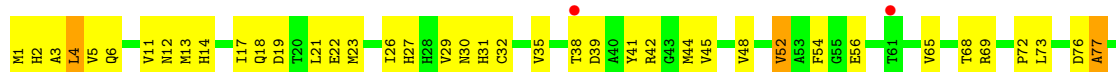
• Molecule 22: RIBOSOMAL PROTEIN L24E



• Molecule 23: RIBOSOMAL PROTEIN L29

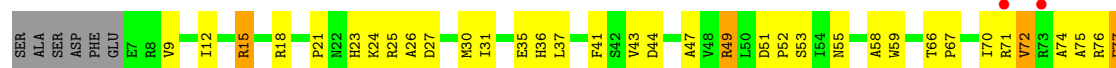


• Molecule 24: RIBOSOMAL PROTEIN L30

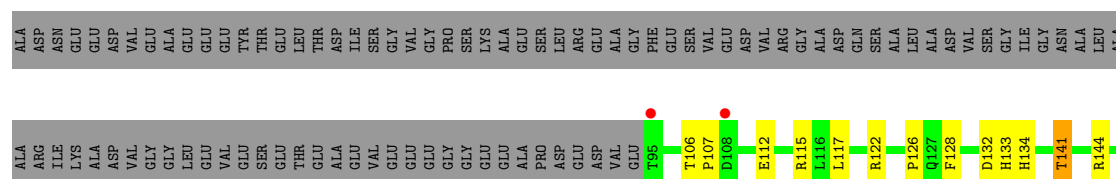




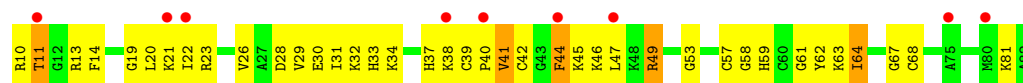
• Molecule 25: RIBOSOMAL PROTEIN L31E



• Molecule 26: RIBOSOMAL PROTEIN L32E



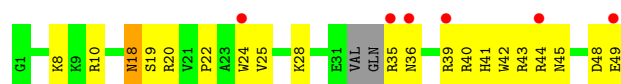
• Molecule 27: RIBOSOMAL PROTEIN L37Ae



• Molecule 28: RIBOSOMAL PROTEIN L37E

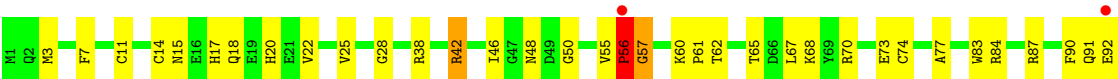


• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (15.00-2.40) 90.6 (85.48-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.222 0.190 , 0.222	Depositor DCC
R_{free} test set	6222 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	98543	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.38	3/66076 (0.0%)	0.71	32/103052 (0.0%)
2	9	0.44	3/2905 (0.1%)	0.85	11/4528 (0.2%)
3	A	0.34	0/1787	0.66	0/2409
4	B	0.34	0/2689	0.64	0/3652
5	C	0.39	0/1883	0.67	0/2551
6	D	0.31	0/1111	0.59	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.33	0/896	0.56	0/1219
9	G	0.25	0/241	0.47	0/324
10	H	0.38	0/1246	0.74	1/1686 (0.1%)
11	I	0.33	0/1135	0.61	0/1530
12	J	0.33	0/1003	0.65	0/1351
13	K	0.34	0/1126	0.68	0/1504
14	L	0.41	0/1633	0.71	1/2180 (0.0%)
15	M	0.29	0/1473	0.64	0/1999
16	N	0.32	0/873	0.61	1/1181 (0.1%)
17	O	0.33	0/1143	0.54	0/1521
18	P	0.35	0/748	0.68	0/1005
19	Q	0.35	0/1172	0.67	0/1578
20	R	0.32	0/648	0.59	1/875 (0.1%)
21	S	0.31	0/957	0.63	0/1289
22	T	0.32	0/417	0.58	0/562
23	U	0.29	0/502	0.54	0/675
24	V	0.33	0/1218	0.62	0/1655
25	W	0.32	0/664	0.60	0/895
26	X	0.34	0/1146	0.63	0/1536
27	Y	0.37	0/575	0.69	0/763
28	Z	0.42	0/437	0.67	0/578
29	1	0.34	0/398	0.54	0/527
30	2	0.38	0/771	0.62	0/1024
All	All	0.37	6/98255 (0.0%)	0.70	47/147027 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	62
2	9	0	2
All	All	1	64

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9	3	A	C2'-O2'	-7.92	1.31	1.41
1	0	1206	U	P-OP2	6.22	1.59	1.49
2	9	3	A	O5'-C5'	6.21	1.54	1.44
1	0	1206	U	C3'-O3'	-5.28	1.34	1.42
1	0	1205	U	C3'-O3'	-5.23	1.34	1.42
2	9	3	A	C5'-C4'	-5.13	1.45	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	O5'-P-OP1	-22.95	83.17	110.70
1	0	1164	U	OP1-P-O3'	-20.79	59.47	105.20
1	0	1165	G	O5'-P-OP2	-15.10	92.11	105.70
2	9	3	A	OP1-P-O3'	-13.36	75.82	105.20
1	0	1164	U	OP2-P-O3'	-13.28	75.98	105.20
2	9	3	A	C5'-C4'-C3'	-11.15	98.16	116.00
2	9	2	U	OP2-P-O3'	-10.56	81.96	105.20
1	0	1563	G	C2'-C3'-O3'	9.58	130.57	109.50
1	0	1942	A	C5'-C4'-C3'	8.93	130.28	116.00
2	9	24	U	C2'-C3'-O3'	8.93	129.14	109.50
1	0	871	G	C5'-C4'-O4'	-8.42	99.00	109.10
1	0	1979	G	C2'-C3'-O3'	8.18	127.49	109.50
2	9	2	U	OP1-P-O3'	7.93	122.65	105.20
1	0	1819	G	C5'-C4'-C3'	7.14	127.43	116.00
2	9	39	U	N1-C1'-C2'	7.07	123.19	114.00
2	9	3	A	OP2-P-O3'	7.00	120.61	105.20
1	0	1206	U	C5'-C4'-C3'	-6.94	104.89	116.00
2	9	103	A	C5'-C4'-O4'	6.87	117.34	109.10
1	0	2316	G	C5'-C4'-C3'	-6.84	105.06	116.00
1	0	1942	A	C5'-C4'-O4'	6.80	117.26	109.10
1	0	1504	A	C1'-O4'-C4'	-6.55	104.66	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2467	A	C1'-O4'-C4'	-6.40	104.78	109.90
1	0	206	G	C5'-C4'-C3'	-6.37	105.81	116.00
1	0	2291	A	N9-C1'-C2'	6.26	122.14	114.00
1	0	1504	A	N9-C1'-C2'	6.21	122.08	114.00
1	0	1559	A	C2'-C3'-O3'	5.91	123.16	113.70
10	H	74	ASN	N-CA-C	-5.82	95.28	111.00
1	0	1942	A	C1'-O4'-C4'	-5.80	105.26	109.90
1	0	1942	A	C4'-C3'-C2'	-5.79	96.81	102.60
1	0	777	U	O4'-C1'-N1	5.70	112.76	108.20
1	0	1164	U	O3'-P-O5'	5.68	114.78	104.00
1	0	1205	U	C4'-C3'-O3'	-5.61	97.63	109.40
1	0	169	A	C5'-C4'-O4'	-5.54	102.46	109.10
1	0	1120	U	C5'-C4'-C3'	-5.52	107.17	116.00
1	0	1829	A	N9-C1'-C2'	-5.47	105.98	112.00
14	L	126	HIS	CB-CA-C	-5.44	99.53	110.40
2	9	103	A	C4'-C3'-C2'	-5.38	97.22	102.60
1	0	2313	C	C5'-C4'-O4'	5.31	115.47	109.10
1	0	1819	G	C4'-C3'-C2'	-5.30	97.30	102.60
1	0	1592	G	N9-C1'-C2'	5.27	120.85	114.00
1	0	841	A	C1'-O4'-C4'	-5.21	105.73	109.90
2	9	103	A	C1'-O4'-C4'	-5.15	105.78	109.90
2	9	24	U	C4'-C3'-C2'	5.11	107.71	102.60
1	0	1165	G	OP1-P-OP2	5.11	127.26	119.60
16	N	66	GLY	N-CA-C	5.04	125.70	113.10
20	R	27	ALA	N-CA-C	-5.03	97.41	111.00
1	0	1563	G	C4'-C3'-O3'	5.01	123.03	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1164	U	Sidechain
1	0	1192	A	Sidechain
1	0	1292	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1501	A	Sidechain
1	0	1524	U	Sidechain
1	0	1794	G	Sidechain
1	0	1809	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2012	U	Sidechain
1	0	2078	U	Sidechain
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2395	A	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2543	G	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2615	U	Sidechain
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	332	G	Sidechain
1	0	333	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	396	U	Sidechain
1	0	452	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	639	A	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
2	9	39	U	Sidechain
2	9	87	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29807	760	0
2	9	2600	0	1326	78	0
3	A	1754	0	1763	109	0
4	B	2624	0	2533	176	0
5	C	1858	0	1816	105	0
6	D	1094	0	1085	130	0
7	E	1357	0	1266	79	0
8	F	885	0	854	59	0
9	G	240	0	231	18	0
10	H	1215	0	1215	150	0
11	I	1119	0	1098	62	0
12	J	993	0	1027	56	0
13	K	1114	0	1072	55	0
14	L	1605	0	1676	141	0
15	M	1444	0	1401	119	0
16	N	864	0	873	31	0
17	O	1133	0	1127	38	0
18	P	734	0	728	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	949	0	923	52	0
22	T	410	0	364	31	0
23	U	499	0	511	28	0
24	V	1195	0	1137	91	0
25	W	654	0	653	44	0
26	X	1130	0	1133	52	0
27	Y	563	0	597	53	0
28	Z	430	0	426	22	0
29	1	393	0	406	32	0
30	2	755	0	728	36	0
31	0	109	0	0	0	0
31	2	1	0	0	0	0
31	9	1	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	S	1	0	0	0	0
31	X	1	0	0	0	0
32	0	2	0	0	0	0
33	0	72	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	2	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	2	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	I	3	0	0	1	0
34	K	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	2	1	0	0	0	0
35	N	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	5938	0	0	173	0
36	1	40	0	0	6	0
36	2	72	0	0	10	0
36	9	135	0	0	14	0
36	A	126	0	0	20	0
36	B	150	0	0	30	0
36	C	172	0	0	30	0
36	D	53	0	0	18	0
36	E	46	0	0	12	0
36	F	28	0	0	7	0
36	G	21	0	0	4	0
36	H	74	0	0	21	0
36	I	56	0	0	5	0
36	J	62	0	0	13	0
36	K	80	0	0	17	0
36	L	127	0	0	19	0
36	M	70	0	0	16	0
36	N	43	0	0	6	0
36	O	68	0	0	1	0
36	P	53	0	0	1	0
36	Q	81	0	0	9	0
36	R	32	0	0	5	0
36	S	39	0	0	5	0
36	T	25	0	0	6	0
36	U	15	0	0	4	0
36	V	67	0	0	10	0
36	W	29	0	0	3	0
36	X	99	0	0	15	0
36	Y	39	0	0	12	0
36	Z	53	0	0	1	0
All	All	98543	0	59503	2453	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 16.

All (2453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.14
10:H:86:ARG:NH1	10:H:133:ILE:HG13	1.62	1.12
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.35	1.07
25:W:37:LEU:HD13	25:W:85:VAL:HG21	1.29	1.06
1:0:960:G:H4'	36:0:6956:HOH:O	1.54	1.06
5:C:236:THR:HG22	5:C:239:ALA:H	1.02	1.06
1:0:1134:G:H4'	10:H:151:MET:HE1	1.34	1.05
21:S:71:VAL:HG11	21:S:90:PRO:HB3	1.39	1.03
2:9:23:U:H4'	2:9:24:U:OP2	1.54	1.02
10:H:162:SER:HB2	10:H:163:PRO:HD3	1.37	1.02
23:U:12:THR:HG22	23:U:15:GLU:HG3	1.40	1.02
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.39	1.02
1:0:156:C:H5''	14:L:171:ARG:HD3	1.39	1.01
1:0:1242:A:H5'	11:I:82:THR:HG23	1.42	1.01
1:0:871:G:C8	1:0:871:G:H5'	1.94	1.01
1:0:1751:G:H2'	1:0:1752:G:H5''	1.43	1.00
10:H:26:LYS:HD2	10:H:28:ILE:HD12	1.41	1.00
14:L:164:THR:HG22	14:L:167:GLY:H	1.23	1.00
10:H:45:GLN:HB3	10:H:163:PRO:HD2	1.38	1.00
1:0:21:G:H5'	19:Q:2:ILE:HA	1.45	0.99
2:9:6:C:H5''	15:M:37:ARG:NH1	1.78	0.99
1:0:856:G:H2'	36:0:4940:HOH:O	1.61	0.99
2:9:56:A:H2'	2:9:57:A:H5''	1.45	0.99
10:H:86:ARG:HH11	10:H:133:ILE:HG13	0.84	0.99
27:Y:10:ARG:HA	36:Y:8415:HOH:O	1.62	0.98
2:9:76:G:H3'	2:9:77:A:H5''	1.46	0.98
10:H:86:ARG:HH11	10:H:133:ILE:CG1	1.77	0.98
12:J:81:ARG:HB2	12:J:87:ARG:HH11	1.24	0.98
12:J:10:GLN:NE2	12:J:10:GLN:H	1.60	0.97
17:O:115:SER:H	17:O:118:GLN:HE21	1.02	0.97
12:J:39:GLY:HA2	36:J:4183:HOH:O	1.63	0.97
1:0:870:G:H2'	1:0:871:G:H5''	1.46	0.97
2:9:3:A:O5'	2:9:3:A:H2'	1.62	0.97
4:B:140:LEU:HA	36:B:8583:HOH:O	1.63	0.95
27:Y:38:LYS:HE2	27:Y:45:LYS:HE2	1.46	0.95
24:V:88:THR:HB	36:V:6679:HOH:O	1.66	0.95
2:9:6:C:H5''	15:M:37:ARG:HH12	1.32	0.95
11:I:76:ASP:HA	36:I:5907:HOH:O	1.67	0.95
12:J:29:LEU:HB3	12:J:55:VAL:HG11	1.46	0.95
14:L:102:GLU:OE1	14:L:164:THR:HG21	1.67	0.95
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.49	0.94
14:L:52:LEU:HD11	36:L:8616:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:83:LEU:HD13	15:M:175:LEU:HD23	1.48	0.94
26:X:200:THR:HG22	26:X:201:GLU:HG3	1.50	0.93
6:D:154:LYS:HD2	6:D:154:LYS:H	1.34	0.93
1:O:871:G:H8	1:O:871:G:H5'	1.30	0.93
24:V:88:THR:HG22	24:V:89:ASP:H	1.33	0.93
20:R:57:THR:HG22	20:R:59:ASP:H	1.34	0.92
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.85	0.92
24:V:137:GLN:HE21	24:V:141:HIS:HE1	1.12	0.92
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.50	0.92
5:C:236:THR:HG22	5:C:239:ALA:N	1.85	0.92
1:O:1835:U:H5	1:O:1840:A:N7	1.68	0.92
36:O:3976:HOH:O	14:L:146:GLN:HG2	1.69	0.91
14:L:106:ASN:ND2	34:L:8518:CL:CL	2.40	0.91
4:B:86:ALA:HA	36:B:8583:HOH:O	1.68	0.91
12:J:10:GLN:N	12:J:10:GLN:HE21	1.67	0.91
10:H:29:ALA:HB3	10:H:65:ARG:HH12	1.33	0.90
1:O:542:A:H5'	1:O:542:A:H8	1.35	0.90
15:M:144:GLY:O	15:M:147:ILE:HG22	1.70	0.89
15:M:47:LEU:HD11	15:M:127:LEU:HD21	1.52	0.89
15:M:23:ARG:HD3	36:M:8549:HOH:O	1.72	0.89
5:C:2:GLN:HB3	36:C:8335:HOH:O	1.73	0.89
36:O:4373:HOH:O	14:L:14:ARG:HG2	1.73	0.89
12:J:81:ARG:HB2	12:J:87:ARG:NH1	1.88	0.88
15:M:87:LEU:HD12	15:M:186:LEU:HD21	1.54	0.88
24:V:6:GLN:HB2	24:V:26:ILE:HD12	1.53	0.88
23:U:42:ASN:HB3	36:U:7247:HOH:O	1.74	0.88
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.53	0.88
3:A:199:HIS:HD2	3:A:201:PHE:H	1.20	0.88
1:O:1116:U:H3	1:O:1246:A:H62	1.20	0.87
1:O:645:U:OP2	13:K:4:LYS:HE2	1.73	0.87
1:O:1164:U:H3	1:O:1192:A:H2	1.21	0.87
24:V:88:THR:HG23	24:V:110:GLN:NE2	1.89	0.87
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.55	0.87
10:H:27:LYS:H	10:H:58:HIS:HD2	1.22	0.87
10:H:162:SER:HB2	10:H:163:PRO:CD	2.04	0.87
1:O:1701:A:H4'	1:O:1702:U:H5''	1.55	0.87
6:D:25:MET:HE2	6:D:41:LEU:HG	1.57	0.87
27:Y:38:LYS:HG2	27:Y:45:LYS:HG2	1.54	0.86
27:Y:46:LYS:HD3	27:Y:59:HIS:HB2	1.58	0.86
1:O:1165:G:H4'	1:O:1174:A:O2'	1.75	0.86
2:9:25:G:H3'	2:9:26:C:H5'	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:132:ASP:HB3	36:C:8365:HOH:O	1.75	0.86
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.39	0.86
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.56	0.85
2:9:23:U:H3'	36:9:8474:HOH:O	1.76	0.85
10:H:55:GLN:HE21	10:H:124:ARG:HE	1.22	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.20	0.85
1:0:2716:G:H5''	4:B:206:THR:HG21	1.59	0.85
5:C:236:THR:CG2	5:C:239:ALA:H	1.88	0.85
12:J:10:GLN:H	12:J:10:GLN:HE21	0.86	0.85
16:N:42:GLU:HB2	36:N:2176:HOH:O	1.74	0.85
1:0:1474:C:H6	1:0:1474:C:H5'	1.42	0.85
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.57	0.85
2:9:24:U:O2'	2:9:25:G:H4'	1.76	0.84
10:H:49:VAL:O	10:H:157:ILE:HG23	1.76	0.84
1:0:1329:A:H2	36:0:4193:HOH:O	1.60	0.84
1:0:381:G:H5''	36:0:3826:HOH:O	1.75	0.84
4:B:238:ASN:HD22	4:B:240:GLY:H	1.26	0.84
5:C:214:THR:HG21	36:C:8403:HOH:O	1.78	0.84
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.59	0.84
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.43	0.84
12:J:74:VAL:HG11	12:J:113:ILE:HG12	1.58	0.84
15:M:7:LYS:HE3	18:P:21:ARG:O	1.77	0.84
2:9:3:A:O5'	2:9:3:A:C2'	2.23	0.83
4:B:321:PRO:HA	36:B:8662:HOH:O	1.78	0.83
7:E:97:VAL:HG12	36:E:4191:HOH:O	1.77	0.83
13:K:133:VAL:HA	36:K:8572:HOH:O	1.77	0.83
19:Q:8:ALA:HB1	19:Q:13:THR:HG21	1.59	0.83
29:1:41:HIS:H	29:1:45:ASN:HD22	1.25	0.83
1:0:560:C:H42	1:0:597:A:H61	1.24	0.83
1:0:2717:C:H2'	1:0:2718:C:H5''	1.60	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.09	0.83
6:D:105:SER:HB2	6:D:131:THR:HG23	1.59	0.83
15:M:113:SER:HB2	36:M:8562:HOH:O	1.78	0.83
14:L:172:GLY:O	14:L:183:VAL:HG11	1.79	0.82
27:Y:58:GLY:HA3	36:Y:8439:HOH:O	1.80	0.82
1:0:214:U:H5'	36:0:5660:HOH:O	1.78	0.82
8:F:91:VAL:HG12	8:F:92:GLY:H	1.45	0.82
1:0:1184:C:H1'	36:0:6994:HOH:O	1.79	0.82
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.61	0.82
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:4:ALA:HB3	36:H:8364:HOH:O	1.80	0.82
1:0:870:G:C2'	1:0:871:G:H5''	2.10	0.82
12:J:14:LYS:HB2	12:J:45:PRO:HG2	1.61	0.82
1:0:962:C:H1'	15:M:5:ARG:NH1	1.93	0.82
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.60	0.81
13:K:79:ASP:HB3	36:K:8558:HOH:O	1.81	0.81
10:H:139:ASP:N	10:H:140:PRO:HD3	1.95	0.81
3:A:191:GLY:HA2	3:A:194:MET:CE	2.10	0.81
23:U:1:THR:HG23	23:U:2:VAL:H	1.44	0.81
1:0:1372:A:H3'	36:0:6711:HOH:O	1.79	0.81
17:O:115:SER:H	17:O:118:GLN:NE2	1.79	0.81
1:0:541:C:H2'	1:0:542:A:H5''	1.62	0.81
30:2:62:THR:HB	36:2:8550:HOH:O	1.79	0.81
1:0:1667:A:H8	1:0:1667:A:H5'	1.45	0.80
2:9:25:G:H3'	2:9:26:C:C5'	2.10	0.80
29:1:22:PRO:HB2	29:1:24:TRP:CD1	2.17	0.80
13:K:68:GLU:HA	36:K:8543:HOH:O	1.82	0.80
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.80
14:L:152:ARG:HG3	36:L:8555:HOH:O	1.82	0.80
15:M:164:ASP:CG	15:M:167:ASP:HA	2.02	0.80
23:U:12:THR:HG22	23:U:15:GLU:CG	2.11	0.80
1:0:1116:U:O2'	1:0:1118:A:H2	1.65	0.80
1:0:1191:A:N1	1:0:1206:U:O4	2.14	0.80
24:V:88:THR:HG23	24:V:110:GLN:HE21	1.45	0.80
1:0:346:U:H4'	36:0:6364:HOH:O	1.82	0.79
36:0:6394:HOH:O	14:L:178:LYS:HB2	1.81	0.79
24:V:4:LEU:HD22	24:V:52:VAL:HG21	1.64	0.79
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.10	0.79
6:D:20:LYS:HA	6:D:75:LEU:O	1.82	0.79
1:0:288:A:H61	1:0:364:C:H42	1.31	0.79
30:2:70:ARG:HD3	36:2:8539:HOH:O	1.81	0.79
3:A:192:VAL:HB	36:A:8596:HOH:O	1.81	0.79
36:0:4053:HOH:O	10:H:151:MET:HE2	1.80	0.79
15:M:49:THR:HG22	15:M:56:ASP:HB2	1.64	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.11	0.78
21:S:61:GLU:HG3	36:S:3851:HOH:O	1.81	0.78
1:0:2710:U:H1'	36:0:7157:HOH:O	1.84	0.78
24:V:137:GLN:HE21	24:V:141:HIS:CE1	2.01	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.78
24:V:122:ARG:HH11	24:V:122:ARG:HG2	1.48	0.78
24:V:88:THR:HG22	24:V:89:ASP:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2506:A:O2'	1:0:2507:G:H8	1.65	0.78
27:Y:40:PRO:HD3	27:Y:47:LEU:HD11	1.66	0.78
1:0:1119:G:H22	1:0:1246:A:H2	1.26	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.10	0.78
1:0:1701:A:H5'	36:0:5802:HOH:O	1.84	0.78
29:1:39:ARG:HG2	36:1:3143:HOH:O	1.83	0.78
1:0:1116:U:HO2'	1:0:1118:A:H2	0.82	0.78
5:C:236:THR:HG21	36:C:8376:HOH:O	1.82	0.78
36:0:6950:HOH:O	21:S:9:LYS:HB2	1.82	0.78
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.65	0.78
14:L:87:MET:HB3	30:2:46:ILE:HG21	1.65	0.78
29:1:24:TRP:CD1	36:1:6863:HOH:O	2.36	0.78
1:0:544:G:H2'	1:0:545:G:H5''	1.65	0.78
10:H:55:GLN:NE2	10:H:124:ARG:HE	1.80	0.78
6:D:27:ILE:HG22	6:D:28:GLY:H	1.48	0.77
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.65	0.77
1:0:559:U:H5'	1:0:559:U:H6	1.49	0.77
36:0:9211:HOH:O	4:B:254:GLN:HG3	1.84	0.77
36:0:4346:HOH:O	11:I:47:THR:HB	1.83	0.77
24:V:149:LEU:HG	24:V:153:MET:HE2	1.67	0.77
30:2:70:ARG:HG2	30:2:77:ALA:HB2	1.65	0.77
26:X:187:VAL:HG23	26:X:192:ASP:HB2	1.65	0.77
1:0:545:G:H8	1:0:545:G:H5'	1.48	0.77
1:0:284:C:H4'	1:0:285:A:O5'	1.83	0.77
2:9:14:G:H5'	2:9:14:G:H8	1.50	0.77
2:9:56:A:C2'	2:9:57:A:H5''	2.14	0.77
36:0:3295:HOH:O	14:L:189:VAL:HG21	1.84	0.77
1:0:1625:U:H4'	36:0:4177:HOH:O	1.84	0.77
10:H:59:ASN:HD22	10:H:59:ASN:N	1.82	0.77
10:H:33:MET:HB2	10:H:83:PHE:HB3	1.67	0.77
12:J:74:VAL:HG13	12:J:113:ILE:HG23	1.67	0.77
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.66	0.77
1:0:2890:A:H1'	22:T:56:ARG:NH2	2.00	0.77
1:0:536:A:H3'	36:0:4557:HOH:O	1.85	0.77
14:L:87:MET:HB3	30:2:46:ILE:HD13	1.66	0.76
36:0:6291:HOH:O	15:M:4:PRO:HD2	1.85	0.76
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.67	0.76
24:V:68:THR:HG23	24:V:69:ARG:HG2	1.67	0.76
27:Y:49:ARG:HD2	36:Y:8430:HOH:O	1.84	0.76
1:0:1130:U:H5'	36:0:7208:HOH:O	1.85	0.76
8:F:96:ALA:HA	36:F:3111:HOH:O	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.21	0.76
14:L:139:PRO:O	14:L:140:ALA:HB3	1.86	0.76
5:C:242:GLU:HG3	36:C:8384:HOH:O	1.85	0.76
8:F:91:VAL:HG12	8:F:92:GLY:N	2.01	0.76
1:0:1751:G:C2'	1:0:1752:G:H5''	2.15	0.76
15:M:164:ASP:OD2	15:M:167:ASP:HA	1.85	0.76
4:B:62:ARG:HA	4:B:65:MET:HE3	1.67	0.76
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.68	0.76
36:0:3235:HOH:O	14:L:157:LEU:HD11	1.85	0.76
14:L:35:PRO:HG2	14:L:38:VAL:HG23	1.67	0.76
20:R:51:GLN:HE21	20:R:53:ASN:HD21	1.34	0.76
1:0:1191:A:C2	1:0:1206:U:O4	2.40	0.75
2:9:3:A:N6	2:9:22:G:H1'	2.01	0.75
2:9:23:U:H6	2:9:23:U:H5''	1.50	0.75
16:N:47:ARG:HH11	16:N:47:ARG:HG3	1.51	0.75
3:A:35:GLY:O	3:A:36:ASP:HB3	1.85	0.75
36:0:5814:HOH:O	6:D:99:ASP:HA	1.85	0.75
1:0:1209:C:H4'	36:0:4791:HOH:O	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75
10:H:59:ASN:HD22	10:H:59:ASN:H	1.34	0.75
11:I:93:ARG:HB3	11:I:93:ARG:HH11	1.49	0.75
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.69	0.75
1:0:541:C:C2'	1:0:542:A:H5''	2.17	0.75
1:0:2054:A:N3	19:Q:128:ARG:NH2	2.35	0.74
19:Q:9:ASP:O	19:Q:13:THR:HB	1.87	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.67	0.74
14:L:87:MET:HG2	30:2:46:ILE:HG21	1.69	0.74
19:Q:18:LEU:HB2	19:Q:143:VAL:HG12	1.67	0.74
24:V:122:ARG:HH21	24:V:154:ARG:HD2	1.51	0.74
26:X:189:ASN:HA	26:X:217:ILE:HD11	1.67	0.74
25:W:78:GLU:HG2	25:W:79:GLU:H	1.52	0.74
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.23	0.74
24:V:72:PRO:HG2	24:V:77:ALA:HB3	1.69	0.74
20:R:57:THR:HG22	20:R:59:ASP:N	2.02	0.74
23:U:39:ALA:N	23:U:40:PRO:HD2	2.03	0.74
1:0:2637:A:H5'	36:0:8785:HOH:O	1.88	0.74
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.74
1:0:21:G:C5'	19:Q:2:ILE:HA	2.17	0.74
1:0:289:G:H22	1:0:363:A:H2	1.36	0.74
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.70	0.74
1:0:1634:G:H3'	36:0:3402:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:39:THR:HG22	19:Q:42:GLU:H	1.53	0.74
10:H:150:LYS:HE2	36:H:8381:HOH:O	1.89	0.73
10:H:162:SER:CB	10:H:163:PRO:HD3	2.17	0.73
6:D:146:LYS:NZ	15:M:107:ASN:HD21	1.86	0.73
6:D:19:GLU:O	6:D:20:LYS:HG2	1.89	0.73
1:O:2840:A:OP1	4:B:211:THR:HG23	1.88	0.73
1:O:1351:G:OP1	5:C:96:LYS:NZ	2.21	0.73
10:H:165:GLY:HA3	36:H:8394:HOH:O	1.87	0.73
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.67	0.73
5:C:1:MET:HG2	5:C:2:GLN:H	1.53	0.73
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.19	0.73
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.71	0.73
17:O:115:SER:OG	17:O:118:GLN:HG3	1.88	0.73
1:O:1328:A:OP1	26:X:169:ARG:HD2	1.87	0.73
1:O:2586:U:H3	1:O:2592:G:H22	1.35	0.73
30:2:65:THR:HG23	30:2:67:LEU:HG	1.70	0.73
1:O:431:G:P	14:L:48:ARG:HH12	2.11	0.73
10:H:46:VAL:HG12	10:H:146:TRP:HZ3	1.53	0.73
13:K:143:THR:HG22	13:K:144:ASP:N	2.03	0.73
1:O:272:A:H3'	36:O:7061:HOH:O	1.88	0.73
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.53	0.73
5:C:236:THR:HA	36:C:8450:HOH:O	1.89	0.73
1:O:657:G:OP1	5:C:27:ARG:NH2	2.18	0.73
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.18	0.73
15:M:48:VAL:CG1	15:M:55:ASP:HB3	2.18	0.73
3:A:131:HIS:O	3:A:132:ASP:HB2	1.89	0.72
1:O:1118:A:H3'	1:O:1118:A:C8	2.24	0.72
27:Y:37:HIS:HB2	27:Y:47:LEU:HB2	1.71	0.72
1:O:1450:C:H4'	1:O:1451:C:OP2	1.88	0.72
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.69	0.72
14:L:104:ARG:O	14:L:108:LYS:HE2	1.88	0.72
1:O:1118:A:H3'	1:O:1118:A:H8	1.54	0.72
1:O:1194:A:C6	1:O:1206:U:C4	2.78	0.72
1:O:506:G:H22	1:O:509:A:H5'	1.53	0.72
24:V:65:VAL:HA	24:V:68:THR:HG22	1.72	0.72
10:H:142:VAL:HG13	36:H:8379:HOH:O	1.89	0.72
10:H:14:TYR:H	10:H:91:HIS:CE1	2.07	0.72
1:O:1666:C:H2'	1:O:1667:A:H5'	1.71	0.72
1:O:1187:U:HO2'	1:O:1189:A:H2	1.35	0.72
1:O:31:C:H2'	36:O:7224:HOH:O	1.89	0.72
4:B:221:GLN:HE22	12:J:42:ASN:HD22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:164:THR:HG22	14:L:167:GLY:N	2.03	0.72
1:O:1594:C:OP2	17:O:120:ARG:HD2	1.89	0.72
1:O:877:G:H5'	1:O:878:G:OP1	1.89	0.71
3:A:199:HIS:CD2	3:A:201:PHE:H	2.07	0.71
24:V:21:LEU:HD22	24:V:26:ILE:HD11	1.72	0.71
1:O:1771:U:H4'	27:Y:20:LEU:HD21	1.71	0.71
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.54	0.71
10:H:41:THR:HA	36:H:8392:HOH:O	1.88	0.71
36:O:3192:HOH:O	14:L:79:LYS:HD3	1.90	0.71
17:O:115:SER:N	17:O:118:GLN:HE21	1.84	0.71
14:L:106:ASN:HD22	14:L:114:VAL:HG23	1.53	0.71
2:9:6:C:OP1	15:M:37:ARG:NH1	2.23	0.71
22:T:14:GLU:O	22:T:17:THR:HB	1.91	0.71
1:O:1170:U:O2'	1:O:1172:G:N7	2.21	0.71
1:O:183:A:H5'	14:L:157:LEU:HD12	1.73	0.71
10:H:26:LYS:HG2	10:H:28:ILE:H	1.55	0.71
14:L:87:MET:HB2	14:L:91:ILE:HD11	1.72	0.71
3:A:210:GLY:HA3	36:A:8590:HOH:O	1.90	0.71
10:H:47:GLU:HB3	10:H:133:ILE:CD1	2.20	0.71
13:K:148:GLU:HA	36:K:8571:HOH:O	1.90	0.71
14:L:87:MET:CB	30:2:46:ILE:HG21	2.20	0.71
1:O:2291:A:C8	1:O:2309:C:H5'	2.25	0.71
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.05	0.71
14:L:35:PRO:CG	14:L:38:VAL:HG23	2.20	0.71
1:O:1119:G:N2	1:O:1246:A:C2	2.55	0.71
7:E:101:GLU:HB2	7:E:116:THR:O	1.91	0.71
11:I:107:ASN:HD21	11:I:109:TYR:HB2	1.56	0.71
19:Q:99:ALA:HB1	19:Q:109:MET:CE	2.20	0.71
1:O:281:U:H2'	1:O:282:C:O4'	1.90	0.71
12:J:81:ARG:HD3	12:J:87:ARG:NH1	2.06	0.71
17:O:59:ARG:NH2	17:O:66:GLN:HE22	1.89	0.70
1:O:2896:A:H5''	36:O:5618:HOH:O	1.90	0.70
9:G:12:ILE:N	9:G:13:PRO:HD3	2.05	0.70
19:Q:18:LEU:HD12	19:Q:143:VAL:HG11	1.71	0.70
15:M:80:SER:HB2	36:M:8537:HOH:O	1.90	0.70
1:O:1166:A:H1'	1:O:1192:A:C2	2.26	0.70
29:1:41:HIS:N	29:1:45:ASN:HD22	1.89	0.70
4:B:103:ASP:HB2	36:B:8598:HOH:O	1.89	0.70
10:H:137:ASN:O	10:H:139:ASP:N	2.25	0.70
11:I:45:VAL:HG23	11:I:130:VAL:O	1.91	0.70
16:N:14:LEU:HD23	16:N:102:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:H8	1.57	0.70
26:X:187:VAL:HG23	26:X:192:ASP:CB	2.22	0.70
10:H:3:GLY:HA2	10:H:57:ARG:HH12	1.57	0.70
13:K:136:ALA:HB3	36:K:8572:HOH:O	1.90	0.70
14:L:113:ARG:NH2	14:L:156:ARG:HG2	2.07	0.70
30:2:73:GLU:HB3	36:2:8560:HOH:O	1.91	0.70
1:0:2468:A:H61	30:2:48:ASN:HD21	1.38	0.70
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.21	0.70
5:C:139:VAL:HG13	36:C:8447:HOH:O	1.91	0.70
7:E:68:HIS:O	7:E:72:MET:HG3	1.92	0.70
1:0:1835:U:C5	1:0:1840:A:N7	2.58	0.69
2:9:39:U:H1'	2:9:44:A:H61	1.56	0.69
36:C:8359:HOH:O	16:N:3:THR:HG21	1.92	0.69
1:0:1603:A:H5'	1:0:1605:G:O4'	1.92	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.24	0.69
29:1:18:ASN:HD21	29:1:40:ARG:H	1.41	0.69
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.75	0.69
1:0:236:A:H4'	1:0:237:G:H5'	1.75	0.69
14:L:164:THR:HG23	14:L:165:SER:N	2.06	0.69
6:D:95:THR:O	6:D:97:GLN:N	2.23	0.69
11:I:107:ASN:ND2	11:I:109:TYR:H	1.89	0.69
12:J:22:ASP:HB2	36:J:5264:HOH:O	1.91	0.69
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.26	0.69
10:H:71:TYR:C	10:H:73:GLN:H	1.96	0.69
2:9:29:C:H2'	2:9:30:C:H5'	1.75	0.69
10:H:31:PHE:HE2	10:H:87:LYS:O	1.76	0.69
1:0:1172:G:H1'	36:0:4485:HOH:O	1.91	0.69
5:C:140:VAL:HB	36:C:8450:HOH:O	1.93	0.69
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.73	0.69
9:G:12:ILE:HA	36:G:4499:HOH:O	1.93	0.69
25:W:71:ARG:HB3	25:W:88:GLU:OE1	1.93	0.69
30:2:57:GLY:HA2	36:2:8526:HOH:O	1.92	0.69
1:0:1377:C:H6	1:0:1377:C:H5'	1.58	0.68
1:0:1474:C:C6	1:0:1474:C:H5'	2.28	0.68
27:Y:38:LYS:HE2	27:Y:45:LYS:CE	2.22	0.68
1:0:182:G:H5'	36:0:4666:HOH:O	1.94	0.68
7:E:100:ASP:HB2	36:E:2789:HOH:O	1.93	0.68
1:0:2346:C:O2'	6:D:52:THR:HG21	1.94	0.68
6:D:37:ALA:O	6:D:40:ILE:HG12	1.94	0.68
10:H:47:GLU:HB3	10:H:133:ILE:HD13	1.75	0.68
21:S:9:LYS:HE3	21:S:13:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:6982:HOH:O	4:B:211:THR:HG21	1.93	0.68
10:H:53:PRO:HG3	10:H:127:GLY:H	1.59	0.68
12:J:34:VAL:HG22	12:J:47:ALA:HB2	1.76	0.68
1:O:1194:A:N6	1:O:1206:U:C4	2.61	0.68
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.22	0.68
24:V:13:MET:CE	24:V:17:ILE:HG22	2.24	0.68
24:V:149:LEU:HG	24:V:153:MET:CE	2.24	0.68
3:A:192:VAL:HG13	36:A:8558:HOH:O	1.92	0.68
1:O:711:G:H1'	36:O:6617:HOH:O	1.93	0.68
5:C:236:THR:H	5:C:239:ALA:HB3	1.59	0.68
24:V:21:LEU:HB3	24:V:26:ILE:HG12	1.76	0.68
6:D:97:GLN:HG2	6:D:97:GLN:O	1.94	0.68
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.74	0.68
5:C:246:ARG:NE	36:C:8424:HOH:O	2.27	0.68
12:J:74:VAL:CG1	12:J:113:ILE:HG12	2.24	0.68
14:L:52:LEU:HD21	36:L:8616:HOH:O	1.93	0.68
36:9:8462:HOH:O	15:M:147:ILE:HB	1.94	0.68
7:E:69:ILE:HA	7:E:72:MET:CE	2.24	0.67
19:Q:39:THR:HB	19:Q:42:GLU:HG3	1.74	0.67
11:I:74:ARG:HB3	11:I:74:ARG:HH11	1.57	0.67
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.75	0.67
14:L:139:PRO:O	14:L:140:ALA:CB	2.40	0.67
24:V:21:LEU:HD22	24:V:26:ILE:CD1	2.25	0.67
1:O:396:U:H1'	36:O:7164:HOH:O	1.95	0.67
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.75	0.67
3:A:33:GLU:O	3:A:34:ASP:HB2	1.94	0.67
4:B:125:GLU:O	4:B:129:ARG:HG3	1.94	0.67
19:Q:111:ILE:HG23	19:Q:145:LEU:HD11	1.76	0.67
23:U:12:THR:CG2	23:U:15:GLU:HG3	2.21	0.67
1:O:1505:U:H6	1:O:1505:U:H5'	1.58	0.67
1:O:1819:G:H2'	1:O:1820:G:H4'	1.76	0.67
8:F:58:GLU:OE1	14:L:27:ARG:NH2	2.23	0.67
24:V:21:LEU:HD21	24:V:48:VAL:HG11	1.76	0.67
1:O:1205:U:C2'	1:O:1206:U:H5''	2.24	0.67
1:O:1701:A:H4'	1:O:1702:U:C5'	2.24	0.67
1:O:2426:G:H1'	36:O:5611:HOH:O	1.92	0.67
1:O:282:C:H1'	1:O:368:C:N4	2.09	0.67
3:A:36:ASP:OD2	3:A:85:ASP:HB2	1.94	0.67
4:B:51:VAL:HG23	4:B:329:TYR:O	1.95	0.67
10:H:136:VAL:HG22	10:H:137:ASN:O	1.94	0.67
14:L:34:GLU:HB3	14:L:35:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:16:ARG:NH1	36:B:8621:HOH:O	2.28	0.67
4:B:62:ARG:HA	4:B:65:MET:CE	2.24	0.67
23:U:64:GLY:O	23:U:65:ASP:HB2	1.93	0.67
1:O:1209:C:H2'	1:O:1210:G:H8	1.59	0.67
1:O:1119:G:H8	11:I:52:GLN:HE22	1.41	0.67
1:O:2748:G:H2'	36:O:7073:HOH:O	1.94	0.67
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.76	0.67
24:V:13:MET:HE3	24:V:17:ILE:HG22	1.76	0.67
1:O:1205:U:H2'	1:O:1206:U:H5''	1.75	0.67
14:L:63:VAL:HG21	14:L:109:PHE:CE1	2.30	0.67
5:C:162:VAL:HG13	5:C:232:LEU:HD21	1.77	0.66
10:H:28:ILE:HA	10:H:62:GLU:OE1	1.94	0.66
27:Y:61:GLY:HA3	36:Y:8427:HOH:O	1.95	0.66
10:H:26:LYS:HD2	10:H:28:ILE:CD1	2.22	0.66
10:H:46:VAL:O	10:H:146:TRP:HH2	1.78	0.66
21:S:47:THR:HB	21:S:100:ASP:HB3	1.77	0.66
24:V:6:GLN:HB2	24:V:26:ILE:CD1	2.25	0.66
1:O:2508:C:H2'	36:O:6273:HOH:O	1.94	0.66
2:9:14:G:H5'	2:9:14:G:C8	2.29	0.66
26:X:141:THR:HG23	36:X:8591:HOH:O	1.94	0.66
26:X:185:VAL:HG12	36:X:8572:HOH:O	1.94	0.66
16:N:32:ARG:O	16:N:32:ARG:HD3	1.94	0.66
25:W:76:ARG:HG3	25:W:76:ARG:HH11	1.60	0.66
1:O:1058:A:H2'	1:O:1060:C:H5''	1.77	0.66
9:G:12:ILE:HG13	36:G:6833:HOH:O	1.94	0.66
1:O:1730:G:H5'	1:O:1731:C:C5	2.31	0.66
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.96	0.66
17:O:18:LYS:O	17:O:21:VAL:HG22	1.95	0.66
1:O:1080:C:H4'	1:O:1081:A:OP1	1.95	0.66
1:O:1766:U:O2	1:O:1778:A:H5'	1.96	0.66
1:O:2908:A:H2'	1:O:2909:G:O4'	1.96	0.66
2:9:6:C:C5'	15:M:37:ARG:NH1	2.57	0.66
28:Z:25:LYS:HE2	36:1:7213:HOH:O	1.93	0.66
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.78	0.66
14:L:138:HIS:ND1	14:L:139:PRO:O	2.22	0.66
16:N:87:THR:O	16:N:91:GLN:HG3	1.96	0.66
19:Q:44:VAL:O	19:Q:48:GLU:HG3	1.94	0.66
1:O:2414:A:H2'	1:O:2415:A:C8	2.30	0.66
14:L:149:TRP:O	14:L:152:ARG:HG2	1.95	0.66
1:O:1684:A:H1'	29:1:43:ARG:HH22	1.60	0.66
1:O:2635:A:O2'	1:O:2636:C:H5'	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:69:A:H5'	1:0:69:A:C8	2.31	0.66
36:0:4461:HOH:O	2:9:103:A:H4'	1.95	0.66
4:B:307:ARG:HB2	4:B:307:ARG:HH11	1.59	0.66
10:H:85:ILE:HB	10:H:132:PHE:CE2	2.31	0.66
4:B:36:PRO:HA	4:B:168:GLY:CA	2.26	0.65
10:H:150:LYS:HB2	10:H:157:ILE:HD12	1.78	0.65
17:O:10:ALA:HA	17:O:13:VAL:HG12	1.78	0.65
1:0:1191:A:H3'	1:0:1192:A:H5''	1.79	0.65
1:0:2533:C:H5'	1:0:2533:C:H6	1.61	0.65
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.65
29:1:41:HIS:H	29:1:45:ASN:ND2	1.94	0.65
4:B:204:GLY:HA3	36:B:8659:HOH:O	1.95	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.65
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.77	0.65
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.11	0.65
1:0:2505:G:O2'	1:0:2506:A:H5'	1.97	0.65
1:0:2878:U:H2'	1:0:2879:A:O4'	1.96	0.65
4:B:141:ARG:HD2	4:B:163:GLU:OE2	1.97	0.65
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.79	0.65
6:D:69:ILE:O	6:D:69:ILE:HG22	1.96	0.65
12:J:32:ILE:HD11	12:J:56:SER:HB3	1.77	0.65
15:M:183:ASP:OD2	15:M:186:LEU:HD12	1.95	0.65
16:N:14:LEU:CD2	16:N:102:ILE:HD11	2.26	0.65
1:0:20:G:H21	19:Q:117:HIS:HD2	1.45	0.65
21:S:41:ARG:HH11	21:S:41:ARG:HG2	1.60	0.65
27:Y:39:CYS:HA	27:Y:47:LEU:HD11	1.77	0.65
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.79	0.65
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.60	0.65
14:L:104:ARG:O	14:L:108:LYS:HG2	1.97	0.65
1:0:1666:C:O2'	1:0:1667:A:H5''	1.97	0.65
1:0:2690:U:O2'	7:E:111:LYS:HE3	1.97	0.65
6:D:99:ASP:HB2	6:D:103:ASN:HB2	1.79	0.65
10:H:166:ASN:N	10:H:166:ASN:HD22	1.94	0.65
21:S:53:GLY:HA3	36:S:6384:HOH:O	1.94	0.65
21:S:9:LYS:HE3	21:S:13:ARG:HH11	1.62	0.65
1:0:2756:U:H3	1:0:2896:A:H2	1.43	0.65
2:9:49:G:H5''	36:9:8462:HOH:O	1.97	0.65
5:C:115:LEU:O	5:C:118:THR:HB	1.97	0.65
11:I:131:THR:HG22	11:I:134:GLU:H	1.61	0.65
21:S:32:ARG:NH1	21:S:38:ARG:HH12	1.95	0.65
24:V:4:LEU:O	24:V:32:CYS:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:23:U:H5''	2:9:23:U:C6	2.32	0.65
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.79	0.65
10:H:3:GLY:HA2	10:H:57:ARG:NH1	2.11	0.65
14:L:94:LYS:HE3	36:L:8582:HOH:O	1.95	0.65
1:0:299:U:H5'	36:0:6860:HOH:O	1.97	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.97	0.65
36:0:7116:HOH:O	27:Y:31:ILE:HG13	1.96	0.65
1:0:2783:A:H3'	36:0:4742:HOH:O	1.96	0.64
7:E:11:VAL:HG12	7:E:12:ASP:N	2.12	0.64
6:D:135:VAL:HG22	6:D:136:ARG:H	1.62	0.64
8:F:99:THR:HA	36:F:3461:HOH:O	1.96	0.64
1:0:603:A:H5''	1:0:604:G:OP1	1.97	0.64
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.79	0.64
10:H:27:LYS:N	10:H:58:HIS:HD2	1.92	0.64
14:L:80:GLY:O	14:L:81:ARG:HD3	1.97	0.64
2:9:69:U:OP1	15:M:4:PRO:HG3	1.98	0.64
25:W:72:VAL:HG22	25:W:85:VAL:HG12	1.78	0.64
7:E:6:GLU:HA	7:E:46:THR:HG22	1.80	0.64
1:0:2672:C:H1'	36:B:8639:HOH:O	1.97	0.64
5:C:76:ARG:HD3	36:C:8369:HOH:O	1.95	0.64
23:U:44:GLY:O	23:U:48:GLU:HG2	1.98	0.64
1:0:1701:A:H5''	1:0:1702:U:H3'	1.80	0.64
3:A:223:ARG:HG3	36:A:8604:HOH:O	1.97	0.64
4:B:185:GLY:HA2	36:B:8638:HOH:O	1.97	0.64
6:D:25:MET:CE	6:D:37:ALA:HB1	2.27	0.64
7:E:7:ILE:HD11	7:E:11:VAL:C	2.18	0.64
7:E:15:GLN:NE2	7:E:40:VAL:O	2.29	0.64
10:H:69:ASN:O	10:H:72:VAL:HG12	1.98	0.64
1:0:259:G:H21	14:L:58:GLN:NE2	1.96	0.64
24:V:154:ARG:C	36:V:4276:HOH:O	2.35	0.64
1:0:1778:A:H2'	1:0:1779:A:H5'	1.80	0.64
1:0:2438:G:H5'	36:0:5690:HOH:O	1.97	0.64
2:9:13:A:O2'	2:9:14:G:H5''	1.98	0.64
1:0:2676:C:H4'	11:I:70:PHE:CE1	2.33	0.64
20:R:43:GLU:HB3	36:R:8341:HOH:O	1.97	0.64
24:V:38:THR:HG22	36:V:3580:HOH:O	1.98	0.64
1:0:2769:C:H2'	1:0:2770:G:O4'	1.98	0.64
10:H:140:PRO:HB3	36:H:8379:HOH:O	1.98	0.64
1:0:1189:A:H3'	36:0:7217:HOH:O	1.97	0.63
1:0:1441:G:H1'	36:0:7301:HOH:O	1.97	0.63
24:V:21:LEU:HD21	24:V:48:VAL:CG1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:64:ARG:HD2	36:L:8586:HOH:O	1.97	0.63
1:0:902:G:N7	13:K:18:HIS:HD2	1.97	0.63
1:0:506:G:H22	1:0:509:A:H5''	1.62	0.63
5:C:27:ARG:HG3	5:C:29:ASP:OD1	1.99	0.63
14:L:30:GLU:O	14:L:34:GLU:HG3	1.98	0.63
19:Q:39:THR:HG23	19:Q:107:GLU:O	1.99	0.63
1:0:1168:C:H2'	1:0:1169:U:O4'	1.99	0.63
1:0:558:C:O2'	1:0:559:U:H5''	1.98	0.63
12:J:62:PRO:HG3	12:J:65:ARG:HH21	1.64	0.63
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.63
5:C:142:ASP:OD1	5:C:237:GLU:HB3	1.99	0.63
6:D:55:LYS:HA	36:D:6752:HOH:O	1.99	0.63
5:C:107:ARG:NE	36:C:8457:HOH:O	2.24	0.63
1:0:962:C:H1'	15:M:5:ARG:HH12	1.62	0.63
26:X:187:VAL:CG2	26:X:192:ASP:HB2	2.28	0.63
6:D:99:ASP:CB	6:D:103:ASN:H	2.12	0.63
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.79	0.63
13:K:73:VAL:HG23	13:K:74:THR:H	1.62	0.63
1:0:2830:U:H3'	36:O:4738:HOH:O	1.97	0.63
1:0:69:A:H5'	1:0:69:A:H8	1.64	0.63
14:L:87:MET:CG	30:2:46:ILE:HG21	2.29	0.63
5:C:16:VAL:HG12	5:C:17:ASP:N	2.14	0.63
14:L:37:VAL:CG1	14:L:63:VAL:HG11	2.28	0.63
26:X:133:HIS:HD2	36:X:8584:HOH:O	1.80	0.63
26:X:212:ARG:HD2	36:X:8605:HOH:O	1.99	0.63
3:A:55:VAL:HG22	3:A:68:ILE:O	1.99	0.62
10:H:44:ALA:HA	10:H:163:PRO:O	1.99	0.62
1:0:1741:U:H5'	1:0:1742:A:OP1	1.99	0.62
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.62
4:B:145:HIS:HD2	4:B:146:THR:O	1.83	0.62
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.33	0.62
15:M:12:ARG:HD3	15:M:18:THR:OG1	1.99	0.62
21:S:24:ARG:HH21	21:S:39:ASN:HD22	1.45	0.62
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.32	0.62
1:0:2851:G:O2'	1:0:2852:A:H5'	1.99	0.62
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.80	0.62
1:0:474:C:O3'	5:C:73:LEU:HD21	1.99	0.62
10:H:130:HIS:CD2	10:H:133:ILE:HD11	2.34	0.62
10:H:35:ASN:ND2	10:H:80:ASN:HA	2.13	0.62
25:W:75:ALA:O	25:W:83:ALA:HA	1.99	0.62
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:7:ILE:HD11	7:E:11:VAL:O	1.98	0.62
10:H:2:PRO:HB2	36:H:8364:HOH:O	1.99	0.62
15:M:37:ARG:NE	36:M:8535:HOH:O	2.32	0.62
19:Q:111:ILE:HG23	19:Q:145:LEU:CD1	2.29	0.62
1:O:1187:U:O2'	1:O:1189:A:H2	1.83	0.62
4:B:7:ARG:CG	4:B:7:ARG:HH11	2.10	0.62
1:O:1008:C:H5''	10:H:16:ARG:HH12	1.64	0.62
15:M:86:LEU:HD12	15:M:125:ALA:HB2	1.82	0.62
24:V:4:LEU:HD22	24:V:52:VAL:CG2	2.29	0.62
1:O:2587:U:H2'	1:O:2589:U:H5''	1.82	0.62
1:O:710:G:OP1	16:N:24:ALA:HB3	2.00	0.62
5:C:79:ARG:O	5:C:87:ARG:HG2	1.99	0.62
15:M:155:GLU:O	15:M:156:GLU:HG3	2.00	0.62
1:O:470:U:O2'	28:Z:16:HIS:HD2	1.82	0.62
1:O:182:G:O3'	14:L:157:LEU:HD13	1.99	0.62
1:O:2638:G:H5'	36:O:4439:HOH:O	2.00	0.62
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.81	0.62
7:E:69:ILE:HA	7:E:72:MET:HE3	1.82	0.62
12:J:55:VAL:HG12	12:J:56:SER:N	2.15	0.62
12:J:75:ARG:CZ	36:J:4172:HOH:O	2.46	0.62
19:Q:18:LEU:HB2	19:Q:143:VAL:CG1	2.29	0.62
24:V:122:ARG:NH2	24:V:154:ARG:HD2	2.14	0.62
1:O:417:G:P	36:O:6944:HOH:O	2.58	0.62
2:9:39:U:H1'	2:9:44:A:N6	2.14	0.62
6:D:149:ARG:NH1	36:D:3066:HOH:O	2.23	0.62
15:M:159:TYR:HB3	15:M:162:ASP:HB2	1.82	0.62
26:X:186:ARG:HG2	26:X:186:ARG:HH11	1.65	0.62
1:O:2578:G:H5'	1:O:2578:G:H8	1.64	0.62
1:O:2346:C:O5'	1:O:2346:C:H6	1.83	0.61
1:O:338:C:H5''	36:C:8421:HOH:O	1.97	0.61
2:9:25:G:C3'	2:9:26:C:H5'	2.27	0.61
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.81	0.61
11:I:103:VAL:HG12	36:I:5907:HOH:O	1.99	0.61
1:O:1118:A:H62	1:O:1244:U:H3	1.48	0.61
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.80	0.61
1:O:338:C:H4'	5:C:174:ILE:CD1	2.30	0.61
6:D:93:LEU:HB3	6:D:97:GLN:OE1	2.01	0.61
10:H:139:ASP:HA	36:H:8369:HOH:O	1.99	0.61
13:K:67:ARG:O	13:K:71:GLU:HG3	1.99	0.61
15:M:71:TRP:CE3	15:M:175:LEU:HD22	2.35	0.61
2:9:48:C:H4'	15:M:141:ARG:HH21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:237:GLU:HB2	36:C:8430:HOH:O	2.00	0.61
6:D:35:ALA:N	36:D:5576:HOH:O	2.32	0.61
10:H:139:ASP:H	10:H:140:PRO:HD3	1.62	0.61
2:9:42:C:H2'	36:9:8497:HOH:O	2.00	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
8:F:107:VAL:O	8:F:111:ILE:HG13	2.00	0.61
10:H:127:GLY:O	10:H:128:ALA:HB3	2.00	0.61
13:K:72:ASN:HB2	36:K:8580:HOH:O	2.00	0.61
1:0:1120:U:H5''	1:0:1120:U:C6	2.36	0.61
7:E:132:THR:HB	36:E:2227:HOH:O	2.01	0.61
20:R:81:ILE:HG23	36:R:8334:HOH:O	2.00	0.61
1:0:1299:G:O6	13:K:6:ARG:HD3	2.01	0.61
15:M:23:ARG:NH1	36:M:8549:HOH:O	2.34	0.61
1:0:2779:G:H21	7:E:143:GLN:NE2	1.98	0.61
1:0:558:C:C2'	1:0:559:U:H5''	2.31	0.61
6:D:23:VAL:O	6:D:23:VAL:HG23	2.01	0.61
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.29	0.61
14:L:169:ARG:HD2	36:L:8590:HOH:O	2.01	0.61
15:M:184:ILE:HG22	15:M:185:GLU:HG3	1.83	0.61
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.61
1:0:1189:A:H1'	1:0:1209:C:O4'	2.01	0.61
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.30	0.61
9:G:23:ILE:O	9:G:27:ILE:HG13	2.01	0.61
36:J:408:HOH:O	22:T:37:GLU:HB3	2.00	0.61
25:W:74:ALA:CB	25:W:85:VAL:HG22	2.31	0.61
1:0:281:U:O2'	1:0:282:C:H5'	2.01	0.61
6:D:38:GLU:HB3	6:D:49:PRO:HG2	1.83	0.61
1:0:553:G:P	26:X:204:ARG:HH22	2.24	0.61
1:0:1525:G:H5'	1:0:1526:A:OP2	2.01	0.60
7:E:79:GLY:HA3	36:E:7046:HOH:O	2.00	0.60
24:V:21:LEU:HD13	24:V:26:ILE:HD11	1.83	0.60
1:0:111:C:O2'	28:Z:20:ARG:HG2	2.01	0.60
1:0:1667:A:C8	1:0:1667:A:H5'	2.34	0.60
8:F:110:GLU:HG2	36:F:6926:HOH:O	2.01	0.60
10:H:118:PRO:HD2	36:H:8339:HOH:O	2.00	0.60
1:0:1244:U:OP1	11:I:18:ILE:HD13	2.01	0.60
1:0:2570:G:H5''	36:0:4423:HOH:O	2.02	0.60
2:9:41:C:O4'	6:D:50:VAL:HG23	2.01	0.60
10:H:83:PHE:HZ	10:H:146:TRP:HE1	1.46	0.60
15:M:47:LEU:HD13	15:M:97:VAL:HG11	1.82	0.60
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.66	0.60
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.60
6:D:166:ILE:HD12	36:D:6326:HOH:O	2.01	0.60
27:Y:53:GLY:HA2	27:Y:67:GLY:O	2.00	0.60
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.02	0.60
4:B:7:ARG:CD	4:B:9:GLY:O	2.50	0.60
4:B:258:GLY:H	4:B:260:HIS:CE1	2.20	0.60
7:E:23:GLU:HG2	7:E:28:SER:CB	2.32	0.60
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.70	0.60
14:L:87:MET:CB	30:2:46:ILE:HD13	2.30	0.60
1:O:1641:A:H2'	1:O:1642:A:H5'	1.83	0.60
4:B:140:LEU:HD23	36:B:8583:HOH:O	2.01	0.60
9:G:12:ILE:N	9:G:13:PRO:CD	2.65	0.60
1:O:447:A:OP1	21:S:2:LYS:HG2	2.02	0.60
3:A:170:VAL:HG22	27:Y:22:ILE:HG23	1.84	0.60
10:H:5:MET:HG3	36:H:8364:HOH:O	2.01	0.60
4:B:238:ASN:HD22	4:B:240:GLY:N	2.00	0.60
23:U:39:ALA:C	23:U:41:GLU:H	2.05	0.60
23:U:55:ARG:O	23:U:59:ILE:HG12	2.02	0.60
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.84	0.60
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.84	0.60
5:C:118:THR:O	5:C:136:VAL:HG13	2.02	0.60
7:E:81:GLU:HG2	7:E:134:SER:CB	2.32	0.60
11:I:74:ARG:CB	11:I:74:ARG:HH11	2.14	0.60
24:V:88:THR:CG2	24:V:89:ASP:H	2.09	0.60
25:W:21:PRO:HG2	25:W:24:LYS:HD3	1.83	0.60
14:L:48:ARG:NH2	36:L:8562:HOH:O	2.34	0.59
15:M:151:ASP:O	15:M:154:LEU:HB2	2.02	0.59
25:W:15:ARG:HH11	25:W:15:ARG:HB3	1.66	0.59
1:O:2310:G:OP2	10:H:114:PRO:HD2	2.01	0.59
11:I:75:PRO:HG2	11:I:105:LEU:HD21	1.84	0.59
13:K:145:LEU:O	13:K:148:GLU:HG3	2.02	0.59
13:K:53:ARG:NH2	13:K:57:VAL:HG12	2.16	0.59
25:W:25:ARG:HD2	36:W:3861:HOH:O	2.02	0.59
4:B:307:ARG:CG	4:B:307:ARG:HH11	2.14	0.59
5:C:12:THR:HB	36:C:8440:HOH:O	2.00	0.59
15:M:38:LYS:HD2	15:M:114:LYS:HE3	1.84	0.59
25:W:30:MET:HE1	25:W:58:ALA:HB3	1.84	0.59
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.84	0.59
20:R:38:ALA:O	20:R:42:GLU:HG3	2.03	0.59
5:C:76:ARG:HG2	5:C:78:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:58:HIS:HA	10:H:61:LEU:HD23	1.84	0.59
10:H:84:ARG:NH2	10:H:135:TRP:HH2	2.00	0.59
13:K:77:ALA:HB3	36:K:8530:HOH:O	2.00	0.59
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.67	0.59
1:0:2721:U:H4'	12:J:87:ARG:HG3	1.84	0.59
29:1:22:PRO:HG2	29:1:25:VAL:CG2	2.32	0.59
14:L:174:ARG:HG3	36:L:8521:HOH:O	2.02	0.59
18:P:64:GLU:HG3	18:P:74:ASP:OD2	2.02	0.59
19:Q:39:THR:HB	19:Q:42:GLU:CG	2.32	0.59
26:X:126:PRO:HG2	26:X:128:PHE:CE1	2.38	0.59
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.14	0.59
6:D:95:THR:C	6:D:97:GLN:H	2.06	0.59
10:H:27:LYS:H	10:H:58:HIS:CD2	2.12	0.59
10:H:56:ILE:HG22	10:H:61:LEU:HD22	1.84	0.59
11:I:131:THR:HG22	11:I:133:GLY:N	2.17	0.59
36:0:5309:HOH:O	14:L:170:CYS:SG	2.32	0.59
15:M:47:LEU:HD12	15:M:92:ALA:HB1	1.85	0.59
1:0:1159:G:H21	1:0:1189:A:H8	1.50	0.59
1:0:558:C:H5'	36:0:4769:HOH:O	2.03	0.59
6:D:65:GLU:HG3	36:D:6752:HOH:O	2.01	0.59
22:T:9:CYS:HA	22:T:52:THR:HG23	1.83	0.59
1:0:1119:G:N2	1:0:1246:A:H2	1.98	0.59
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.59
13:K:133:VAL:HB	36:K:8557:HOH:O	2.02	0.59
14:L:114:VAL:HG21	14:L:159:THR:HG21	1.85	0.59
15:M:43:VAL:HG11	15:M:81:ALA:HA	1.85	0.59
24:V:80:ASP:O	24:V:84:VAL:HG23	2.03	0.59
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.03	0.58
1:0:1166:A:H1'	1:0:1192:A:N1	2.17	0.58
1:0:2004:U:H4'	36:0:4818:HOH:O	2.03	0.58
1:0:1329:A:C2	36:0:4193:HOH:O	2.45	0.58
1:0:1528:A:H2'	1:0:1529:G:O4'	2.03	0.58
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
3:A:88:ILE:HG22	3:A:88:ILE:O	2.02	0.58
4:B:307:ARG:CB	4:B:307:ARG:HH11	2.16	0.58
36:0:3172:HOH:O	14:L:79:LYS:HD2	2.02	0.58
27:Y:28:ASP:O	27:Y:31:ILE:HG22	2.03	0.58
1:0:285:A:H2'	1:0:286:U:O4'	2.03	0.58
1:0:316:A:H5'	21:S:54:ASP:OD2	2.02	0.58
1:0:31:C:H4'	36:0:6950:HOH:O	2.02	0.58
29:1:22:PRO:HG2	29:1:25:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:25:VAL:HG22	30:2:68:LYS:HG3	1.84	0.58
2:9:92:G:H22	10:H:52:LYS:NZ	2.01	0.58
3:A:164:ARG:NE	36:A:8591:HOH:O	2.35	0.58
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.21	0.58
15:M:78:MET:HB2	15:M:79:PRO:HD3	1.86	0.58
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.67	0.58
27:Y:62:TYR:CE2	27:Y:64:ILE:HG23	2.38	0.58
28:Z:21:ARG:HD2	28:Z:37:CYS:SG	2.43	0.58
1:0:1887:U:OP1	27:Y:21:LYS:HE3	2.03	0.58
1:0:2064:U:H5'	1:0:2652:U:O3'	2.04	0.58
1:0:485:A:N3	1:0:487:G:H5''	2.18	0.58
3:A:175:LYS:HE2	36:A:8579:HOH:O	2.03	0.58
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.68	0.58
36:0:3353:HOH:O	10:H:11:LYS:HE2	2.03	0.58
13:K:114:VAL:HG11	36:K:8572:HOH:O	2.02	0.58
15:M:62:HIS:HB3	15:M:65:ASP:OD1	2.03	0.58
10:H:45:GLN:HE21	10:H:135:TRP:HE1	1.51	0.58
10:H:46:VAL:HG12	10:H:146:TRP:CZ3	2.37	0.58
36:0:3496:HOH:O	21:S:82:THR:HA	2.03	0.58
26:X:144:ARG:NH1	36:X:8578:HOH:O	2.33	0.58
1:0:2862:G:H4'	4:B:336:GLN:O	2.03	0.58
1:0:328:U:O4'	5:C:202:THR:HG22	2.03	0.58
20:R:81:ILE:HG12	36:R:8334:HOH:O	2.03	0.58
3:A:37:VAL:HG22	36:A:8599:HOH:O	2.04	0.58
7:E:172:PRO:HB3	36:E:6931:HOH:O	2.03	0.58
13:K:143:THR:CG2	13:K:144:ASP:N	2.66	0.58
14:L:108:LYS:HE3	36:L:8614:HOH:O	2.04	0.58
4:B:267:LYS:HD3	36:B:8528:HOH:O	2.02	0.58
22:T:52:THR:HG22	22:T:54:THR:N	2.19	0.58
23:U:58:THR:O	23:U:62:GLU:HG3	2.04	0.58
27:Y:13:ARG:NH1	36:Y:8421:HOH:O	2.37	0.58
1:0:1118:A:H8	1:0:1119:G:H5''	1.67	0.57
1:0:1878:G:H1'	36:0:5640:HOH:O	2.03	0.57
13:K:143:THR:HG22	13:K:144:ASP:H	1.69	0.57
13:K:73:VAL:HG23	13:K:74:THR:N	2.19	0.57
13:K:90:ARG:NH2	13:K:121:ILE:HD11	2.19	0.57
15:M:154:LEU:O	15:M:155:GLU:HB3	2.04	0.57
1:0:1181:A:H2'	1:0:1182:C:O4'	2.03	0.57
4:B:62:ARG:CA	4:B:65:MET:HE3	2.34	0.57
15:M:34:LEU:HA	15:M:47:LEU:HD23	1.86	0.57
22:T:13:ILE:HG12	22:T:32:CYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1173:A:H2'	36:0:3856:HOH:O	2.04	0.57
1:0:371:U:H2'	1:0:372:A:H8	1.69	0.57
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.86	0.57
4:B:175:LEU:C	4:B:175:LEU:HD23	2.24	0.57
7:E:15:GLN:HG2	7:E:19:ASP:O	2.04	0.57
22:T:31:PHE:CG	22:T:37:GLU:HG2	2.39	0.57
22:T:52:THR:CG2	22:T:54:THR:HB	2.34	0.57
1:0:1120:U:H6	1:0:1120:U:H5''	1.69	0.57
1:0:1679:C:H5'	36:0:8834:HOH:O	2.05	0.57
1:0:2456:A:H5'	36:0:5210:HOH:O	2.04	0.57
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.16	0.57
36:0:4077:HOH:O	5:C:50:GLU:HG2	2.03	0.57
6:D:91:ALA:HB1	36:D:5198:HOH:O	2.03	0.57
8:F:37:THR:O	8:F:41:GLU:HG3	2.04	0.57
36:0:7216:HOH:O	14:L:154:ARG:HB2	2.04	0.57
4:B:329:TYR:CE2	22:T:15:PRO:HG2	2.38	0.57
23:U:39:ALA:N	23:U:40:PRO:CD	2.66	0.57
3:A:53:ALA:HB3	36:A:8608:HOH:O	2.05	0.57
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.31	0.57
3:A:164:ARG:HB2	27:Y:68:CYS:SG	2.44	0.57
1:0:2241:C:O2'	1:0:2242:U:H5'	2.04	0.57
1:0:2630:G:O6	3:A:206:ARG:NH2	2.37	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.34	0.57
2:9:20:G:O2'	2:9:21:G:H5'	2.05	0.57
7:E:31:ARG:NH1	36:E:5919:HOH:O	2.36	0.57
11:I:75:PRO:HG2	11:I:105:LEU:CD2	2.33	0.57
15:M:48:VAL:HG11	15:M:55:ASP:HB3	1.85	0.57
24:V:122:ARG:CZ	36:V:5817:HOH:O	2.53	0.57
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.57
6:D:86:THR:O	6:D:90:LEU:HG	2.05	0.57
12:J:115:ARG:HG3	12:J:116:GLU:N	2.19	0.57
20:R:33:SER:OG	20:R:36:GLU:HG3	2.05	0.57
23:U:4:HIS:HB3	36:U:6622:HOH:O	2.05	0.57
24:V:106:THR:OG1	24:V:109:GLU:HG3	2.04	0.57
25:W:31:ILE:O	25:W:35:GLU:HG3	2.05	0.57
1:0:2420:G:O2'	1:0:2421:G:H5'	2.04	0.57
1:0:449:A:N7	5:C:43:LYS:HG2	2.18	0.57
4:B:162:MET:HG3	4:B:310:ARG:NH1	2.19	0.57
9:G:12:ILE:HG22	9:G:12:ILE:O	2.05	0.57
10:H:48:LEU:HG	10:H:157:ILE:HG21	1.87	0.57
14:L:38:VAL:C	14:L:63:VAL:HG13	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:90:LEU:HB2	15:M:186:LEU:HD22	1.85	0.57
17:O:121:ASP:HB2	36:O:198:HOH:O	2.05	0.57
22:T:46:ALA:HB1	22:T:52:THR:HG21	1.87	0.57
26:X:144:ARG:NE	36:X:8615:HOH:O	2.37	0.57
1:O:1441:G:O2'	1:O:1442:A:H5'	2.05	0.57
1:O:2533:C:C6	1:O:2533:C:H5'	2.39	0.57
2:9:55:U:H4'	2:9:56:A:C8	2.39	0.57
2:9:76:G:C3'	2:9:77:A:H5''	2.28	0.57
4:B:162:MET:HG3	4:B:310:ARG:CZ	2.35	0.57
3:A:105:VAL:HG12	3:A:106:CYS:N	2.20	0.57
5:C:1:MET:HG2	5:C:2:GLN:N	2.18	0.57
8:F:50:VAL:HG21	8:F:63:ILE:HG21	1.87	0.57
12:J:34:VAL:CG2	12:J:47:ALA:HB2	2.33	0.57
14:L:60:ILE:C	14:L:61:ILE:HD12	2.25	0.57
15:M:154:LEU:HG	15:M:155:GLU:H	1.68	0.57
36:J:1387:HOH:O	22:T:20:MET:HE3	2.03	0.57
26:X:165:GLU:HB3	36:X:8597:HOH:O	2.04	0.57
1:O:797:A:O4'	27:Y:10:ARG:N	2.37	0.57
28:Z:28:HIS:CD2	28:Z:30:LYS:HB2	2.40	0.57
1:O:2419:U:H5''	1:O:2420:G:H5'	1.87	0.56
6:D:136:ARG:HD2	6:D:155:HIS:O	2.04	0.56
8:F:101:ALA:HB2	8:F:108:LEU:CD2	2.34	0.56
14:L:61:ILE:HG13	36:L:8624:HOH:O	2.04	0.56
5:C:214:THR:HG23	36:C:8436:HOH:O	2.05	0.56
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.04	0.56
10:H:14:TYR:N	10:H:91:HIS:CE1	2.74	0.56
10:H:166:ASN:N	10:H:166:ASN:ND2	2.52	0.56
20:R:51:GLN:HE21	20:R:53:ASN:ND2	2.02	0.56
24:V:125:HIS:CD2	24:V:127:GLY:H	2.23	0.56
1:O:738:G:H3'	36:O:6569:HOH:O	2.05	0.56
4:B:82:VAL:HG12	4:B:82:VAL:O	2.05	0.56
8:F:99:THR:O	8:F:100:ASP:HB2	2.05	0.56
20:R:51:GLN:NE2	20:R:53:ASN:HD21	2.00	0.56
24:V:31:HIS:HB3	36:V:5420:HOH:O	2.05	0.56
24:V:81:ASP:OD1	24:V:92:ASP:HB2	2.04	0.56
26:X:220:GLU:HG2	36:X:8551:HOH:O	2.04	0.56
1:O:200:U:H2'	36:O:9957:HOH:O	2.03	0.56
1:O:2676:C:H4'	11:I:70:PHE:HE1	1.70	0.56
1:O:289:G:N2	1:O:363:A:H2	2.00	0.56
3:A:121:ALA:O	3:A:124:VAL:HG22	2.05	0.56
6:D:103:ASN:ND2	6:D:134:LEU:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:93:LEU:HG	36:D:3862:HOH:O	2.05	0.56
10:H:75:SER:HB3	10:H:79:ALA:HB1	1.88	0.56
25:W:12:ILE:HD12	25:W:36:HIS:ND1	2.20	0.56
1:O:183:A:C5'	14:L:157:LEU:HD12	2.36	0.56
1:O:2718:C:H6	1:O:2718:C:H5'	1.70	0.56
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.56
1:O:380:A:H5''	14:L:48:ARG:NH2	2.21	0.56
15:M:64:SER:C	15:M:66:LEU:H	2.09	0.56
1:O:280:C:H2'	1:O:281:U:O4'	2.06	0.56
1:O:2890:A:H1'	22:T:56:ARG:HH21	1.70	0.56
1:O:2548:C:OP2	4:B:5:ARG:NH2	2.39	0.56
6:D:49:PRO:HG3	36:D:5828:HOH:O	2.05	0.56
11:I:130:VAL:HG12	11:I:131:THR:N	2.19	0.56
16:N:96:VAL:HA	36:N:4258:HOH:O	2.04	0.56
17:O:13:VAL:HG21	17:O:41:ARG:HG2	1.87	0.56
21:S:9:LYS:CE	21:S:13:ARG:NH1	2.68	0.56
1:O:1116:U:O2'	1:O:1118:A:C2	2.48	0.56
1:O:2781:U:H1'	7:E:139:GLU:OE2	2.05	0.56
1:O:2815:G:OP2	11:I:99:GLU:HG2	2.06	0.56
17:O:38:GLU:HA	17:O:41:ARG:NH1	2.21	0.56
19:Q:106:GLY:HA2	19:Q:109:MET:HE3	1.87	0.56
22:T:11:THR:HG22	22:T:53:ASP:OD2	2.06	0.56
10:H:109:ASP:HB2	36:H:8345:HOH:O	2.05	0.56
4:B:215:VAL:HB	4:B:234:ARG:HH12	1.70	0.56
10:H:47:GLU:HG2	10:H:133:ILE:HD12	1.87	0.56
12:J:62:PRO:HG3	12:J:65:ARG:NH2	2.20	0.56
14:L:37:VAL:HG13	14:L:63:VAL:HG11	1.88	0.56
15:M:159:TYR:HE2	15:M:163:PHE:HE2	1.54	0.56
24:V:108:ARG:HE	24:V:114:PRO:HG3	1.71	0.56
1:O:1119:G:H8	11:I:52:GLN:NE2	2.04	0.56
9:G:63:ARG:O	9:G:67:LEU:HG	2.05	0.56
10:H:39:GLY:O	10:H:41:THR:N	2.39	0.56
1:O:2081:A:H4'	11:I:69:TYR:CE1	2.41	0.56
18:P:11:ARG:HD3	36:P:5620:HOH:O	2.04	0.56
25:W:78:GLU:CG	25:W:79:GLU:H	2.18	0.56
1:O:797:A:C4'	27:Y:10:ARG:N	2.69	0.56
1:O:1134:G:H4'	10:H:151:MET:CE	2.23	0.56
1:O:1209:C:H2'	1:O:1210:G:C8	2.39	0.56
1:O:2821:C:H4'	4:B:116:PRO:HB3	1.88	0.56
3:A:212:PRO:HB2	36:A:8562:HOH:O	2.06	0.56
36:O:5761:HOH:O	3:A:22:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:11:HIS:C	6:D:13:MET:H	2.09	0.56
29:1:35:ARG:HB2	36:1:2691:HOH:O	2.06	0.55
6:D:10:PHE:CG	6:D:11:HIS:N	2.74	0.55
15:M:87:LEU:CD1	15:M:186:LEU:HD21	2.33	0.55
19:Q:18:LEU:HD12	19:Q:143:VAL:CG1	2.36	0.55
1:0:1086:A:C6	24:V:11:VAL:HG11	2.41	0.55
1:0:1667:A:H2'	1:0:1668:U:C6	2.41	0.55
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.88	0.55
5:C:16:VAL:HG12	5:C:17:ASP:H	1.69	0.55
5:C:98:ARG:NH1	36:C:8357:HOH:O	2.36	0.55
15:M:11:ARG:NH2	36:M:8521:HOH:O	2.39	0.55
25:W:25:ARG:HG2	36:W:5356:HOH:O	2.05	0.55
1:0:1524:U:OP1	1:0:1524:U:H4'	2.06	0.55
1:0:2604:A:H5'	36:0:5307:HOH:O	2.06	0.55
1:0:263:U:O4'	8:F:59:ILE:HD13	2.05	0.55
1:0:567:U:H5''	36:V:5817:HOH:O	2.06	0.55
36:0:6547:HOH:O	3:A:211:LYS:HG2	2.06	0.55
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.88	0.55
13:K:104:ASP:HB3	36:K:8563:HOH:O	2.07	0.55
27:Y:58:GLY:CA	36:Y:8439:HOH:O	2.47	0.55
30:2:18:GLN:OE1	30:2:73:GLU:HB3	2.05	0.55
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.88	0.55
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.21	0.55
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.42	0.55
7:E:11:VAL:HG13	7:E:23:GLU:O	2.05	0.55
26:X:144:ARG:CZ	36:X:8615:HOH:O	2.53	0.55
1:0:1185:U:H2'	1:0:1186:C:C6	2.41	0.55
36:0:5728:HOH:O	4:B:2:GLN:HA	2.05	0.55
9:G:64:ASN:HD22	9:G:64:ASN:N	2.03	0.55
10:H:97:LYS:HD3	10:H:117:LYS:HE2	1.88	0.55
10:H:139:ASP:N	10:H:140:PRO:CD	2.68	0.55
14:L:94:LYS:CE	36:L:8582:HOH:O	2.54	0.55
26:X:216:ARG:HD3	36:X:8571:HOH:O	2.05	0.55
1:0:2064:U:H5'	1:0:2652:U:H4'	1.88	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
6:D:174:VAL:HG13	36:D:6555:HOH:O	2.07	0.55
6:D:36:ASN:HA	36:D:7500:HOH:O	2.07	0.55
6:D:62:ASP:HA	36:D:4233:HOH:O	2.06	0.55
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.37	0.55
11:I:133:GLY:O	11:I:137:GLU:HG3	2.07	0.55
14:L:164:THR:HB	36:L:8519:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H5'	1:0:1868:G:C5'	2.36	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.55
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.06	0.55
14:L:74:ARG:HG3	14:L:74:ARG:HH11	1.72	0.55
36:0:8907:HOH:O	14:L:94:LYS:HE2	2.06	0.55
15:M:61:ALA:HB3	15:M:88:ALA:HB2	1.89	0.55
21:S:111:ARG:HB3	21:S:119:ALA:HB2	1.89	0.55
2:9:55:U:H4'	2:9:56:A:H8	1.70	0.55
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.72	0.55
1:0:2898:G:H4'	4:B:288:GLY:HA2	1.88	0.55
6:D:58:VAL:HG12	6:D:59:GLY:N	2.22	0.55
24:V:21:LEU:HB3	24:V:26:ILE:CG1	2.36	0.55
25:W:43:VAL:CG1	25:W:47:ALA:HB3	2.37	0.55
1:0:1123:A:C6	1:0:1238:C:H5'	2.42	0.55
1:0:1137:G:H1'	36:0:3386:HOH:O	2.06	0.55
1:0:1299:G:N2	36:0:4193:HOH:O	2.39	0.55
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.55
1:0:1615:A:H5'	36:0:3690:HOH:O	2.07	0.55
1:0:57:C:H5''	36:0:6278:HOH:O	2.06	0.55
10:H:59:ASN:H	10:H:59:ASN:ND2	2.04	0.55
26:X:235:GLU:CD	26:X:235:GLU:H	2.10	0.55
1:0:1669:A:H2'	1:0:1670:G:C8	2.42	0.55
1:0:2717:C:O2'	1:0:2718:C:H5''	2.06	0.55
6:D:154:LYS:H	6:D:154:LYS:CD	2.10	0.55
6:D:51:ARG:HD3	36:D:7636:HOH:O	2.07	0.55
8:F:101:ALA:HB2	8:F:108:LEU:HD22	1.88	0.55
11:I:107:ASN:HD22	11:I:109:TYR:H	1.52	0.55
11:I:99:GLU:HA	36:I:7377:HOH:O	2.06	0.55
15:M:170:GLU:O	15:M:174:GLU:HG3	2.07	0.55
15:M:49:THR:CG2	15:M:56:ASP:HB2	2.36	0.55
16:N:38:ARG:NH1	36:N:7674:HOH:O	2.40	0.55
17:O:80:ARG:HG2	17:O:87:ARG:CZ	2.37	0.55
19:Q:25:PHE:CE2	19:Q:29:LYS:HE2	2.42	0.55
20:R:23:LYS:HE2	36:R:8329:HOH:O	2.06	0.55
30:2:17:HIS:O	30:2:18:GLN:HG3	2.07	0.54
26:X:189:ASN:C	26:X:189:ASN:HD22	2.10	0.54
1:0:138:U:H5''	1:0:139:C:OP2	2.08	0.54
8:F:58:GLU:CD	14:L:27:ARG:HH22	2.10	0.54
17:O:16:VAL:HG12	17:O:17:GLY:N	2.22	0.54
25:W:74:ALA:HB2	25:W:85:VAL:HG13	1.88	0.54
26:X:112:GLU:CD	26:X:115:ARG:NH1	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:ARG:NH1	4:B:11:LEU:HD22	2.22	0.54
10:H:129:ASN:N	10:H:129:ASN:HD22	2.04	0.54
14:L:55:LYS:HB2	14:L:60:ILE:CD1	2.38	0.54
14:L:61:ILE:HA	36:L:8624:HOH:O	2.07	0.54
19:Q:33:ARG:NH1	36:Q:8541:HOH:O	2.39	0.54
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.54
1:0:1189:A:H1'	1:0:1209:C:H1'	1.89	0.54
1:0:2502:C:H2'	1:0:2503:A:H5'	1.89	0.54
1:0:283:U:H5''	1:0:284:C:P	2.47	0.54
1:0:542:A:H2'	1:0:543:G:O4'	2.07	0.54
13:K:143:THR:HG22	13:K:145:LEU:H	1.72	0.54
14:L:37:VAL:HG21	14:L:108:LYS:CG	2.38	0.54
19:Q:119:VAL:HG12	19:Q:119:VAL:O	2.07	0.54
1:0:21:G:H5''	19:Q:1:GLY:O	2.07	0.54
1:0:1268:C:O2'	26:X:169:ARG:HB2	2.07	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.06	0.54
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.89	0.54
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.89	0.54
23:U:39:ALA:O	23:U:41:GLU:N	2.41	0.54
25:W:9:VAL:HG22	25:W:88:GLU:OE2	2.07	0.54
1:0:1189:A:O2'	1:0:1208:C:H2'	2.07	0.54
1:0:2488:A:H61	1:0:2534:C:H42	1.55	0.54
2:9:25:G:H2'	36:9:8458:HOH:O	2.08	0.54
2:9:49:G:H2'	2:9:50:G:O4'	2.07	0.54
4:B:85:ARG:NH1	36:B:8639:HOH:O	2.41	0.54
10:H:53:PRO:HA	10:H:125:VAL:O	2.07	0.54
12:J:87:ARG:CZ	36:J:4854:HOH:O	2.55	0.54
15:M:110:THR:HB	15:M:113:SER:OG	2.07	0.54
16:N:39:THR:O	16:N:115:ARG:NH2	2.40	0.54
36:0:9462:HOH:O	25:W:23:HIS:HD2	1.90	0.54
1:0:1333:U:H2'	1:0:1334:C:C6	2.43	0.54
1:0:2094:G:H4'	4:B:245:SER:HB3	1.89	0.54
1:0:244:C:OP2	8:F:38:LYS:HE3	2.08	0.54
11:I:93:ARG:HB3	11:I:93:ARG:NH1	2.22	0.54
14:L:164:THR:CG2	14:L:165:SER:N	2.71	0.54
24:V:139:GLY:O	24:V:141:HIS:HD2	1.90	0.54
1:0:2265:U:H2'	1:0:2266:A:C8	2.43	0.54
1:0:797:A:H5'	27:Y:10:ARG:HG2	1.90	0.54
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.33	0.54
17:O:103:THR:O	17:O:107:GLU:HG3	2.08	0.54
27:Y:38:LYS:HD3	36:Y:8425:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1384:C:H5'	25:W:30:MET:HG2	1.90	0.54
1:0:282:C:H1'	1:0:368:C:H42	1.71	0.54
3:A:100:PRO:HG2	3:A:103:VAL:CG2	2.34	0.54
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.90	0.54
4:B:7:ARG:HG2	4:B:7:ARG:NH1	2.15	0.54
5:C:77:ALA:O	5:C:78:ARG:HG3	2.07	0.54
10:H:35:ASN:HD21	10:H:80:ASN:HA	1.73	0.54
26:X:106:THR:HG23	26:X:107:PRO:HD2	1.90	0.54
1:0:1730:G:H5'	1:0:1731:C:C6	2.43	0.54
1:0:2289:G:H21	1:0:2291:A:H2	1.52	0.54
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.54
2:9:44:A:O4'	6:D:76:ARG:NE	2.41	0.54
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.90	0.54
4:B:248:ARG:O	4:B:251:VAL:CG1	2.56	0.54
4:B:162:MET:CE	4:B:308:LEU:HD21	2.38	0.54
8:F:47:LEU:HD22	8:F:108:LEU:CD1	2.38	0.54
10:H:71:TYR:C	10:H:73:GLN:N	2.59	0.54
1:0:2815:G:N7	11:I:80:LYS:NZ	2.55	0.54
12:J:30:LYS:O	12:J:55:VAL:HG13	2.07	0.54
1:0:1044:C:H3'	1:0:1045:G:H5''	1.90	0.53
1:0:1919:A:H4'	36:0:4360:HOH:O	2.08	0.53
1:0:2301:A:H5''	1:0:2302:A:H5'	1.89	0.53
1:0:500:G:H21	19:Q:98:ASN:HD21	1.56	0.53
4:B:297:VAL:HB	36:B:8610:HOH:O	2.08	0.53
6:D:81:GLU:O	6:D:85:GLN:HG3	2.08	0.53
6:D:99:ASP:O	6:D:159:PRO:HG3	2.07	0.53
10:H:45:GLN:HG3	10:H:135:TRP:NE1	2.23	0.53
14:L:172:GLY:C	14:L:183:VAL:HG11	2.26	0.53
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.37	0.53
36:0:8593:HOH:O	4:B:214:PRO:HD2	2.08	0.53
11:I:107:ASN:C	11:I:107:ASN:HD22	2.12	0.53
27:Y:30:GLU:HA	27:Y:33:HIS:CB	2.39	0.53
1:0:2526:C:O2'	1:0:2527:U:H5'	2.08	0.53
1:0:2812:A:N7	36:0:7048:HOH:O	2.34	0.53
29:1:19:SER:HB3	36:1:4479:HOH:O	2.09	0.53
29:1:48:ASP:O	29:1:49:GLU:HB2	2.08	0.53
8:F:39:SER:CB	8:F:45:ALA:HB2	2.39	0.53
10:H:147:ARG:HA	10:H:150:LYS:NZ	2.24	0.53
15:M:154:LEU:HG	15:M:155:GLU:N	2.22	0.53
1:0:775:G:OP1	28:Z:16:HIS:HE1	1.91	0.53
1:0:272:A:H5'	1:0:273:G:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3:A:OP2	2:9:3:A:C8	2.61	0.53
4:B:16:ARG:NE	36:B:8555:HOH:O	2.25	0.53
6:D:57:THR:HG23	6:D:63:ILE:CB	2.38	0.53
7:E:36:PRO:HD3	11:I:127:ILE:HD12	1.90	0.53
8:F:47:LEU:HB2	8:F:108:LEU:HD11	1.90	0.53
9:G:12:ILE:HD12	36:G:692:HOH:O	2.07	0.53
11:I:19:MET:HE3	11:I:132:LEU:HD11	1.89	0.53
12:J:82:ARG:NH2	12:J:115:ARG:HG2	2.23	0.53
13:K:143:THR:CG2	13:K:144:ASP:H	2.20	0.53
17:O:91:LYS:O	17:O:95:GLU:HG3	2.08	0.53
24:V:19:ASP:O	24:V:23:MET:HG3	2.09	0.53
1:O:703:G:O2'	1:O:704:C:H5'	2.09	0.53
30:2:60:LYS:HG3	30:2:61:PRO:HD2	1.90	0.53
3:A:132:ASP:OD1	3:A:133:ARG:N	2.41	0.53
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.23	0.53
6:D:38:GLU:OE2	6:D:51:ARG:CZ	2.57	0.53
8:F:91:VAL:CG1	8:F:92:GLY:H	2.18	0.53
27:Y:11:THR:OG1	27:Y:23:ARG:HB2	2.09	0.53
1:O:2591:C:H2'	1:O:2592:G:O4'	2.09	0.53
1:O:920:C:H5''	1:O:921:G:O5'	2.08	0.53
5:C:27:ARG:HG2	5:C:30:LEU:HG	1.91	0.53
12:J:58:THR:HG22	12:J:59:LYS:HG3	1.91	0.53
17:O:105:LEU:HD21	17:O:137:LEU:HD21	1.91	0.53
21:S:49:GLU:HB3	21:S:59:GLU:CG	2.38	0.53
23:U:56:ILE:O	23:U:60:GLN:HG3	2.08	0.53
3:A:76:VAL:HG23	27:Y:63:LYS:HB3	1.89	0.53
28:Z:8:GLN:HE22	28:Z:11:LYS:NZ	2.07	0.53
1:O:1523:G:H2'	1:O:1524:U:C6	2.44	0.53
1:O:2717:C:H2'	1:O:2718:C:C5'	2.35	0.53
4:B:42:ALA:HB1	4:B:308:LEU:HD11	1.89	0.53
8:F:22:VAL:HG21	8:F:104:ALA:HB2	1.90	0.53
14:L:185:PRO:HG2	14:L:189:VAL:HG11	1.91	0.53
36:O:9045:HOH:O	17:O:81:LYS:HG2	2.08	0.53
23:U:64:GLY:O	23:U:65:ASP:CB	2.57	0.53
24:V:141:HIS:HB2	24:V:146:ILE:HG12	1.89	0.53
4:B:119:HIS:O	4:B:121:PRO:HD3	2.09	0.53
7:E:166:VAL:HG12	36:E:3134:HOH:O	2.08	0.53
10:H:144:GLU:OE1	10:H:144:GLU:HA	2.08	0.53
19:Q:106:GLY:HA2	19:Q:109:MET:CE	2.39	0.53
19:Q:132:ARG:NH1	36:Q:8580:HOH:O	2.41	0.53
22:T:14:GLU:OE1	22:T:15:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:41:TYR:O	24:V:45:VAL:HG13	2.09	0.53
27:Y:30:GLU:HA	27:Y:33:HIS:HB3	1.90	0.53
1:0:2072:G:C6	1:0:2533:C:H1'	2.44	0.53
1:0:2507:G:H2'	1:0:2510:C:H42	1.74	0.53
1:0:2638:G:H1'	36:0:7295:HOH:O	2.08	0.53
1:0:2896:A:OP1	25:W:15:ARG:NH1	2.42	0.53
2:9:23:U:H3'	2:9:24:U:H5''	1.91	0.53
36:0:8627:HOH:O	5:C:103:ASN:HB3	2.08	0.53
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.90	0.53
8:F:19:ALA:O	8:F:22:VAL:HG22	2.09	0.53
26:X:178:HIS:CG	26:X:179:PRO:HD2	2.44	0.53
1:0:1299:G:H5'	36:0:3580:HOH:O	2.09	0.53
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.09	0.53
1:0:1353:C:P	36:0:4189:HOH:O	2.67	0.53
5:C:180:SER:HB2	36:C:8444:HOH:O	2.09	0.53
8:F:100:ASP:HB3	36:F:5691:HOH:O	2.09	0.53
13:K:125:PHE:CZ	13:K:140:VAL:HG13	2.44	0.53
8:F:2:VAL:HG11	14:L:23:LEU:HD23	1.89	0.53
19:Q:104:PHE:HB2	19:Q:109:MET:HE1	1.90	0.53
1:0:2787:C:H5	36:0:4141:HOH:O	1.91	0.52
4:B:138:GLY:O	4:B:139:ASP:O	2.26	0.52
5:C:246:ARG:NH2	36:C:8424:HOH:O	2.41	0.52
1:0:317:A:H5''	21:S:52:ARG:HD2	1.91	0.52
3:A:164:ARG:CZ	36:A:8591:HOH:O	2.57	0.52
4:B:17:LYS:O	4:B:260:HIS:HD2	1.93	0.52
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.36	0.52
6:D:99:ASP:HB2	6:D:103:ASN:H	1.75	0.52
6:D:99:ASP:HB3	6:D:103:ASN:H	1.74	0.52
6:D:163:VAL:HA	36:D:6326:HOH:O	2.09	0.52
11:I:45:VAL:HG21	11:I:129:PHE:CD1	2.45	0.52
12:J:109:LEU:HD13	12:J:113:ILE:HD11	1.91	0.52
1:0:2415:A:C2	15:M:25:ARG:HB3	2.44	0.52
16:N:7:LEU:HD22	36:N:5650:HOH:O	2.09	0.52
25:W:30:MET:CE	25:W:58:ALA:HB3	2.39	0.52
26:X:184:GLU:OE1	26:X:204:ARG:NH1	2.42	0.52
1:0:2329:C:O2'	1:0:2330:U:H5'	2.10	0.52
3:A:211:LYS:HD3	36:A:8613:HOH:O	2.09	0.52
10:H:55:GLN:HE22	10:H:91:HIS:CD2	2.27	0.52
1:0:184:G:H5''	14:L:153:THR:HG22	1.91	0.52
16:N:47:ARG:NH1	16:N:47:ARG:HG3	2.22	0.52
1:0:949:U:O2'	18:P:40:HIS:HE1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:39:THR:HB	19:Q:42:GLU:CD	2.30	0.52
20:R:56:ASN:O	29:1:8:LYS:HE2	2.09	0.52
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.52
6:D:105:SER:CB	6:D:131:THR:HG23	2.35	0.52
14:L:77:PHE:HD2	36:L:8526:HOH:O	1.91	0.52
18:P:40:HIS:CE1	18:P:94:GLN:HA	2.45	0.52
1:0:396:U:O2'	1:0:418:C:H4'	2.10	0.52
30:2:87:ARG:NH1	36:2:8525:HOH:O	2.43	0.52
19:Q:17:MET:HE1	19:Q:19:ARG:NH2	2.24	0.52
27:Y:11:THR:CG2	27:Y:23:ARG:HB2	2.40	0.52
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.43	0.52
1:0:2524:G:H21	1:0:2526:C:N4	2.07	0.52
2:9:23:U:C3'	2:9:24:U:H5''	2.39	0.52
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.40	0.52
3:A:94:LEU:N	3:A:94:LEU:HD23	2.24	0.52
6:D:146:LYS:NZ	15:M:107:ASN:ND2	2.56	0.52
7:E:22:VAL:O	7:E:28:SER:HA	2.10	0.52
19:Q:132:ARG:CZ	36:Q:8580:HOH:O	2.57	0.52
1:0:2090:G:H2'	1:0:2091:G:C8	2.44	0.52
1:0:2769:C:O2'	1:0:2770:G:H5'	2.09	0.52
3:A:179:MET:HG2	3:A:186:TRP:CB	2.40	0.52
4:B:310:ARG:NH2	36:B:8558:HOH:O	2.41	0.52
5:C:246:ARG:CZ	36:C:8424:HOH:O	2.56	0.52
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.92	0.52
11:I:88:PRO:O	11:I:94:GLY:HA3	2.10	0.52
15:M:169:PRO:O	15:M:172:PHE:HB3	2.10	0.52
15:M:37:ARG:NH2	36:M:8535:HOH:O	2.43	0.52
1:0:1197:G:N2	36:0:5753:HOH:O	2.43	0.52
1:0:1878:G:O2'	1:0:1879:U:C6	2.60	0.52
1:0:960:G:H2'	1:0:960:G:N3	2.25	0.52
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.40	0.52
6:D:94:ALA:O	6:D:95:THR:O	2.27	0.52
8:F:99:THR:HG23	8:F:99:THR:O	2.09	0.52
1:0:182:G:O3'	14:L:157:LEU:CD1	2.57	0.52
27:Y:29:VAL:O	27:Y:33:HIS:HB2	2.10	0.52
1:0:1213:C:O2'	1:0:1214:G:H5'	2.10	0.52
1:0:1497:G:H4'	1:0:1627:G:O2'	2.10	0.52
1:0:1503:U:H2'	1:0:1504:A:O4'	2.10	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.75	0.52
1:0:88:G:H5'	1:0:88:G:H8	1.75	0.52
12:J:10:GLN:NE2	12:J:10:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:12:TRP:CE2	14:L:20:ILE:HD11	2.45	0.52
14:L:137:ASP:HA	14:L:142:LYS:HE3	1.91	0.52
14:L:182:LYS:HB2	14:L:194:ALA:HB2	1.92	0.52
1:O:2300:A:H4'	1:O:2301:A:O5'	2.10	0.52
1:O:2768:A:O2'	1:O:2769:C:H5'	2.10	0.52
1:O:2837:U:H2'	36:O:6360:HOH:O	2.10	0.52
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.40	0.52
4:B:175:LEU:O	4:B:175:LEU:HD23	2.09	0.52
5:C:151:GLN:O	5:C:154:VAL:HB	2.10	0.52
6:D:27:ILE:HG22	6:D:28:GLY:N	2.20	0.52
7:E:43:ASP:HA	36:E:5864:HOH:O	2.10	0.52
8:F:46:GLU:N	36:F:3461:HOH:O	2.42	0.52
13:K:149:ARG:O	13:K:150:GLN:HB2	2.10	0.52
36:9:8514:HOH:O	15:M:107:ASN:HB3	2.09	0.52
1:O:710:G:P	16:N:24:ALA:HB3	2.50	0.52
19:Q:29:LYS:HB3	36:Q:8530:HOH:O	2.08	0.52
20:R:57:THR:CG2	20:R:58:MET:N	2.73	0.52
1:O:1450:C:C4'	1:O:1451:C:OP2	2.57	0.51
1:O:1462:C:H2'	1:O:1463:A:C8	2.46	0.51
1:O:88:G:C6	29:1:24:TRP:CZ3	2.98	0.51
2:9:1:U:O3'	2:9:3:A:H5'	2.10	0.51
4:B:305:ASP:O	4:B:306:LYS:HB2	2.11	0.51
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.71	0.51
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.93	0.51
6:D:135:VAL:HG22	6:D:136:ARG:N	2.25	0.51
6:D:50:VAL:O	6:D:71:ALA:HA	2.10	0.51
15:M:157:PRO:HA	36:M:8527:HOH:O	2.09	0.51
22:T:33:SER:O	22:T:37:GLU:HG3	2.10	0.51
1:O:2506:A:O2'	1:O:2507:G:O5'	2.27	0.51
36:O:7089:HOH:O	30:2:60:LYS:HG3	2.11	0.51
14:L:37:VAL:HG21	14:L:108:LYS:HG3	1.91	0.51
14:L:114:VAL:HB	14:L:159:THR:HG23	1.90	0.51
14:L:81:ARG:HG3	14:L:85:ARG:HB2	1.91	0.51
18:P:75:ILE:CD1	18:P:84:ILE:HD11	2.41	0.51
25:W:37:LEU:CD1	25:W:85:VAL:HG21	2.20	0.51
26:X:144:ARG:NH2	36:X:8615:HOH:O	2.44	0.51
3:A:170:VAL:HG13	27:Y:22:ILE:HG21	1.92	0.51
1:O:1878:G:H4'	36:O:3624:HOH:O	2.10	0.51
1:O:2812:A:C2	1:O:2814:A:N6	2.68	0.51
1:O:283:U:H5''	1:O:284:C:OP2	2.11	0.51
1:O:538:C:H5''	1:O:539:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:29:C:C2'	2:9:30:C:H5'	2.40	0.51
1:0:470:U:O2'	28:Z:16:HIS:CD2	2.62	0.51
2:9:49:G:O2'	2:9:50:G:H5'	2.10	0.51
3:A:34:ASP:OD1	3:A:35:GLY:N	2.40	0.51
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.92	0.51
10:H:59:ASN:ND2	10:H:59:ASN:N	2.55	0.51
14:L:84:LYS:HE2	36:L:8576:HOH:O	2.10	0.51
21:S:80:GLU:OE2	21:S:84:GLY:HA2	2.11	0.51
26:X:155:ARG:NH1	36:X:8559:HOH:O	2.44	0.51
1:0:1118:A:C8	1:0:1119:G:H5''	2.45	0.51
1:0:1236:A:H2'	1:0:1237:U:O4'	2.11	0.51
36:0:5650:HOH:O	29:1:20:ARG:HB3	2.11	0.51
6:D:11:HIS:O	6:D:12:GLU:HB3	2.10	0.51
6:D:65:GLU:HA	36:D:6752:HOH:O	2.09	0.51
7:E:69:ILE:HA	7:E:72:MET:HE2	1.92	0.51
19:Q:18:LEU:HG	19:Q:91:LEU:HD13	1.91	0.51
23:U:49:LEU:O	23:U:53:ILE:HG13	2.11	0.51
25:W:74:ALA:HB1	25:W:85:VAL:HG22	1.92	0.51
1:0:2251:G:H2'	1:0:2252:A:C8	2.46	0.51
2:9:23:U:H6	2:9:23:U:C5'	2.21	0.51
6:D:58:VAL:CG1	6:D:59:GLY:N	2.72	0.51
8:F:91:VAL:CG1	8:F:92:GLY:N	2.72	0.51
12:J:106:GLY:HA3	36:J:5264:HOH:O	2.09	0.51
14:L:87:MET:HB2	14:L:91:ILE:CD1	2.39	0.51
15:M:71:TRP:HE3	15:M:175:LEU:HD22	1.76	0.51
19:Q:132:ARG:HG2	19:Q:133:ALA:N	2.26	0.51
21:S:92:ASP:OD1	21:S:94:SER:HB3	2.11	0.51
24:V:38:THR:HG22	24:V:39:ASP:N	2.26	0.51
1:0:1972:U:H2'	1:0:1973:A:C5'	2.41	0.51
1:0:475:G:OP1	5:C:73:LEU:HD22	2.11	0.51
14:L:113:ARG:HH21	14:L:156:ARG:HG2	1.74	0.51
16:N:96:VAL:HG13	16:N:100:GLN:HB2	1.93	0.51
22:T:52:THR:HG22	22:T:54:THR:HB	1.93	0.51
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.51
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.76	0.51
4:B:156:LYS:HE3	36:B:8635:HOH:O	2.09	0.51
6:D:170:TYR:O	6:D:171:ASP:HB3	2.10	0.51
6:D:25:MET:CE	6:D:41:LEU:HG	2.34	0.51
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.28	0.51
10:H:75:SER:C	10:H:79:ALA:HB2	2.31	0.51
13:K:57:VAL:O	13:K:57:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1470:A:OP1	14:L:93:ARG:HD2	2.11	0.51
1:0:1044:C:H5''	36:0:8542:HOH:O	2.10	0.51
1:0:1862:C:H1'	36:0:6742:HOH:O	2.10	0.51
3:A:93:THR:HG23	3:A:154:ALA:O	2.11	0.51
14:L:52:LEU:HD13	14:L:116:ASN:HB3	1.93	0.51
2:9:6:C:C5'	15:M:37:ARG:HH12	2.12	0.51
26:X:187:VAL:HB	36:X:8572:HOH:O	2.10	0.51
1:0:1592:G:O2'	1:0:1593:C:O4'	2.27	0.51
1:0:1787:C:OP1	17:O:68:LYS:HE2	2.11	0.51
1:0:2672:C:O2'	1:0:2673:U:H5'	2.11	0.51
10:H:75:SER:O	10:H:79:ALA:HB2	2.11	0.51
15:M:152:GLU:C	15:M:154:LEU:H	2.13	0.51
15:M:180:LEU:O	15:M:181:ASP:HB3	2.10	0.51
15:M:182:GLY:O	15:M:183:ASP:O	2.28	0.51
17:O:10:ALA:HA	17:O:13:VAL:CG1	2.41	0.51
24:V:119:HIS:HD2	24:V:120:PRO:O	1.94	0.51
25:W:18:ARG:NH1	36:W:4132:HOH:O	2.41	0.51
1:0:1180:U:H2'	1:0:1181:A:O4'	2.11	0.50
1:0:1194:A:N6	1:0:1206:U:O4	2.44	0.50
1:0:2842:G:H2'	1:0:2843:A:H5'	1.92	0.50
4:B:14:GLY:HA2	4:B:15:PRO:C	2.31	0.50
4:B:41:PHE:CE1	4:B:79:MET:HG3	2.45	0.50
10:H:71:TYR:O	10:H:73:GLN:N	2.44	0.50
24:V:5:VAL:O	24:V:52:VAL:HG22	2.11	0.50
25:W:43:VAL:HG12	25:W:44:ASP:N	2.25	0.50
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.26	0.50
1:0:2361:A:H8	1:0:2361:A:H5'	1.76	0.50
1:0:899:C:H5'	36:0:9711:HOH:O	2.11	0.50
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.50
14:L:69:LYS:HG2	14:L:127:LYS:HG3	1.93	0.50
1:0:2363:G:O3'	18:P:11:ARG:NH1	2.44	0.50
24:V:122:ARG:HH22	24:V:154:ARG:C	2.15	0.50
24:V:38:THR:HG22	24:V:39:ASP:H	1.77	0.50
27:Y:19:GLY:O	27:Y:23:ARG:HG2	2.10	0.50
1:0:1733:A:H4'	4:B:212:GLN:HA	1.92	0.50
4:B:168:GLY:O	4:B:169:GLY:O	2.30	0.50
12:J:74:VAL:HG12	12:J:75:ARG:HG3	1.92	0.50
13:K:97:VAL:HG12	13:K:98:GLU:O	2.12	0.50
14:L:63:VAL:HG21	14:L:109:PHE:CZ	2.47	0.50
6:D:146:LYS:HZ3	15:M:107:ASN:HD21	1.57	0.50
21:S:49:GLU:OE2	21:S:97:ARG:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:3572:HOH:O	4:B:27:ASN:HB2	2.10	0.50
4:B:63:GLU:HG3	4:B:63:GLU:O	2.11	0.50
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.47	0.50
10:H:48:LEU:HD13	10:H:146:TRP:HB3	1.93	0.50
10:H:65:ARG:HB3	36:H:8383:HOH:O	2.12	0.50
11:I:74:ARG:O	11:I:78:ILE:HG12	2.11	0.50
12:J:87:ARG:NE	36:J:4854:HOH:O	2.44	0.50
13:K:61:ALA:HA	36:K:8563:HOH:O	2.12	0.50
1:O:818:A:O2'	27:Y:13:ARG:HD3	2.11	0.50
30:2:56:PRO:N	36:2:8549:HOH:O	2.43	0.50
2:9:35:C:H5''	36:9:8452:HOH:O	2.12	0.50
4:B:27:ASN:H	4:B:27:ASN:HD22	1.59	0.50
4:B:320:GLN:HG3	4:B:321:PRO:HD2	1.94	0.50
5:C:233:THR:HG22	5:C:234:VAL:N	2.26	0.50
10:H:56:ILE:HG21	10:H:61:LEU:HD13	1.94	0.50
12:J:28:GLU:HB3	12:J:59:LYS:HB2	1.93	0.50
24:V:125:HIS:HD2	24:V:127:GLY:H	1.58	0.50
1:O:1834:C:H2'	1:O:1840:A:N6	2.26	0.50
1:O:188:C:H5''	14:L:163:LEU:HD21	1.94	0.50
1:O:2004:U:H2'	1:O:2004:U:O2	2.10	0.50
1:O:371:U:H2'	1:O:372:A:C8	2.45	0.50
2:9:54:A:O2'	2:9:55:U:H5'	2.12	0.50
3:A:194:MET:CE	3:A:199:HIS:HB2	2.42	0.50
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.94	0.50
4:B:333:GLU:HB2	22:T:14:GLU:OE2	2.10	0.50
2:9:92:G:H2'	2:9:93:A:C8	2.47	0.50
15:M:139:TRP:N	36:M:8572:HOH:O	2.45	0.50
15:M:77:ASN:OD1	15:M:80:SER:HB2	2.12	0.50
1:O:1559:A:H1'	36:O:5381:HOH:O	2.11	0.50
1:O:1717:A:H5''	17:O:54:LYS:HB2	1.94	0.50
4:B:248:ARG:HG2	36:B:8577:HOH:O	2.11	0.50
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.77	0.50
14:L:43:PRO:HG3	14:L:62:VAL:HG21	1.94	0.50
22:T:39:ASN:ND2	22:T:44:ARG:HH11	2.10	0.50
26:X:186:ARG:NH1	26:X:186:ARG:HG2	2.26	0.50
1:O:1527:A:H1'	1:O:1528:A:C8	2.46	0.50
1:O:2756:U:N3	1:O:2896:A:H2	2.09	0.50
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.41	0.50
6:D:57:THR:HG23	6:D:63:ILE:CG2	2.41	0.50
12:J:29:LEU:HB3	12:J:55:VAL:CG1	2.30	0.50
25:W:78:GLU:HG2	25:W:79:GLU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:107:PRO:HB3	26:X:182:PHE:CE2	2.47	0.50
27:Y:30:GLU:O	27:Y:33:HIS:HB3	2.12	0.50
1:0:175:G:H2'	14:L:192:ALA:HB3	1.94	0.49
1:0:1996:U:O2'	1:0:1997:A:H5'	2.12	0.49
1:0:2320:U:H4'	1:0:2321:A:O4'	2.12	0.49
1:0:920:C:H5'	1:0:921:G:C4	2.47	0.49
1:0:2434:A:O3'	30:2:28:GLY:HA3	2.12	0.49
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.12	0.49
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.42	0.49
6:D:99:ASP:CB	6:D:103:ASN:HB2	2.41	0.49
7:E:10:ASP:HA	36:E:3707:HOH:O	2.11	0.49
10:H:47:GLU:CB	10:H:133:ILE:HD13	2.42	0.49
10:H:147:ARG:HA	10:H:150:LYS:HZ2	1.77	0.49
17:O:71:LYS:HG3	17:O:71:LYS:O	2.12	0.49
22:T:47:ARG:CG	36:T:4381:HOH:O	2.60	0.49
25:W:41:PHE:O	25:W:43:VAL:HG23	2.11	0.49
1:0:1060:C:H6	1:0:1060:C:H5'	1.77	0.49
1:0:1164:U:N3	1:0:1192:A:H2	2.02	0.49
1:0:1289:C:O2'	1:0:1290:G:H5'	2.12	0.49
1:0:1656:A:H2'	1:0:1657:A:O4'	2.12	0.49
1:0:1972:U:H2'	1:0:1973:A:H5'	1.95	0.49
1:0:344:C:H2'	1:0:345:G:O4'	2.11	0.49
1:0:644:G:N3	1:0:644:G:H5'	2.27	0.49
1:0:380:A:OP2	14:L:9:ARG:HD2	2.11	0.49
19:Q:29:LYS:HD3	36:Q:8530:HOH:O	2.11	0.49
28:Z:10:LYS:HG3	36:Z:8430:HOH:O	2.11	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.12	0.49
1:0:1266:U:H4'	26:X:115:ARG:HH21	1.76	0.49
1:0:1500:U:P	17:O:41:ARG:HH22	2.35	0.49
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.27	0.49
1:0:654:A:OP2	16:N:38:ARG:HD3	2.12	0.49
26:X:107:PRO:HB3	26:X:182:PHE:CD2	2.48	0.49
1:0:407:A:H5'	36:O:5542:HOH:O	2.12	0.49
1:0:559:U:H5'	1:0:559:U:C6	2.39	0.49
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.49
12:J:45:PRO:HB2	36:J:7169:HOH:O	2.13	0.49
1:0:656:G:OP2	16:N:37:ARG:HD2	2.12	0.49
1:0:1595:G:O2'	1:0:1596:U:H5'	2.12	0.49
1:0:538:C:OP2	26:X:134:HIS:HE1	1.96	0.49
1:0:396:U:OP2	30:2:38:ARG:NH1	2.44	0.49
3:A:128:LEU:HG	36:A:8576:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:219:ASN:O	5:C:222:ASP:OD1	2.30	0.49
14:L:155:HIS:CE1	14:L:158:ARG:HE	2.29	0.49
36:O:6950:HOH:O	21:S:9:LYS:HD2	2.12	0.49
22:T:44:ARG:HB3	36:T:3805:HOH:O	2.11	0.49
7:E:11:VAL:CG1	7:E:12:ASP:N	2.75	0.49
11:I:42:GLU:O	11:I:131:THR:HG23	2.12	0.49
1:O:1010:C:H4'	15:M:4:PRO:HB2	1.95	0.49
21:S:71:VAL:HG11	21:S:90:PRO:CB	2.28	0.49
30:2:55:VAL:HB	30:2:56:PRO:HD2	1.95	0.49
4:B:279:THR:OG1	4:B:290:VAL:HB	2.12	0.49
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.47	0.49
10:H:130:HIS:CG	10:H:133:ILE:HD11	2.46	0.49
11:I:47:THR:HG22	11:I:48:GLY:N	2.28	0.49
13:K:148:GLU:HB2	36:K:8587:HOH:O	2.11	0.49
14:L:78:ASN:C	14:L:79:LYS:HG2	2.33	0.49
15:M:73:ALA:HB2	15:M:163:PHE:CZ	2.48	0.49
22:T:52:THR:HG22	22:T:54:THR:H	1.77	0.49
24:V:126:ASP:HB3	24:V:135:GLY:O	2.12	0.49
1:O:2472:C:O2'	1:O:2634:G:H4'	2.12	0.49
22:T:47:ARG:HG3	36:T:4381:HOH:O	2.13	0.49
1:O:1172:G:H5'	36:O:6784:HOH:O	2.13	0.49
1:O:1192:A:N3	36:O:3910:HOH:O	2.45	0.49
1:O:1204:C:C4	1:O:1205:U:C5	3.00	0.49
1:O:2316:G:H4'	36:O:5611:HOH:O	2.12	0.49
1:O:2756:U:N3	1:O:2896:A:C2	2.72	0.49
1:O:447:A:O2'	1:O:448:G:H5'	2.13	0.49
1:O:558:C:C2'	1:O:559:U:C5'	2.91	0.49
36:O:5713:HOH:O	29:1:44:ARG:HG2	2.13	0.49
4:B:27:ASN:HB3	36:B:8632:HOH:O	2.12	0.49
5:C:246:ARG:NH1	36:C:8372:HOH:O	2.46	0.49
21:S:38:ARG:NH1	36:S:6217:HOH:O	2.45	0.49
24:V:65:VAL:HA	24:V:68:THR:CG2	2.42	0.49
27:Y:26:VAL:O	27:Y:30:GLU:HG3	2.13	0.49
4:B:41:PHE:CD2	4:B:190:MET:HE3	2.47	0.49
4:B:7:ARG:HD2	4:B:9:GLY:O	2.12	0.49
7:E:92:PRO:HB2	36:E:4917:HOH:O	2.12	0.49
11:I:45:VAL:HG22	11:I:46:ILE:N	2.27	0.49
13:K:120:LEU:HD12	13:K:133:VAL:HG21	1.95	0.49
15:M:139:TRP:HA	15:M:139:TRP:CE3	2.48	0.49
1:O:256:C:H2'	1:O:257:G:O4'	2.13	0.48
1:O:281:U:H3'	36:O:6729:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:24:U:H4'	2:9:25:G:OP1	2.13	0.48
3:A:130:THR:HG22	3:A:131:HIS:O	2.12	0.48
1:0:820:G:C6	3:A:171:LYS:HB2	2.48	0.48
2:9:41:C:C6	6:D:50:VAL:HG21	2.47	0.48
8:F:50:VAL:CG2	8:F:63:ILE:HG21	2.42	0.48
14:L:182:LYS:HD2	14:L:193:LYS:HB2	1.95	0.48
24:V:84:VAL:HG12	36:V:6679:HOH:O	2.13	0.48
26:X:189:ASN:ND2	26:X:192:ASP:H	2.11	0.48
27:Y:30:GLU:HB3	27:Y:34:LYS:HE3	1.95	0.48
1:0:1730:G:C5'	1:0:1731:C:C6	2.96	0.48
1:0:2256:G:H2'	1:0:2257:G:C5'	2.43	0.48
29:1:24:TRP:NE1	36:1:6863:HOH:O	2.43	0.48
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.96	0.48
14:L:5:TYR:HE2	14:L:46:LEU:HD13	1.78	0.48
21:S:41:ARG:NH1	21:S:41:ARG:HG2	2.28	0.48
1:0:1234:U:N3	4:B:244:PRO:HB3	2.29	0.48
1:0:681:G:N3	1:0:681:G:H5'	2.29	0.48
4:B:248:ARG:O	4:B:251:VAL:HG12	2.13	0.48
5:C:150:THR:HA	5:C:203:ALA:O	2.14	0.48
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.43	0.48
8:F:113:ASP:O	8:F:117:GLU:HG3	2.13	0.48
19:Q:68:HIS:CD2	19:Q:76:ASP:HB2	2.48	0.48
1:0:2768:A:H5''	36:0:3935:HOH:O	2.13	0.48
14:L:115:LEU:HD13	14:L:116:ASN:HB2	1.95	0.48
36:0:5044:HOH:O	14:L:58:GLN:HG3	2.13	0.48
20:R:73:ASP:OD1	20:R:75:GLN:HB2	2.13	0.48
26:X:172:THR:HG22	26:X:173:ALA:N	2.29	0.48
28:Z:28:HIS:CD2	28:Z:31:LYS:HG3	2.48	0.48
1:0:1699:C:H4'	36:0:5960:HOH:O	2.14	0.48
6:D:10:PHE:CD1	6:D:11:HIS:N	2.81	0.48
13:K:62:ALA:HB2	13:K:103:ALA:CB	2.43	0.48
14:L:74:ARG:NH1	14:L:74:ARG:HG3	2.28	0.48
1:0:2044:G:OP1	25:W:23:HIS:HE1	1.97	0.48
26:X:126:PRO:HG2	26:X:128:PHE:CZ	2.47	0.48
26:X:200:THR:HG22	26:X:201:GLU:CG	2.33	0.48
1:0:1192:A:H3'	1:0:1193:A:H5'	1.94	0.48
1:0:1484:G:H2'	36:0:8618:HOH:O	2.13	0.48
1:0:168:C:O2'	1:0:169:A:H5'	2.13	0.48
1:0:1940:C:H4'	36:0:6871:HOH:O	2.12	0.48
1:0:2256:G:H2'	1:0:2257:G:H5'	1.95	0.48
1:0:278:A:H2'	1:0:279:C:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:26:LYS:HD3	10:H:89:PRO:CG	2.42	0.48
21:S:41:ARG:NH1	21:S:42:VAL:O	2.46	0.48
1:0:121:U:OP2	29:1:10:ARG:NH2	2.39	0.48
1:0:2420:G:H4'	36:0:3602:HOH:O	2.13	0.48
2:9:42:C:O2	6:D:76:ARG:NH1	2.47	0.48
4:B:207:LYS:HG2	4:B:304:PRO:HB3	1.94	0.48
5:C:140:VAL:HG12	5:C:141:SER:N	2.29	0.48
7:E:77:THR:OG1	7:E:78:GLU:N	2.45	0.48
15:M:37:ARG:CZ	36:M:8535:HOH:O	2.62	0.48
24:V:3:ALA:O	24:V:54:PHE:HA	2.14	0.48
27:Y:38:LYS:HG3	36:Y:8431:HOH:O	2.14	0.48
1:0:1666:C:C2'	1:0:1667:A:C5'	2.92	0.48
1:0:1819:G:H2'	1:0:1820:G:C4'	2.44	0.48
1:0:2326:U:H4'	1:0:2412:G:H4'	1.96	0.48
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.79	0.48
1:0:2896:A:N3	1:0:2896:A:H2'	2.29	0.48
30:2:48:ASN:ND2	30:2:50:GLY:H	2.11	0.48
2:9:91:C:H2'	2:9:92:G:O4'	2.13	0.48
10:H:26:LYS:HD3	10:H:89:PRO:HG3	1.95	0.48
26:X:122:ARG:NH2	36:X:8536:HOH:O	2.46	0.48
27:Y:46:LYS:NZ	36:Y:8442:HOH:O	2.46	0.48
1:0:1028:U:H1'	36:0:3157:HOH:O	2.14	0.48
1:0:2073:G:OP2	1:0:2490:A:H5'	2.14	0.48
1:0:450:C:OP1	5:C:184:ARG:NH2	2.31	0.48
6:D:101:THR:HG22	36:D:7400:HOH:O	2.14	0.48
6:D:67:ASP:OD2	6:D:69:ILE:HD11	2.13	0.48
7:E:95:VAL:O	7:E:126:ILE:HD13	2.13	0.48
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.43	0.48
10:H:55:GLN:HE21	10:H:124:ARG:NE	2.02	0.48
12:J:75:ARG:HG2	12:J:90:PHE:CD2	2.49	0.48
15:M:58:LEU:HD12	15:M:58:LEU:N	2.29	0.48
17:O:59:ARG:HH22	17:O:66:GLN:HE22	1.60	0.48
21:S:41:ARG:O	21:S:43:ASN:ND2	2.47	0.48
24:V:122:ARG:HH11	24:V:122:ARG:CG	2.19	0.48
24:V:130:HIS:O	24:V:136:GLY:HA3	2.14	0.48
1:0:1477:C:H5'	1:0:1868:G:H5''	1.95	0.48
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.48
1:0:941:G:O2'	1:0:942:U:H5'	2.13	0.48
4:B:162:MET:CE	4:B:310:ARG:HD3	2.44	0.48
10:H:46:VAL:O	10:H:146:TRP:CH2	2.63	0.48
1:0:1003:U:O2'	10:H:90:PHE:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:73:HIS:CD2	21:S:88:PRO:HG3	2.49	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.47
1:0:1667:A:H2'	1:0:1668:U:H6	1.78	0.47
1:0:2443:C:H3'	36:0:9984:HOH:O	2.14	0.47
1:0:584:U:H3'	36:0:5614:HOH:O	2.12	0.47
1:0:656:G:H5'	16:N:3:THR:HG22	1.96	0.47
3:A:36:ASP:O	3:A:38:ILE:N	2.47	0.47
4:B:144:THR:HG22	4:B:145:HIS:N	2.28	0.47
15:M:79:PRO:HG3	15:M:142:THR:O	2.14	0.47
15:M:171:HIS:CE1	36:M:8569:HOH:O	2.67	0.47
15:M:32:PRO:HD2	15:M:99:GLU:O	2.14	0.47
1:0:1409:G:H5'	36:0:3237:HOH:O	2.14	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.47
1:0:1909:A:N1	1:0:2128:G:H1'	2.28	0.47
1:0:2791:U:H1'	1:0:2792:A:H5''	1.95	0.47
2:9:64:C:H2'	2:9:65:A:H5'	1.97	0.47
6:D:167:GLU:OE2	6:D:173:GLU:HG2	2.13	0.47
36:0:6749:HOH:O	14:L:13:LYS:HE2	2.13	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.96	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.47
6:D:94:ALA:HB3	6:D:174:VAL:HA	1.96	0.47
10:H:157:ILE:CG2	10:H:158:ASN:N	2.77	0.47
1:0:182:G:H4'	14:L:157:LEU:HD13	1.96	0.47
26:X:154:ARG:HH12	26:X:155:ARG:HG3	1.79	0.47
1:0:1166:A:H61	1:0:1180:U:H3	1.61	0.47
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.47
1:0:1500:U:OP2	17:O:41:ARG:NH2	2.48	0.47
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.14	0.47
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.43	0.47
7:E:31:ARG:HH12	7:E:68:HIS:CE1	2.32	0.47
8:F:58:GLU:HA	8:F:61:MET:HG3	1.96	0.47
9:G:20:VAL:O	9:G:24:VAL:HG23	2.15	0.47
10:H:84:ARG:CZ	10:H:135:TRP:HH2	2.26	0.47
15:M:184:ILE:HG22	15:M:185:GLU:N	2.27	0.47
18:P:30:VAL:O	18:P:30:VAL:HG12	2.14	0.47
21:S:18:GLU:O	21:S:21:LYS:HG2	2.15	0.47
1:0:2670:G:O2'	1:0:2671:U:H5'	2.15	0.47
1:0:2769:C:H2'	1:0:2770:G:C5'	2.44	0.47
1:0:432:G:O2'	1:0:433:C:H5'	2.14	0.47
30:2:3:MET:O	30:2:90:PHE:HA	2.14	0.47
3:A:51:ARG:NH2	3:A:69:LEU:HD13	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:32:ASP:HA	36:B:8575:HOH:O	2.13	0.47
6:D:59:GLY:C	6:D:61:PHE:H	2.18	0.47
8:F:46:GLU:O	8:F:73:PRO:HD2	2.14	0.47
10:H:163:PRO:O	10:H:164:ALA:HB2	2.14	0.47
36:O:4483:HOH:O	10:H:57:ARG:HG3	2.14	0.47
17:O:98:ILE:HD12	17:O:102:ARG:NE	2.30	0.47
17:O:105:LEU:CD2	17:O:137:LEU:HD21	2.45	0.47
21:S:63:ILE:HD11	21:S:75:GLU:HB2	1.95	0.47
22:T:17:THR:HG22	22:T:18:GLY:N	2.30	0.47
25:W:76:ARG:HG3	25:W:76:ARG:NH1	2.28	0.47
25:W:76:ARG:O	25:W:77:PHE:HB3	2.14	0.47
1:O:2488:A:H2	36:O:6800:HOH:O	1.96	0.47
7:E:132:THR:O	7:E:132:THR:HG23	2.15	0.47
10:H:111:MET:O	10:H:114:PRO:HD3	2.14	0.47
10:H:132:PHE:O	10:H:133:ILE:HD13	2.13	0.47
10:H:149:ALA:C	10:H:151:MET:H	2.17	0.47
10:H:150:LYS:HG2	36:H:8381:HOH:O	2.14	0.47
15:M:90:LEU:CB	15:M:186:LEU:HD22	2.44	0.47
25:W:70:ILE:O	25:W:70:ILE:HG23	2.14	0.47
1:O:621:C:H5'	26:X:132:ASP:OD2	2.15	0.47
1:O:1681:G:H5''	1:O:1682:A:H5'	1.96	0.47
1:O:2361:A:H5''	36:O:8523:HOH:O	2.15	0.47
1:O:2724:U:H2'	1:O:2725:G:O4'	2.14	0.47
1:O:581:G:H5'	36:O:7219:HOH:O	2.14	0.47
1:O:671:A:O2'	1:O:672:G:H2'	2.15	0.47
4:B:168:GLY:N	4:B:174:ARG:HD3	2.29	0.47
7:E:21:THR:HG23	7:E:30:THR:OG1	2.15	0.47
10:H:127:GLY:O	10:H:128:ALA:CB	2.63	0.47
10:H:86:ARG:HD3	10:H:130:HIS:HD2	1.80	0.47
10:H:150:LYS:HE2	36:H:8377:HOH:O	2.14	0.47
13:K:53:ARG:HH22	13:K:57:VAL:HG12	1.79	0.47
36:9:8462:HOH:O	15:M:147:ILE:HD12	2.14	0.47
24:V:110:GLN:NE2	24:V:110:GLN:HA	2.30	0.47
1:O:119:A:H2'	1:O:120:A:H5''	1.95	0.47
1:O:1878:G:O2'	1:O:1879:U:P	2.73	0.47
1:O:2720:C:O2	12:J:87:ARG:NH2	2.48	0.47
5:C:107:ARG:NH2	36:C:8457:HOH:O	2.39	0.47
7:E:108:LEU:HB3	36:E:1306:HOH:O	2.15	0.47
8:F:117:GLU:C	8:F:119:ARG:H	2.18	0.47
6:D:146:LYS:HZ1	15:M:107:ASN:HD21	1.60	0.47
26:X:115:ARG:NE	36:X:8557:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1003:U:O2	10:H:90:PHE:CZ	2.68	0.47
1:0:1181:A:C2	1:0:1192:A:C8	3.03	0.47
1:0:2010:A:H2'	36:0:5476:HOH:O	2.15	0.47
1:0:2563:U:H2'	1:0:2565:C:O5'	2.14	0.47
29:1:18:ASN:ND2	29:1:40:ARG:H	2.09	0.47
14:L:173:LEU:HD23	14:L:183:VAL:HG12	1.97	0.47
15:M:143:ARG:HA	15:M:172:PHE:CD2	2.50	0.47
25:W:9:VAL:HG13	25:W:88:GLU:OE2	2.15	0.47
1:0:2353:A:H4'	1:0:2354:A:O5'	2.13	0.47
1:0:291:C:H2'	1:0:292:G:O4'	2.15	0.47
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.80	0.47
14:L:57:LYS:HE2	14:L:140:ALA:O	2.14	0.47
17:O:16:VAL:CG1	17:O:17:GLY:N	2.78	0.47
22:T:49:LEU:HD11	36:T:3805:HOH:O	2.15	0.47
1:0:1185:U:H5'	36:0:6994:HOH:O	2.15	0.47
1:0:1250:C:O2'	1:0:1251:C:H5'	2.15	0.47
1:0:1753:C:O2	4:B:229:ARG:NH2	2.46	0.47
30:2:7:PHE:HE2	30:2:22:VAL:HG21	1.80	0.47
4:B:82:VAL:HG12	4:B:101:TRP:CE3	2.50	0.47
4:B:307:ARG:HD3	36:B:8524:HOH:O	2.15	0.47
4:B:79:MET:HE3	4:B:144:THR:HG21	1.97	0.47
4:B:80:ARG:HD3	36:B:8611:HOH:O	2.15	0.47
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.45	0.47
10:H:136:VAL:HG23	36:H:8343:HOH:O	2.14	0.47
13:K:101:ASP:C	13:K:103:ALA:H	2.18	0.47
1:0:189:A:OP1	14:L:171:ARG:NH2	2.47	0.47
1:0:1120:U:H5'	1:0:1121:G:OP2	2.15	0.46
1:0:1741:U:O2'	1:0:2723:G:H4'	2.15	0.46
1:0:283:U:H5	1:0:284:C:N4	2.12	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.15	0.46
5:C:13:ASP:OD1	5:C:13:ASP:O	2.33	0.46
10:H:150:LYS:NZ	36:H:8377:HOH:O	2.47	0.46
7:E:34:TRP:O	11:I:127:ILE:HD11	2.15	0.46
16:N:25:VAL:HG23	16:N:26:TRP:N	2.30	0.46
24:V:21:LEU:CD2	24:V:48:VAL:HG11	2.43	0.46
1:0:1167:G:O2'	1:0:1168:C:H5'	2.15	0.46
1:0:1505:U:C6	1:0:1505:U:H5'	2.46	0.46
1:0:603:A:H4'	1:0:604:G:O5'	2.15	0.46
2:9:24:U:C6	36:9:8477:HOH:O	2.56	0.46
3:A:223:ARG:NH1	36:A:8518:HOH:O	2.48	0.46
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:153:THR:HG22	36:D:5234:HOH:O	2.15	0.46
16:N:25:VAL:HG23	16:N:26:TRP:H	1.80	0.46
24:V:41:TYR:HA	24:V:44:MET:HE3	1.97	0.46
1:O:204:A:C2'	1:O:205:U:H5'	2.45	0.46
6:D:55:LYS:O	6:D:56:ARG:HB2	2.14	0.46
10:H:47:GLU:CB	10:H:133:ILE:CD1	2.91	0.46
13:K:21:ARG:N	36:K:8531:HOH:O	2.48	0.46
15:M:37:ARG:HD3	15:M:37:ARG:HA	1.71	0.46
17:O:38:GLU:HA	17:O:41:ARG:HH11	1.78	0.46
24:V:41:TYR:CD2	24:V:44:MET:HE3	2.50	0.46
26:X:112:GLU:OE2	26:X:115:ARG:NH1	2.49	0.46
1:O:585:C:H6	36:O:5614:HOH:O	1.97	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.50	0.46
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.98	0.46
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.97	0.46
8:F:60:VAL:HG12	8:F:60:VAL:O	2.16	0.46
11:I:46:ILE:HA	36:I:1123:HOH:O	2.15	0.46
12:J:66:ARG:HH11	12:J:66:ARG:HG2	1.80	0.46
1:O:1439:C:OP1	29:1:41:HIS:HE1	1.97	0.46
1:O:816:G:C6	1:O:817:G:N1	2.83	0.46
4:B:241:PRO:HD2	36:B:8661:HOH:O	2.14	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46
11:I:70:PHE:CD2	11:I:70:PHE:O	2.68	0.46
12:J:4:LEU:HD22	12:J:116:GLU:HB3	1.98	0.46
14:L:37:VAL:HG12	14:L:63:VAL:HG11	1.97	0.46
15:M:100:ALA:O	15:M:129:ILE:HG23	2.16	0.46
15:M:7:LYS:HE2	36:M:8514:HOH:O	2.14	0.46
15:M:89:GLY:O	15:M:92:ALA:HB3	2.15	0.46
24:V:4:LEU:HD23	24:V:54:PHE:HB3	1.97	0.46
1:O:128:A:H3'	1:O:128:A:C8	2.50	0.46
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.46
1:O:2730:G:O2'	1:O:2731:G:H5'	2.15	0.46
2:9:107:C:H5	36:9:8436:HOH:O	1.97	0.46
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.45	0.46
5:C:214:THR:HB	36:C:8325:HOH:O	2.16	0.46
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.97	0.46
12:J:101:ASN:O	12:J:102:GLU:HB2	2.15	0.46
14:L:167:GLY:O	14:L:171:ARG:HG3	2.15	0.46
18:P:66:LYS:HB2	18:P:70:ALA:O	2.16	0.46
21:S:27:LEU:HD23	21:S:98:VAL:HB	1.98	0.46
1:O:2831:C:H2'	1:O:2832:C:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	16:N:3:THR:CG2	2.46	0.46
2:9:3:A:H61	2:9:22:G:H1'	1.75	0.46
2:9:88:G:OP1	24:V:130:HIS:NE2	2.46	0.46
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.15	0.46
4:B:75:GLU:C	4:B:77:PRO:HD3	2.35	0.46
6:D:128:LEU:N	36:D:6007:HOH:O	2.49	0.46
8:F:101:ALA:HA	36:F:5413:HOH:O	2.16	0.46
1:0:2502:C:C4'	10:H:151:MET:HG2	2.46	0.46
10:H:157:ILE:HG22	10:H:158:ASN:N	2.30	0.46
11:I:93:ARG:CB	11:I:93:ARG:HH11	2.23	0.46
20:R:8:PRO:HD2	23:U:32:ALA:HA	1.98	0.46
25:W:9:VAL:HG13	25:W:88:GLU:OE1	2.16	0.46
1:0:1119:G:H2'	11:I:52:GLN:NE2	2.31	0.46
1:0:2403:C:H3'	36:O:4722:HOH:O	2.16	0.46
1:0:2649:A:H5'	1:0:2649:A:H8	1.80	0.46
1:0:474:C:O3'	5:C:73:LEU:CD2	2.64	0.46
1:0:88:G:C6	29:1:24:TRP:CE3	3.04	0.46
4:B:7:ARG:NH1	4:B:11:LEU:CD2	2.79	0.46
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.51	0.46
8:F:107:VAL:HG23	36:F:6617:HOH:O	2.16	0.46
14:L:38:VAL:HG12	14:L:38:VAL:O	2.15	0.46
1:0:431:G:OP1	14:L:48:ARG:NH1	2.49	0.46
22:T:9:CYS:CA	22:T:52:THR:HG23	2.45	0.46
24:V:38:THR:HB	36:V:5390:HOH:O	2.15	0.46
25:W:66:THR:HG23	25:W:67:PRO:HD2	1.98	0.46
28:Z:28:HIS:HD2	28:Z:30:LYS:H	1.62	0.46
1:0:1592:G:HO2'	1:0:1593:C:C4'	2.29	0.46
1:0:1603:A:H5''	1:0:1605:G:H5'	1.97	0.46
1:0:1735:C:O2'	1:0:1736:A:H5'	2.15	0.46
1:0:2415:A:H2'	1:0:2416:G:H5'	1.96	0.46
1:0:2883:A:H2'	1:0:2884:G:O4'	2.16	0.46
4:B:102:THR:HG21	4:B:182:VAL:O	2.16	0.46
4:B:55:ASN:HB3	4:B:64:GLY:H	1.81	0.46
10:H:141:ASN:HA	36:H:8365:HOH:O	2.16	0.46
10:H:134:ALA:HB3	10:H:142:VAL:HG21	1.97	0.46
11:I:19:MET:CE	11:I:132:LEU:HD11	2.46	0.46
1:0:1789:G:O6	17:O:73:HIS:HE1	1.98	0.46
1:0:2679:G:H2'	1:0:2681:A:OP2	2.16	0.46
2:9:31:C:H2'	2:9:32:G:O4'	2.16	0.46
2:9:39:U:H3'	2:9:40:C:H5''	1.98	0.46
2:9:3:A:H2	2:9:21:G:N3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.78	0.46
1:0:475:G:C5'	5:C:73:LEU:HD23	2.46	0.46
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.45	0.46
15:M:5:ARG:HG3	18:P:18:PRO:CB	2.46	0.46
1:0:1418:U:OP1	29:1:42:TRP:HB3	2.16	0.45
1:0:2768:A:H3'	36:0:3935:HOH:O	2.15	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.16	0.45
1:0:820:G:C5	3:A:171:LYS:HB2	2.51	0.45
1:0:88:G:N7	29:1:28:LYS:HD2	2.30	0.45
3:A:48:ASP:HB3	36:A:8608:HOH:O	2.17	0.45
4:B:221:GLN:HE22	12:J:42:ASN:ND2	2.08	0.45
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.31	0.45
4:B:72:THR:HB	36:B:8610:HOH:O	2.15	0.45
12:J:79:PRO:HB2	36:J:782:HOH:O	2.15	0.45
23:U:55:ARG:NH2	36:U:4428:HOH:O	2.40	0.45
26:X:154:ARG:NH1	26:X:155:ARG:HG3	2.31	0.45
1:0:2297:U:H1'	36:0:4686:HOH:O	2.17	0.45
1:0:2559:C:H4'	36:0:6780:HOH:O	2.16	0.45
30:2:73:GLU:HB2	36:2:8527:HOH:O	2.16	0.45
4:B:60:SER:C	4:B:62:ARG:H	2.18	0.45
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.46	0.45
8:F:28:ALA:HB3	8:F:99:THR:O	2.15	0.45
10:H:150:LYS:HA	10:H:153:VAL:HG22	1.97	0.45
10:H:84:ARG:CZ	10:H:135:TRP:CH2	2.99	0.45
17:O:120:ARG:NH2	17:O:123:TYR:CD2	2.84	0.45
18:P:25:PRO:HA	18:P:26:PRO:HD3	1.84	0.45
20:R:32:ALA:HA	20:R:36:GLU:OE1	2.16	0.45
21:S:40:VAL:HG22	21:S:41:ARG:N	2.31	0.45
22:T:50:GLU:CD	36:T:7349:HOH:O	2.53	0.45
1:0:1666:C:C2'	1:0:1667:A:H5'	2.44	0.45
1:0:2401:A:H5'	36:0:9000:HOH:O	2.16	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
1:0:821:U:H5''	36:0:9559:HOH:O	2.14	0.45
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.16	0.45
5:C:33:LYS:HE2	36:C:8362:HOH:O	2.16	0.45
10:H:26:LYS:HA	10:H:58:HIS:CD2	2.51	0.45
11:I:90:LYS:HB2	34:I:8502:CL:CL	2.53	0.45
15:M:86:LEU:O	15:M:90:LEU:HG	2.16	0.45
20:R:6:LYS:HB2	20:R:27:ALA:O	2.15	0.45
23:U:57:LYS:HA	23:U:60:GLN:HE21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:776:A:OP1	28:Z:28:HIS:HE1	2.00	0.45
1:0:1730:G:C5'	1:0:1731:C:H6	2.29	0.45
1:0:2912:C:H2'	1:0:2913:A:O4'	2.17	0.45
30:2:65:THR:HB	30:2:83:TRP:H	1.81	0.45
4:B:16:ARG:NH2	36:B:8555:HOH:O	2.44	0.45
4:B:280:VAL:HG13	4:B:333:GLU:O	2.17	0.45
6:D:166:ILE:O	6:D:169:THR:N	2.49	0.45
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.97	0.45
10:H:81:TYR:C	10:H:81:TYR:CD1	2.89	0.45
15:M:154:LEU:CG	15:M:155:GLU:H	2.26	0.45
15:M:71:TRP:N	36:M:8540:HOH:O	2.49	0.45
36:0:6931:HOH:O	21:S:2:LYS:HE2	2.14	0.45
1:0:1218:U:H2'	1:0:1219:U:C6	2.51	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
4:B:205:VAL:O	4:B:307:ARG:NE	2.49	0.45
4:B:275:GLY:O	4:B:291:ASP:HA	2.17	0.45
4:B:1:PRO:O	4:B:2:GLN:HB2	2.16	0.45
5:C:234:VAL:HG22	5:C:234:VAL:O	2.17	0.45
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.99	0.45
12:J:27:ARG:HD2	36:J:4747:HOH:O	2.17	0.45
24:V:11:VAL:O	24:V:12:ASN:HB2	2.16	0.45
1:0:1268:C:O2'	1:0:1269:G:H5'	2.15	0.45
1:0:1314:U:H2'	36:0:5390:HOH:O	2.16	0.45
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.30	0.45
2:9:2:U:OP2	2:9:3:A:H5'	2.16	0.45
3:A:8:ARG:HG2	36:A:8553:HOH:O	2.16	0.45
12:J:98:VAL:HG22	12:J:102:GLU:C	2.36	0.45
12:J:78:LYS:HA	12:J:79:PRO:HD3	1.86	0.45
1:0:797:A:H4'	27:Y:10:ARG:N	2.31	0.45
1:0:1086:A:N6	24:V:11:VAL:HG11	2.32	0.45
1:0:420:U:H2'	1:0:421:C:C6	2.52	0.45
1:0:814:G:H4'	36:0:9643:HOH:O	2.16	0.45
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.17	0.45
4:B:127:GLN:HG3	36:B:8647:HOH:O	2.16	0.45
5:C:162:VAL:HG12	5:C:162:VAL:O	2.17	0.45
7:E:93:MET:HE1	7:E:165:GLY:N	2.32	0.45
8:F:50:VAL:HG11	8:F:60:VAL:HG11	1.97	0.45
18:P:31:GLU:CD	18:P:93:ARG:HH12	2.20	0.45
24:V:129:LYS:HG2	36:V:1990:HOH:O	2.17	0.45
1:0:1176:C:H1'	36:0:3439:HOH:O	2.16	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:514:G:O5'	1:0:514:G:H8	1.99	0.45
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.81	0.45
5:C:39:GLN:O	5:C:43:LYS:HD3	2.17	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.46	0.45
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.99	0.45
19:Q:84:ALA:O	19:Q:88:PHE:HD1	1.99	0.45
21:S:45:GLY:C	36:S:3851:HOH:O	2.55	0.45
1:0:1168:C:H5	36:0:7027:HOH:O	1.99	0.45
1:0:1183:C:N4	36:0:3910:HOH:O	2.48	0.45
1:0:1684:A:O2'	1:0:1685:A:H5''	2.17	0.45
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.45
1:0:566:A:H2'	1:0:567:U:O4'	2.17	0.45
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.17	0.45
7:E:32:ARG:O	7:E:33:LEU:HD23	2.16	0.45
10:H:113:ALA:N	10:H:114:PRO:CD	2.80	0.45
14:L:67:ILE:CD1	14:L:104:ARG:HD2	2.47	0.45
15:M:167:ASP:O	15:M:168:LEU:HD23	2.17	0.45
27:Y:33:HIS:HE1	27:Y:49:ARG:NE	2.15	0.45
1:0:1162:G:H2'	36:0:6102:HOH:O	2.17	0.45
1:0:1636:G:O2'	1:0:1637:A:H5'	2.16	0.45
1:0:2642:G:H2'	1:0:2643:G:O4'	2.17	0.45
29:1:18:ASN:HA	29:1:18:ASN:HD22	1.59	0.45
2:9:51:A:H5'	15:M:160:SER:HB3	1.99	0.45
3:A:17:ARG:HD2	36:A:8542:HOH:O	2.17	0.45
5:C:153:VAL:O	5:C:157:LEU:HG	2.17	0.45
5:C:164:ALA:O	5:C:167:ASP:HB2	2.17	0.45
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.47	0.45
7:E:20:ILE:HD12	7:E:33:LEU:HD12	2.00	0.45
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.17	0.45
11:I:142:ASN:O	11:I:144:THR:N	2.50	0.45
1:0:926:A:O2'	13:K:41:HIS:HD2	2.00	0.45
21:S:74:VAL:HB	21:S:77:VAL:HG21	1.99	0.45
23:U:1:THR:HG23	23:U:2:VAL:N	2.22	0.45
23:U:55:ARG:NE	36:U:4428:HOH:O	2.37	0.45
36:0:5586:HOH:O	27:Y:34:LYS:HE2	2.17	0.45
1:0:1182:C:H1'	1:0:1192:A:H8	1.82	0.44
1:0:2326:U:H4'	1:0:2412:G:C4'	2.47	0.44
1:0:2467:A:O2'	1:0:2468:A:H2'	2.17	0.44
1:0:2777:G:O2'	1:0:2778:A:H5'	2.17	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
8:F:28:ALA:CB	8:F:99:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:27:ILE:HD12	9:G:70:ALA:HB1	1.99	0.44
11:I:63:ILE:HG22	11:I:64:GLY:N	2.31	0.44
12:J:75:ARG:HE	12:J:94:ALA:HB3	1.82	0.44
19:Q:14:ALA:HB3	19:Q:147:LEU:HB2	1.99	0.44
24:V:122:ARG:NE	36:V:5817:HOH:O	2.50	0.44
1:O:2505:G:H8	36:O:5154:HOH:O	2.00	0.44
1:O:2515:C:H2'	1:O:2516:G:O4'	2.17	0.44
1:O:870:G:C3'	1:O:871:G:H5''	2.47	0.44
30:2:84:ARG:HD3	36:2:8550:HOH:O	2.17	0.44
2:9:2:U:OP2	2:9:2:U:H4'	2.17	0.44
3:A:165:THR:HG22	36:A:8620:HOH:O	2.17	0.44
4:B:198:GLU:HB3	36:B:8601:HOH:O	2.16	0.44
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.47	0.44
36:O:7244:HOH:O	5:C:94:THR:HG21	2.16	0.44
6:D:76:ARG:O	6:D:77:ASP:HB2	2.18	0.44
10:H:14:TYR:N	10:H:91:HIS:HE1	2.16	0.44
14:L:122:GLU:HB2	14:L:126:HIS:O	2.17	0.44
14:L:186:SER:O	14:L:189:VAL:HG12	2.17	0.44
19:Q:125:ARG:HG2	36:Q:8540:HOH:O	2.17	0.44
24:V:13:MET:HE1	24:V:18:GLN:HA	2.00	0.44
1:O:2388:C:H5'	18:P:83:THR:O	2.17	0.44
4:B:125:GLU:OE2	4:B:129:ARG:NH1	2.50	0.44
4:B:36:PRO:HA	4:B:168:GLY:HA2	1.95	0.44
10:H:31:PHE:HA	10:H:85:ILE:CG2	2.48	0.44
10:H:35:ASN:ND2	10:H:79:ALA:O	2.51	0.44
11:I:22:VAL:O	11:I:26:VAL:HG23	2.16	0.44
15:M:47:LEU:CD1	15:M:97:VAL:HG11	2.47	0.44
21:S:52:ARG:HB2	21:S:95:ASN:HB3	1.99	0.44
1:O:1555:G:H4'	1:O:1630:A:H2	1.83	0.44
1:O:2112:A:H2'	1:O:2113:G:C8	2.52	0.44
1:O:2338:G:H2'	6:D:129:ASP:OD1	2.17	0.44
1:O:2456:A:H2'	1:O:2457:U:C6	2.52	0.44
7:E:152:THR:HG21	7:E:165:GLY:HA2	1.99	0.44
13:K:125:PHE:CE1	13:K:140:VAL:HG13	2.53	0.44
15:M:154:LEU:O	15:M:155:GLU:CB	2.66	0.44
17:O:10:ALA:CA	17:O:13:VAL:HG12	2.45	0.44
24:V:108:ARG:HE	24:V:114:PRO:CG	2.30	0.44
27:Y:59:HIS:HA	36:Y:8442:HOH:O	2.18	0.44
28:Z:25:LYS:HD2	29:1:49:GLU:H	1.82	0.44
1:O:1006:A:N1	1:O:2311:A:H1'	2.33	0.44
1:O:2781:U:H2'	1:O:2782:G:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.26	0.44
5:C:236:THR:O	5:C:237:GLU:C	2.55	0.44
6:D:140:ARG:O	6:D:144:ARG:HG2	2.17	0.44
6:D:169:THR:O	6:D:170:TYR:HB2	2.17	0.44
10:H:110:GLY:N	36:H:8393:HOH:O	2.50	0.44
10:H:43:PRO:HD2	10:H:137:ASN:HA	1.99	0.44
10:H:57:ARG:O	10:H:61:LEU:HD22	2.18	0.44
13:K:128:GLY:O	13:K:132:LYS:HG3	2.17	0.44
15:M:11:ARG:HG3	15:M:14:ARG:NH1	2.33	0.44
15:M:91:ARG:HG3	15:M:186:LEU:HD23	1.99	0.44
19:Q:25:PHE:CE2	19:Q:29:LYS:CE	3.00	0.44
24:V:42:ARG:O	24:V:45:VAL:HG22	2.17	0.44
26:X:187:VAL:HG12	26:X:205:ILE:HA	1.99	0.44
28:Z:25:LYS:O	28:Z:25:LYS:HG2	2.18	0.44
1:O:1029:U:O2'	1:O:1273:C:OP1	2.31	0.44
1:O:2314:G:C2'	1:O:2315:C:H5'	2.47	0.44
1:O:484:A:N1	1:O:506:G:H4'	2.32	0.44
5:C:13:ASP:N	36:C:8440:HOH:O	2.50	0.44
6:D:95:THR:C	6:D:97:GLN:N	2.68	0.44
13:K:92:ASP:OD1	13:K:94:ARG:HB2	2.17	0.44
15:M:161:GLY:O	15:M:162:ASP:C	2.55	0.44
36:O:6063:HOH:O	27:Y:22:ILE:HG13	2.17	0.44
1:O:1211:G:O2'	1:O:1212:C:H5'	2.17	0.44
1:O:130:C:H5'	36:O:4724:HOH:O	2.17	0.44
1:O:2005:G:OP2	1:O:2005:G:H3'	2.18	0.44
6:D:23:VAL:CG2	6:D:23:VAL:O	2.64	0.44
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.99	0.44
1:O:1119:G:C8	11:I:52:GLN:NE2	2.85	0.44
11:I:6:PHE:O	11:I:8:ALA:N	2.51	0.44
12:J:55:VAL:CG1	12:J:56:SER:N	2.81	0.44
15:M:182:GLY:N	36:M:8573:HOH:O	2.51	0.44
28:Z:8:GLN:HE22	28:Z:11:LYS:HZ2	1.65	0.44
1:O:590:A:H2'	1:O:591:A:H5'	2.00	0.44
4:B:146:THR:O	4:B:159:PRO:HB3	2.17	0.44
36:O:5034:HOH:O	4:B:298:LYS:HD3	2.17	0.44
5:C:7:ASP:OD1	5:C:11:ASN:O	2.36	0.44
7:E:84:MET:HE1	7:E:133:VAL:HG21	1.98	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.48	0.44
21:S:71:VAL:CG1	21:S:72:ILE:N	2.80	0.44
24:V:122:ARG:NH1	24:V:122:ARG:CG	2.80	0.44
24:V:26:ILE:HG13	24:V:26:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:5:VAL:HG22	24:V:32:CYS:HB2	2.00	0.44
26:X:106:THR:CG2	26:X:107:PRO:HD2	2.47	0.44
27:Y:11:THR:HG23	27:Y:11:THR:O	2.17	0.44
1:O:1980:U:O2	1:O:2008:U:H4'	2.18	0.44
1:O:2064:U:H4'	1:O:2653:A:OP1	2.18	0.44
1:O:2812:A:H1'	36:O:5305:HOH:O	2.18	0.44
14:L:107:ARG:NH1	36:L:8577:HOH:O	2.48	0.44
14:L:183:VAL:HG12	14:L:184:ARG:N	2.32	0.44
15:M:108:SER:HA	15:M:109:PRO:HD3	1.79	0.44
36:O:5789:HOH:O	17:O:59:ARG:HD3	2.17	0.44
24:V:90:TYR:N	24:V:90:TYR:CD1	2.85	0.44
1:O:1902:G:H2'	1:O:1903:U:O4'	2.18	0.43
1:O:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:O:2383:G:H1'	36:O:6223:HOH:O	2.17	0.43
1:O:2769:C:H2'	1:O:2770:G:H5'	2.00	0.43
1:O:314:G:N2	1:O:316:A:H3'	2.33	0.43
1:O:321:A:H1'	36:O:6554:HOH:O	2.18	0.43
1:O:338:C:H4'	5:C:174:ILE:HD12	1.99	0.43
1:O:40:C:H4'	36:O:6522:HOH:O	2.18	0.43
1:O:42:C:H1'	36:O:4186:HOH:O	2.18	0.43
1:O:816:G:H5'	1:O:1598:A:H4'	1.98	0.43
3:A:135:VAL:N	36:A:8598:HOH:O	2.50	0.43
8:F:21:GLU:O	8:F:24:ARG:HG3	2.17	0.43
11:I:26:VAL:HG13	11:I:36:VAL:HG11	1.99	0.43
13:K:121:ILE:HG12	13:K:141:GLU:HB2	1.99	0.43
14:L:125:ARG:NH1	36:L:8596:HOH:O	2.50	0.43
1:O:1423:C:O2'	1:O:1424:A:H5'	2.18	0.43
1:O:1669:A:H2'	1:O:1670:G:H8	1.82	0.43
2:9:59:C:H6	2:9:59:C:O5'	2.01	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.53	0.43
3:A:1:GLY:HA2	3:A:197:VAL:HG23	2.00	0.43
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.99	0.43
6:D:173:GLU:HG3	6:D:174:VAL:N	2.33	0.43
7:E:7:ILE:HG22	7:E:45:ASP:O	2.19	0.43
10:H:26:LYS:HG2	10:H:28:ILE:N	2.29	0.43
13:K:6:ARG:NH2	36:K:8548:HOH:O	2.47	0.43
14:L:55:LYS:O	14:L:60:ILE:HD12	2.18	0.43
21:S:38:ARG:HG3	21:S:38:ARG:HH11	1.82	0.43
27:Y:57:CYS:SG	27:Y:59:HIS:HB3	2.58	0.43
1:O:1342:C:O2'	1:O:1343:C:H5'	2.18	0.43
1:O:2083:A:N6	11:I:90:LYS:HE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2419:U:H5''	1:0:2420:G:C5'	2.47	0.43
1:0:2782:G:O6	1:0:2790:C:H5''	2.18	0.43
1:0:2832:C:H5	36:0:6736:HOH:O	2.01	0.43
2:9:31:C:H1'	36:9:8392:HOH:O	2.18	0.43
2:9:4:G:OP1	2:9:59:C:O2'	2.33	0.43
2:9:56:A:C3'	2:9:57:A:H5''	2.49	0.43
4:B:254:GLN:HG2	4:B:255:GLY:N	2.32	0.43
5:C:14:GLY:N	36:C:8440:HOH:O	2.49	0.43
1:0:1109:U:O4	11:I:21:ARG:HA	2.18	0.43
13:K:53:ARG:NH2	13:K:57:VAL:CG1	2.82	0.43
20:R:29:ASP:OD1	20:R:31:ARG:HG3	2.19	0.43
24:V:90:TYR:CE2	24:V:99:ALA:HB2	2.54	0.43
1:0:426:G:H2'	1:0:427:C:O4'	2.18	0.43
1:0:653:C:H2'	1:0:654:A:C8	2.53	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.43
3:A:179:MET:HG2	3:A:186:TRP:CG	2.53	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.43
4:B:307:ARG:NH1	4:B:307:ARG:CG	2.79	0.43
11:I:39:VAL:CG1	11:I:107:ASN:HB2	2.49	0.43
13:K:65:ASP:CG	13:K:111:ALA:HB3	2.38	0.43
13:K:72:ASN:OD1	13:K:75:LEU:HD12	2.19	0.43
15:M:67:ALA:HA	15:M:71:TRP:H	1.83	0.43
22:T:13:ILE:HG12	22:T:32:CYS:CB	2.47	0.43
24:V:22:GLU:HG2	24:V:27:HIS:CD2	2.54	0.43
25:W:15:ARG:NH1	25:W:15:ARG:HB3	2.32	0.43
25:W:12:ILE:HG23	25:W:36:HIS:CG	2.53	0.43
27:Y:38:LYS:CE	27:Y:45:LYS:HE2	2.34	0.43
1:0:1206:U:H2'	1:0:1207:A:O4'	2.18	0.43
1:0:1235:G:C1'	11:I:63:ILE:HG23	2.48	0.43
1:0:1973:A:C8	1:0:1973:A:H5'	2.44	0.43
30:2:91:GLN:O	30:2:92:GLU:HB2	2.18	0.43
3:A:105:VAL:CG1	3:A:106:CYS:N	2.81	0.43
36:0:8729:HOH:O	3:A:11:ARG:HD3	2.19	0.43
4:B:279:THR:CG2	4:B:280:VAL:N	2.81	0.43
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.49	0.43
10:H:30:GLN:H	10:H:65:ARG:NH1	2.17	0.43
11:I:103:VAL:CG1	36:I:5907:HOH:O	2.64	0.43
13:K:90:ARG:NH1	13:K:119:THR:HG21	2.34	0.43
13:K:130:ARG:HA	36:K:8557:HOH:O	2.18	0.43
21:S:24:ARG:HH21	21:S:39:ASN:ND2	2.13	0.43
26:X:117:LEU:HD12	26:X:174:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:41:VAL:HG12	27:Y:42:CYS:N	2.33	0.43
1:O:1467:C:OP1	14:L:35:PRO:HB2	2.19	0.43
1:O:2851:G:C2'	1:O:2852:A:H5'	2.49	0.43
1:O:1787:C:H4'	1:O:2883:A:O4'	2.18	0.43
1:O:716:G:C2'	1:O:717:C:O5'	2.67	0.43
29:1:36:ASN:HB3	29:1:39:ARG:NE	2.34	0.43
2:9:92:G:H22	10:H:52:LYS:HZ2	1.65	0.43
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.99	0.43
8:F:28:ALA:HB3	8:F:99:THR:HG23	2.00	0.43
13:K:146:GLY:C	13:K:148:GLU:H	2.22	0.43
14:L:25:TRP:HE3	14:L:26:HIS:HD2	1.66	0.43
14:L:38:VAL:O	14:L:63:VAL:HG13	2.18	0.43
23:U:23:LEU:HD12	23:U:56:ILE:HD12	2.00	0.43
1:O:1592:G:O2'	1:O:1593:C:O5'	2.36	0.43
1:O:1657:A:H2'	1:O:1658:A:C8	2.54	0.43
1:O:559:U:H2'	1:O:560:C:O4'	2.19	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
6:D:84:LEU:HA	6:D:87:ALA:HB3	2.01	0.43
8:F:26:THR:HG21	8:F:103:ALA:HB2	1.99	0.43
10:H:113:ALA:N	10:H:114:PRO:HD3	2.33	0.43
14:L:153:THR:O	14:L:156:ARG:HG3	2.18	0.43
26:X:187:VAL:HB	26:X:203:VAL:HG22	1.99	0.43
1:O:1328:A:C8	26:X:169:ARG:HD3	2.54	0.43
1:O:1613:C:H2'	1:O:1614:G:O4'	2.18	0.43
1:O:1857:A:N6	1:O:2247:C:H1'	2.34	0.43
1:O:716:G:H2'	1:O:717:C:O5'	2.19	0.43
1:O:88:G:N1	29:1:24:TRP:CE3	2.87	0.43
5:C:33:LYS:HD2	36:C:8459:HOH:O	2.18	0.43
6:D:23:VAL:HG23	6:D:41:LEU:HD22	1.99	0.43
6:D:99:ASP:HB2	6:D:103:ASN:CB	2.47	0.43
7:E:80:TRP:O	7:E:134:SER:HA	2.18	0.43
14:L:146:GLN:NE2	36:L:8643:HOH:O	2.51	0.43
15:M:149:GLU:O	15:M:152:GLU:HB2	2.19	0.43
24:V:48:VAL:CG1	24:V:48:VAL:O	2.65	0.43
27:Y:13:ARG:NH1	27:Y:14:PHE:CE2	2.87	0.43
27:Y:34:LYS:HE2	36:Y:8426:HOH:O	2.18	0.43
1:O:777:U:O2'	28:Z:11:LYS:HG2	2.19	0.43
2:9:27:C:H1'	36:9:8431:HOH:O	2.19	0.43
3:A:103:VAL:HA	3:A:104:PRO:HD3	1.89	0.43
3:A:105:VAL:HG13	3:A:155:THR:O	2.19	0.43
1:O:1194:A:C6	1:O:1206:U:N3	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:H5'	30:2:42:ARG:NH1	2.34	0.43
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.01	0.43
4:B:277:GLU:N	4:B:278:PRO:HD2	2.33	0.43
4:B:320:GLN:HG3	4:B:321:PRO:CD	2.48	0.43
4:B:74:ILE:HG13	36:B:8610:HOH:O	2.18	0.43
6:D:77:ASP:HB3	6:D:78:GLU:H	1.58	0.43
6:D:84:LEU:C	6:D:86:THR:H	2.22	0.43
8:F:21:GLU:HA	8:F:24:ARG:HE	1.83	0.43
14:L:49:ALA:C	14:L:54:TYR:HB3	2.39	0.43
1:0:2274:A:H1'	14:L:86:MET:SD	2.59	0.43
15:M:163:PHE:HE1	15:M:171:HIS:HD1	1.67	0.43
16:N:21:SER:OG	16:N:106:PRO:HB2	2.19	0.43
1:0:2365:G:H4'	18:P:45:PRO:O	2.18	0.43
19:Q:29:LYS:NZ	36:Q:8538:HOH:O	2.52	0.43
20:R:29:ASP:OD1	20:R:31:ARG:NH1	2.52	0.43
21:S:49:GLU:HB3	21:S:59:GLU:HG3	2.01	0.43
28:Z:25:LYS:HZ3	28:Z:25:LYS:HG2	1.75	0.43
1:0:1634:G:H2'	1:0:1635:U:C6	2.54	0.42
1:0:514:G:OP1	1:0:514:G:H2'	2.19	0.42
1:0:869:G:OP1	14:L:79:LYS:HE2	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
4:B:268:ARG:NE	36:B:8612:HOH:O	2.51	0.42
4:B:62:ARG:CB	4:B:65:MET:HE3	2.49	0.42
6:D:67:ASP:O	6:D:69:ILE:HG13	2.18	0.42
12:J:34:VAL:HB	36:J:7169:HOH:O	2.19	0.42
12:J:99:ASP:OD1	12:J:101:ASN:N	2.51	0.42
14:L:134:ILE:HG23	14:L:141:ILE:HD13	2.01	0.42
21:S:3:GLN:HA	21:S:4:PRO:HD3	1.83	0.42
24:V:88:THR:CG2	24:V:89:ASP:N	2.69	0.42
1:0:564:G:H1'	36:0:5829:HOH:O	2.20	0.42
1:0:736:A:H2'	1:0:737:A:O4'	2.19	0.42
1:0:834:G:H4'	1:0:835:U:OP2	2.19	0.42
1:0:834:G:H3'	1:0:835:U:H4'	2.00	0.42
11:I:75:PRO:HD3	11:I:136:SER:OG	2.18	0.42
12:J:55:VAL:HG12	12:J:56:SER:H	1.83	0.42
23:U:20:LEU:HD22	23:U:60:GLN:HE22	1.84	0.42
24:V:139:GLY:O	24:V:141:HIS:CD2	2.71	0.42
25:W:26:ALA:HB1	25:W:59:TRP:CE2	2.54	0.42
1:0:1406:A:H4'	1:0:1407:A:H5''	2.00	0.42
1:0:2608:C:H2'	36:0:3085:HOH:O	2.19	0.42
1:0:488:U:O2'	21:S:82:THR:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:9:GLU:HG3	7:E:10:ASP:N	2.33	0.42
11:I:130:VAL:CG1	11:I:131:THR:N	2.81	0.42
13:K:1:THR:N	36:K:8540:HOH:O	2.53	0.42
23:U:12:THR:OG1	23:U:13:PRO:HD2	2.20	0.42
1:O:1173:A:H4'	1:O:1174:A:C8	2.54	0.42
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.48	0.42
4:B:280:VAL:CG1	4:B:334:SER:HA	2.49	0.42
9:G:64:ASN:ND2	9:G:64:ASN:N	2.66	0.42
10:H:62:GLU:HA	36:H:8383:HOH:O	2.19	0.42
12:J:125:ALA:C	12:J:127:ALA:H	2.21	0.42
15:M:33:ARG:NH1	15:M:103:ASP:OD2	2.46	0.42
15:M:139:TRP:HA	15:M:139:TRP:HE3	1.84	0.42
18:P:32:GLU:O	18:P:93:ARG:NH2	2.53	0.42
24:V:54:PHE:CZ	24:V:140:LYS:HB2	2.54	0.42
24:V:76:ASP:O	24:V:77:ALA:C	2.58	0.42
25:W:43:VAL:CG1	25:W:44:ASP:N	2.81	0.42
1:O:1477:C:C5'	1:O:1868:G:H5''	2.50	0.42
1:O:2289:G:N2	1:O:2291:A:C2	2.80	0.42
1:O:23:G:H1'	1:O:520:A:N6	2.35	0.42
1:O:2842:G:C2'	1:O:2843:A:H5'	2.49	0.42
1:O:289:G:O2'	1:O:290:C:H5'	2.20	0.42
1:O:37:A:H2'	1:O:38:G:C8	2.55	0.42
1:O:661:G:C5	1:O:686:A:C2	3.07	0.42
1:O:827:A:H2'	1:O:828:G:O4'	2.19	0.42
2:9:20:G:H3'	36:9:8434:HOH:O	2.19	0.42
6:D:57:THR:HA	6:D:63:ILE:HA	2.00	0.42
7:E:9:GLU:HA	36:E:5240:HOH:O	2.18	0.42
15:M:44:ARG:HG3	15:M:45:ALA:N	2.35	0.42
15:M:47:LEU:HD12	15:M:92:ALA:CB	2.48	0.42
16:N:43:VAL:HG12	16:N:44:ASN:O	2.19	0.42
22:T:52:THR:HG21	22:T:54:THR:HB	2.00	0.42
1:O:1098:A:H2'	1:O:1099:G:O4'	2.19	0.42
1:O:1123:A:C2	1:O:1129:C:H4'	2.54	0.42
1:O:1367:A:H2'	1:O:1368:U:O4'	2.20	0.42
2:9:64:C:C2'	2:9:65:A:H5'	2.49	0.42
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.91	0.42
6:D:19:GLU:O	6:D:133:ASN:HB3	2.20	0.42
10:H:136:VAL:HG22	10:H:137:ASN:N	2.35	0.42
15:M:42:HIS:CG	15:M:62:HIS:HE1	2.38	0.42
15:M:73:ALA:HB1	15:M:74:PRO:CD	2.49	0.42
16:N:26:TRP:CE3	16:N:26:TRP:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:1:MET:HB2	24:V:103:GLU:HG2	2.00	0.42
27:Y:32:LYS:HB3	27:Y:32:LYS:HE2	1.76	0.42
1:0:1236:A:C8	11:I:63:ILE:HD11	2.55	0.42
1:0:1279:U:H5''	36:0:9100:HOH:O	2.20	0.42
1:0:1804:A:H2'	1:0:1805:G:C8	2.54	0.42
1:0:2001:G:O2'	1:0:2002:C:H5'	2.20	0.42
1:0:2061:C:C2'	1:0:2062:A:H5'	2.49	0.42
1:0:545:G:H2'	1:0:546:C:O4'	2.20	0.42
5:C:16:VAL:CG1	5:C:17:ASP:N	2.81	0.42
5:C:35:VAL:HG21	5:C:227:GLY:HA2	2.00	0.42
6:D:44:ILE:HG12	6:D:83:PHE:CE1	2.53	0.42
8:F:58:GLU:HA	8:F:61:MET:HE2	2.01	0.42
9:G:19:GLU:O	9:G:23:ILE:HG13	2.20	0.42
11:I:71:TYR:CD1	11:I:72:PRO:HD2	2.54	0.42
14:L:191:GLY:O	14:L:192:ALA:HB3	2.20	0.42
14:L:42:ARG:HA	14:L:43:PRO:HD3	1.85	0.42
15:M:120:GLU:HG3	15:M:136:LEU:HD13	2.02	0.42
21:S:69:LYS:O	21:S:71:VAL:HG23	2.20	0.42
28:Z:2:GLY:O	28:Z:6:PRO:HG2	2.19	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.42
1:0:1878:G:O2'	1:0:1879:U:H6	2.03	0.42
1:0:1883:U:O2'	1:0:1884:G:H5'	2.19	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.85	0.42
1:0:2415:A:N3	15:M:26:LEU:HD13	2.35	0.42
1:0:249:G:O2'	1:0:250:C:H5'	2.20	0.42
1:0:2653:A:H2'	1:0:2654:C:C6	2.55	0.42
1:0:2681:A:H4'	1:0:2682:C:H5'	2.02	0.42
1:0:2820:A:H2'	1:0:2821:C:O4'	2.19	0.42
1:0:644:G:H1'	36:0:5924:HOH:O	2.19	0.42
3:A:33:GLU:CD	3:A:33:GLU:H	2.23	0.42
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.35	0.42
6:D:86:THR:HG23	36:D:7477:HOH:O	2.20	0.42
7:E:31:ARG:NH1	7:E:68:HIS:CD2	2.88	0.42
10:H:117:LYS:HB2	36:H:8339:HOH:O	2.19	0.42
1:0:2502:C:H4'	10:H:151:MET:HG2	2.02	0.42
10:H:94:ARG:NH2	36:H:8332:HOH:O	2.50	0.42
14:L:99:ARG:HD2	14:L:167:GLY:HA2	2.01	0.42
16:N:54:GLU:O	16:N:55:ASP:HB2	2.20	0.42
19:Q:132:ARG:NH2	36:Q:8580:HOH:O	2.52	0.42
1:0:306:A:P	21:S:38:ARG:HH21	2.43	0.42
1:0:1855:G:H8	3:A:144:GLU:OE2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:139:VAL:CG1	36:C:8447:HOH:O	2.61	0.42
22:T:9:CYS:O	22:T:52:THR:HG23	2.20	0.42
1:0:1175:G:H1'	1:0:1193:A:H2'	2.02	0.42
1:0:1524:U:O2'	1:0:1525:G:OP2	2.34	0.42
1:0:2257:G:H4'	1:0:2259:C:C2	2.55	0.42
1:0:2649:A:H5'	1:0:2649:A:C8	2.55	0.42
1:0:324:G:O2'	1:0:325:U:H5'	2.20	0.42
29:1:19:SER:O	29:1:36:ASN:ND2	2.53	0.42
12:J:72:VAL:HG11	12:J:121:PHE:CD1	2.55	0.42
15:M:127:LEU:HA	15:M:127:LEU:HD12	1.85	0.42
1:0:1058:A:H2'	1:0:1060:C:C5'	2.47	0.41
1:0:1139:U:H2'	1:0:1140:C:C6	2.55	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.55	0.41
1:0:2578:G:C8	1:0:2578:G:H5'	2.51	0.41
1:0:613:C:H2'	1:0:614:U:H6	1.85	0.41
1:0:88:G:H2'	1:0:89:G:C8	2.54	0.41
3:A:200:PRO:HD3	36:A:8521:HOH:O	2.20	0.41
4:B:145:HIS:CD2	4:B:146:THR:O	2.68	0.41
4:B:315:VAL:HG23	4:B:316:ARG:HG2	2.01	0.41
8:F:26:THR:HG21	8:F:103:ALA:CB	2.48	0.41
9:G:67:LEU:O	9:G:71:LEU:HG	2.20	0.41
10:H:13:ALA:HA	10:H:91:HIS:CE1	2.55	0.41
1:0:2601:A:N1	12:J:38:SER:HB2	2.35	0.41
18:P:40:HIS:HD2	18:P:60:THR:OG1	2.03	0.41
19:Q:96:VAL:HG13	19:Q:106:GLY:HA3	2.02	0.41
21:S:37:GLN:OE1	21:S:118:SER:HA	2.19	0.41
24:V:146:ILE:HA	24:V:146:ILE:HD13	1.88	0.41
24:V:29:VAL:O	24:V:30:ASN:HB2	2.19	0.41
1:0:1385:G:O3'	25:W:49:ARG:NH1	2.52	0.41
28:Z:28:HIS:HD2	28:Z:31:LYS:H	1.68	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.55	0.41
1:0:757:C:OP1	13:K:27:ARG:HD2	2.20	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.20	0.41
2:9:24:U:C5	36:9:8477:HOH:O	2.72	0.41
2:9:28:U:H2'	2:9:29:C:C6	2.55	0.41
3:A:30:ARG:HB3	3:A:30:ARG:HE	1.68	0.41
1:0:2821:C:H4'	4:B:116:PRO:CB	2.49	0.41
4:B:305:ASP:O	4:B:306:LYS:CB	2.67	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.21	0.41
10:H:83:PHE:HE1	10:H:146:TRP:CZ2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1003:U:O2	10:H:90:PHE:HZ	2.03	0.41
14:L:125:ARG:CZ	36:L:8596:HOH:O	2.68	0.41
14:L:65:VAL:HG21	14:L:105:ALA:HB2	2.01	0.41
15:M:73:ALA:N	36:M:8569:HOH:O	2.53	0.41
15:M:61:ALA:CB	15:M:88:ALA:HB2	2.50	0.41
36:O:3538:HOH:O	18:P:13:LYS:HE3	2.19	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.41
1:0:2589:U:H2'	1:0:2590:U:C6	2.55	0.41
1:0:2667:G:H1'	1:0:2914:A:N3	2.34	0.41
1:0:2668:G:H2'	1:0:2669:U:C6	2.55	0.41
1:0:2712:G:H5'	36:J:4183:HOH:O	2.19	0.41
1:0:303:C:H2'	1:0:304:G:O4'	2.21	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.21	0.41
1:0:858:U:H2'	1:0:859:C:C6	2.55	0.41
2:9:105:A:H2'	2:9:106:C:O4'	2.20	0.41
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.85	0.41
36:O:3589:HOH:O	8:F:31:LYS:HE3	2.19	0.41
10:H:46:VAL:CG1	10:H:146:TRP:HZ3	2.29	0.41
10:H:83:PHE:CE1	10:H:146:TRP:NE1	2.87	0.41
15:M:143:ARG:HH12	15:M:173:ASP:CG	2.21	0.41
1:0:1593:C:OP1	17:O:117:SER:CB	2.68	0.41
17:O:94:TRP:CZ2	17:O:98:ILE:HG13	2.55	0.41
21:S:38:ARG:HG3	21:S:38:ARG:NH1	2.34	0.41
21:S:78:THR:HB	21:S:87:VAL:O	2.21	0.41
25:W:76:ARG:HA	25:W:82:GLU:O	2.20	0.41
26:X:154:ARG:HB3	26:X:154:ARG:HH11	1.84	0.41
1:0:1413:A:H2'	1:0:1414:A:O4'	2.20	0.41
1:0:1545:C:H2'	1:0:1546:G:O4'	2.21	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.41
1:0:553:G:P	26:X:204:ARG:NH2	2.93	0.41
1:0:1881:A:OP1	3:A:199:HIS:HE1	2.04	0.41
3:A:223:ARG:NE	36:A:8575:HOH:O	2.54	0.41
4:B:41:PHE:HB3	4:B:190:MET:CE	2.50	0.41
4:B:258:GLY:N	4:B:260:HIS:CE1	2.86	0.41
4:B:60:SER:C	4:B:62:ARG:N	2.73	0.41
5:C:65:ARG:HG3	5:C:67:GLN:HB2	2.03	0.41
8:F:34:ASN:HA	14:L:4:ALA:HB2	2.02	0.41
15:M:163:PHE:O	15:M:164:ASP:O	2.37	0.41
20:R:30:ASP:HA	20:R:62:LYS:HE3	2.03	0.41
23:U:39:ALA:C	23:U:41:GLU:N	2.74	0.41
1:0:1205:U:O2	1:0:1205:U:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1406:A:N1	36:0:5553:HOH:O	2.37	0.41
1:0:1926:G:H2'	1:0:1927:A:C8	2.56	0.41
1:0:2421:G:H3'	1:0:2422:U:C5'	2.51	0.41
1:0:903:U:OP2	13:K:11:ARG:NH1	2.51	0.41
36:0:3919:HOH:O	3:A:11:ARG:CZ	2.69	0.41
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.41
4:B:71:VAL:CG1	4:B:296:LEU:HB3	2.48	0.41
1:0:2346:C:H4'	6:D:52:THR:HG22	2.03	0.41
7:E:101:GLU:OE2	7:E:115:ARG:HD3	2.21	0.41
36:0:9135:HOH:O	8:F:38:LYS:HE2	2.20	0.41
1:0:262:A:OP2	8:F:91:VAL:HG11	2.20	0.41
7:E:35:TYR:HA	11:I:127:ILE:HD12	2.03	0.41
12:J:90:PHE:CD1	12:J:90:PHE:N	2.89	0.41
13:K:89:PHE:N	36:K:8570:HOH:O	2.54	0.41
15:M:159:TYR:CE2	15:M:163:PHE:HE2	2.36	0.41
16:N:14:LEU:HD23	16:N:102:ILE:CD1	2.48	0.41
16:N:23:GLY:C	36:N:3062:HOH:O	2.58	0.41
16:N:26:TRP:HE3	16:N:26:TRP:HA	1.84	0.41
16:N:98:LEU:HA	16:N:98:LEU:HD12	1.88	0.41
1:0:793:A:H5''	17:O:83:LYS:HG2	2.03	0.41
21:S:71:VAL:HG12	21:S:72:ILE:N	2.34	0.41
23:U:42:ASN:O	23:U:44:GLY:N	2.53	0.41
24:V:146:ILE:HG22	24:V:147:ASP:N	2.35	0.41
1:0:588:G:O6	24:V:154:ARG:NH1	2.53	0.41
25:W:30:MET:HE1	25:W:55:ASN:HA	2.03	0.41
28:Z:28:HIS:CD2	28:Z:31:LYS:H	2.38	0.41
1:0:1752:G:H2'	36:0:7080:HOH:O	2.19	0.41
1:0:513:A:H3'	36:0:3363:HOH:O	2.20	0.41
1:0:2346:C:H4'	6:D:52:THR:CG2	2.50	0.41
9:G:63:ARG:N	36:G:2569:HOH:O	2.53	0.41
10:H:48:LEU:CD1	10:H:157:ILE:HG21	2.50	0.41
14:L:78:ASN:O	14:L:79:LYS:HG2	2.21	0.41
16:N:77:ALA:HA	16:N:96:VAL:O	2.20	0.41
21:S:1:SER:N	36:S:5837:HOH:O	2.53	0.41
24:V:6:GLN:HA	24:V:52:VAL:HG23	2.02	0.41
36:0:3697:HOH:O	26:X:186:ARG:HD2	2.21	0.41
1:0:1525:G:C5'	1:0:1526:A:OP2	2.68	0.41
1:0:305:A:C5	1:0:329:A:C2	3.09	0.41
1:0:660:A:H4'	1:0:661:G:O5'	2.21	0.41
1:0:677:C:H4'	5:C:246:ARG:NH2	2.36	0.41
3:A:36:ASP:HB2	3:A:83:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:205:VAL:HA	4:B:260:HIS:O	2.21	0.41
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.35	0.41
7:E:37:ASP:OD1	11:I:125:SER:HB3	2.21	0.41
10:H:62:GLU:O	10:H:66:VAL:HG23	2.21	0.41
18:P:16:ASN:HA	18:P:16:ASN:HD22	1.71	0.41
21:S:48:VAL:HG22	21:S:97:ARG:O	2.21	0.41
21:S:48:VAL:HG13	21:S:49:GLU:N	2.35	0.41
23:U:1:THR:HG23	23:U:2:VAL:HG23	2.02	0.41
24:V:14:HIS:HB2	24:V:17:ILE:HD12	2.03	0.41
1:0:1878:G:H5''	36:0:9307:HOH:O	2.20	0.41
1:0:2241:C:H2'	1:0:2242:U:C6	2.56	0.41
1:0:2346:C:O3'	6:D:52:THR:HG23	2.20	0.41
1:0:2597:U:H2'	1:0:2598:U:H5'	2.03	0.41
1:0:2779:G:H21	7:E:143:GLN:HE22	1.69	0.41
1:0:40:C:O5'	1:0:40:C:H6	2.04	0.41
1:0:412:C:H2'	1:0:413:G:O4'	2.21	0.41
1:0:771:G:OP2	14:L:79:LYS:HE3	2.21	0.41
2:9:3:A:H61	2:9:22:G:C1'	2.34	0.41
4:B:129:ARG:NH2	4:B:176:ASP:OD1	2.52	0.41
6:D:15:GLU:HA	6:D:16:PRO:HD3	1.87	0.41
7:E:11:VAL:HG11	7:E:22:VAL:HG13	2.02	0.41
13:K:104:ASP:O	13:K:105:TYR:HB3	2.21	0.41
19:Q:149:GLU:HA	19:Q:150:PRO:HD3	1.95	0.41
27:Y:42:CYS:SG	27:Y:44:PHE:HB2	2.61	0.41
1:0:2748:G:H5'	36:0:7073:HOH:O	2.21	0.41
36:0:4589:HOH:O	4:B:216:LYS:HA	2.21	0.41
4:B:254:GLN:NE2	36:B:8595:HOH:O	2.51	0.41
6:D:151:ILE:HA	6:D:152:PRO:HD3	1.93	0.41
6:D:153:THR:O	6:D:156:ARG:HB2	2.20	0.41
6:D:64:ARG:HG2	6:D:66:GLY:O	2.21	0.41
7:E:20:ILE:CD1	7:E:33:LEU:HD12	2.50	0.41
10:H:114:PRO:O	10:H:115:PHE:C	2.58	0.41
1:0:2413:A:N7	15:M:109:PRO:HB3	2.35	0.41
15:M:66:LEU:HA	15:M:66:LEU:HD12	1.95	0.41
19:Q:47:LEU:O	19:Q:51:ILE:HG13	2.21	0.41
28:Z:25:LYS:HD2	29:1:49:GLU:N	2.35	0.41
1:0:625:U:H5''	1:0:1044:C:N4	2.35	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.88	0.41
1:0:141:C:P	36:0:3373:HOH:O	2.79	0.41
1:0:1462:C:H2'	1:0:1463:A:H8	1.84	0.41
1:0:1615:A:H4'	36:0:5402:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.41
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.41
1:0:638:C:H2'	1:0:639:A:C8	2.56	0.41
1:0:694:A:H2'	1:0:695:C:H5'	2.02	0.41
4:B:223:ARG:HG3	4:B:232:TRP:O	2.21	0.41
5:C:95:GLU:HG3	36:C:8475:HOH:O	2.20	0.41
6:D:48:MET:HA	6:D:49:PRO:HD3	1.78	0.41
7:E:7:ILE:HA	7:E:8:PRO:HD3	1.89	0.41
10:H:85:ILE:HB	10:H:132:PHE:HE2	1.84	0.41
12:J:101:ASN:O	12:J:102:GLU:CB	2.69	0.41
14:L:134:ILE:O	14:L:136:PRO:HD3	2.20	0.41
14:L:138:HIS:C	14:L:139:PRO:O	2.54	0.41
19:Q:39:THR:CG2	19:Q:42:GLU:HG3	2.50	0.41
25:W:51:ASP:O	25:W:53:SER:N	2.54	0.41
25:W:37:LEU:HD21	25:W:72:VAL:HG11	2.02	0.41
28:Z:17:THR:HA	29:1:49:GLU:HA	2.03	0.41
1:0:1524:U:O2'	1:0:1525:G:P	2.78	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
1:0:2506:A:H1'	36:0:5574:HOH:O	2.21	0.41
1:0:2718:C:C6	1:0:2718:C:H5'	2.52	0.41
30:2:15:ASN:ND2	36:2:8547:HOH:O	2.53	0.41
30:2:65:THR:HG23	30:2:67:LEU:CG	2.45	0.41
4:B:88:GLU:HG3	4:B:88:GLU:O	2.20	0.41
5:C:115:LEU:HA	5:C:115:LEU:HD12	1.89	0.41
6:D:18:ILE:HD13	6:D:84:LEU:HD12	2.03	0.41
10:H:150:LYS:CB	10:H:157:ILE:HD12	2.46	0.41
1:0:1242:A:C5'	11:I:82:THR:HG23	2.30	0.41
14:L:133:LEU:O	14:L:134:ILE:HD13	2.21	0.41
15:M:164:ASP:OD1	15:M:167:ASP:HA	2.19	0.41
17:O:131:PHE:CD1	17:O:137:LEU:HD13	2.55	0.41
22:T:49:LEU:CD1	36:T:3805:HOH:O	2.69	0.41
1:0:1377:C:H1'	36:0:6797:HOH:O	2.19	0.40
1:0:1393:A:H2'	1:0:1394:C:C6	2.57	0.40
1:0:157:G:H4'	14:L:95:LYS:HE3	2.04	0.40
1:0:1878:G:H5''	36:0:4675:HOH:O	2.20	0.40
1:0:1947:G:H2'	1:0:1948:G:C8	2.56	0.40
1:0:204:A:H2'	1:0:205:U:H5'	2.03	0.40
1:0:2478:U:O2'	1:0:2479:A:H5'	2.21	0.40
1:0:2691:A:OP1	1:0:2691:A:H8	2.04	0.40
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.40
1:0:2909:G:H2'	1:0:2910:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:377:C:H5	36:0:9820:HOH:O	2.04	0.40
1:0:708:A:H2'	1:0:709:G:O4'	2.20	0.40
3:A:128:LEU:HD21	3:A:131:HIS:CE1	2.55	0.40
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.35	0.40
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.85	0.40
4:B:286:ASN:O	4:B:306:LYS:HE3	2.20	0.40
4:B:82:VAL:CG1	4:B:82:VAL:O	2.67	0.40
4:B:84:LEU:HD13	4:B:84:LEU:O	2.21	0.40
6:D:103:ASN:ND2	6:D:133:ASN:HD22	2.18	0.40
1:0:166:A:N7	13:K:25:GLY:HA2	2.36	0.40
13:K:24:ALA:HB2	13:K:30:ARG:HD2	2.03	0.40
14:L:45:ARG:CZ	14:L:48:ARG:HG3	2.50	0.40
1:0:317:A:OP1	21:S:52:ARG:O	2.39	0.40
24:V:4:LEU:HA	24:V:4:LEU:HD23	1.94	0.40
24:V:2:HIS:HD2	24:V:56:GLU:N	2.19	0.40
27:Y:23:ARG:NH1	36:Y:8404:HOH:O	2.53	0.40
1:0:1614:G:H2'	36:0:4136:HOH:O	2.21	0.40
1:0:1677:U:OP2	29:1:8:LYS:NZ	2.51	0.40
1:0:2256:G:C2'	1:0:2257:G:H5'	2.51	0.40
1:0:2471:G:N3	1:0:2633:A:H2	2.18	0.40
30:2:11:CYS:HB2	30:2:20:HIS:CE1	2.57	0.40
5:C:196:THR:HG23	36:C:8400:HOH:O	2.22	0.40
6:D:59:GLY:O	6:D:61:PHE:N	2.42	0.40
7:E:156:ASP:OD2	7:E:157:LYS:HG3	2.19	0.40
9:G:64:ASN:O	9:G:68:GLU:HG3	2.21	0.40
12:J:118:ALA:C	12:J:120:ARG:H	2.24	0.40
36:0:9057:HOH:O	14:L:84:LYS:HD3	2.21	0.40
22:T:6:CYS:HA	22:T:13:ILE:HD11	2.03	0.40
1:0:1194:A:C5	1:0:1206:U:N3	2.90	0.40
1:0:151:A:H2'	1:0:152:A:O4'	2.22	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.22	0.40
1:0:419:A:H1'	1:0:1921:A:C2	2.57	0.40
1:0:934:C:H2'	1:0:935:G:C8	2.57	0.40
30:2:74:CYS:N	36:2:8560:HOH:O	2.54	0.40
5:C:46:TYR:CE1	5:C:92:PRO:HB3	2.56	0.40
6:D:99:ASP:HB2	6:D:103:ASN:CA	2.51	0.40
6:D:10:PHE:CE1	6:D:11:HIS:HB3	2.55	0.40
11:I:46:ILE:HG12	11:I:53:ILE:HD13	2.03	0.40
13:K:73:VAL:HG11	13:K:118:LEU:HD21	2.01	0.40
14:L:95:LYS:HG2	14:L:99:ARG:HB3	2.02	0.40
15:M:138:ASP:C	36:M:8572:HOH:O	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:175:LEU:HD12	15:M:175:LEU:HA	1.86	0.40
17:O:16:VAL:CG1	17:O:20:ARG:HB2	2.52	0.40
19:Q:119:VAL:HG21	19:Q:142:ASP:CG	2.42	0.40
19:Q:61:GLN:NE2	36:Q:8538:HOH:O	2.53	0.40
1:O:1166:A:N3	1:O:1166:A:H2'	2.37	0.40
1:O:1756:G:H1'	36:O:5783:HOH:O	2.21	0.40
1:O:398:U:H2'	1:O:399:C:C6	2.56	0.40
1:O:771:G:P	14:L:79:LYS:HG3	2.61	0.40
3:A:192:VAL:O	3:A:207:GLN:HG2	2.22	0.40
3:A:35:GLY:O	3:A:36:ASP:CB	2.62	0.40
4:B:132:HIS:HB2	4:B:137:LEU:HD22	2.03	0.40
4:B:275:GLY:C	36:B:8656:HOH:O	2.59	0.40
6:D:94:ALA:HB3	6:D:174:VAL:CA	2.52	0.40
14:L:87:MET:HG2	30:2:46:ILE:CG2	2.45	0.40
16:N:32:ARG:NE	36:N:3360:HOH:O	2.54	0.40
20:R:53:ASN:ND2	36:R:8320:HOH:O	2.55	0.40
24:V:13:MET:HE3	24:V:17:ILE:CG2	2.48	0.40
1:O:2019:A:H5'	36:O:4048:HOH:O	2.20	0.40
1:O:2255:A:H2'	1:O:2256:G:O4'	2.21	0.40
1:O:2289:G:N2	1:O:2291:A:H2	2.19	0.40
1:O:370:G:O2'	1:O:371:U:H5'	2.22	0.40
1:O:517:U:H1'	36:O:7111:HOH:O	2.22	0.40
1:O:894:A:C2	5:C:87:ARG:NH2	2.90	0.40
2:9:31:C:O2'	2:9:32:G:H5'	2.21	0.40
2:9:92:G:H22	10:H:52:LYS:HZ1	1.68	0.40
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.49	0.40
4:B:189:ALA:HB1	36:B:8568:HOH:O	2.21	0.40
4:B:215:VAL:HB	4:B:234:ARG:NH1	2.35	0.40
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.93	0.40
14:L:23:LEU:O	14:L:26:HIS:HB2	2.21	0.40
17:O:13:VAL:HG13	17:O:14:LEU:N	2.36	0.40
19:Q:82:GLU:HG3	19:Q:83:LYS:N	2.35	0.40
21:S:14:ALA:HA	21:S:15:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/239 (98%)	216 (92%)	14 (6%)	5 (2%)	8	9
4	B	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	9
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/176 (76%)	97 (72%)	28 (21%)	9 (7%)	1	0
7	E	170/177 (96%)	161 (95%)	8 (5%)	1 (1%)	28	41
8	F	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	11	13
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	4	4
11	I	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	8	9
12	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	22	33
13	K	141/164 (86%)	121 (86%)	19 (14%)	1 (1%)	25	37
14	L	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	32	46
15	M	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	4	3
16	N	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	O	141/148 (95%)	138 (98%)	3 (2%)	0	100	100
18	P	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
19	Q	148/154 (96%)	143 (97%)	4 (3%)	1 (1%)	25	37
20	R	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	S	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	4
24	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	25	37
25	W	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	6	6
26	X	140/240 (58%)	140 (100%)	0	0	100	100
27	Y	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	6	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	1	42/48 (88%)	42 (100%)	0	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	8	9
All	All	3633/4235 (86%)	3372 (93%)	209 (6%)	52 (1%)	13	18

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO
6	D	173	GLU
10	H	162	SER
13	K	80	ASP
15	M	154	LEU
15	M	164	ASP
15	M	183	ASP
23	U	43	PRO
3	A	34	ASP
3	A	37	VAL
3	A	132	ASP
4	B	34	GLY
4	B	169	GLY
6	D	11	HIS
6	D	20	LYS
8	F	101	ALA
10	H	164	ALA
11	I	7	ASP
11	I	143	LYS
15	M	162	ASP
30	2	56	PRO
30	2	57	GLY
4	B	184	ASP
6	D	171	ASP
10	H	40	PRO
10	H	138	PRO
11	I	5	GLU
14	L	140	ALA
15	M	167	ASP
15	M	181	ASP

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Mol	Chain	Res	Type
24	V	77	ALA
25	W	77	PHE
27	Y	81	LYS
4	B	185	GLY
6	D	61	PHE
10	H	72	VAL
15	M	65	ASP
4	B	107	SER
8	F	64	PRO
6	D	96	SER
12	J	119	GLN
23	U	40	PRO
4	B	2	GLN
27	Y	41	VAL
7	E	44	GLY
19	Q	81	PRO
3	A	211	LYS
25	W	52	PRO
3	A	112	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	166 (93%)	13 (7%)	16	26
4	B	282/282 (100%)	264 (94%)	18 (6%)	20	32
5	C	193/193 (100%)	179 (93%)	14 (7%)	16	26
6	D	117/147 (80%)	106 (91%)	11 (9%)	10	15
7	E	152/155 (98%)	148 (97%)	4 (3%)	51	72
8	F	92/92 (100%)	91 (99%)	1 (1%)	78	90
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	122/122 (100%)	109 (89%)	13 (11%)	8	10
11	I	118/121 (98%)	109 (92%)	9 (8%)	15	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	J	106/106 (100%)	103 (97%)	3 (3%)	49	70
13	K	112/126 (89%)	108 (96%)	4 (4%)	40	60
14	L	166/166 (100%)	157 (95%)	9 (5%)	26	41
15	M	149/149 (100%)	143 (96%)	6 (4%)	36	55
16	N	93/93 (100%)	91 (98%)	2 (2%)	57	76
17	O	113/116 (97%)	111 (98%)	2 (2%)	64	81
18	P	79/79 (100%)	75 (95%)	4 (5%)	28	44
19	Q	117/121 (97%)	114 (97%)	3 (3%)	51	72
20	R	71/73 (97%)	71 (100%)	0	100	100
21	S	105/105 (100%)	101 (96%)	4 (4%)	38	58
22	T	44/52 (85%)	44 (100%)	0	100	100
23	U	51/56 (91%)	50 (98%)	1 (2%)	60	79
24	V	130/130 (100%)	122 (94%)	8 (6%)	21	34
25	W	66/73 (90%)	62 (94%)	4 (6%)	22	34
26	X	120/195 (62%)	110 (92%)	10 (8%)	13	20
27	Y	56/56 (100%)	52 (93%)	4 (7%)	17	27
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	54	74
30	2	79/79 (100%)	76 (96%)	3 (4%)	38	58
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	28	45

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	68	ILE
3	A	69	LEU
3	A	78	ASP
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG

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Mol	Chain	Res	Type
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	53	LEU
4	B	63	GLU
4	B	84	LEU
4	B	97	LEU
4	B	98	THR
4	B	103	ASP
4	B	162	MET
4	B	234	ARG
4	B	251	VAL
4	B	254	GLN
4	B	256	GLN
4	B	264	GLU
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS
6	D	50	VAL
6	D	61	PHE
6	D	95	THR
6	D	99	ASP
6	D	100	ASP
6	D	131	THR
6	D	133	ASN

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Mol	Chain	Res	Type
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	54	ASP
7	E	102	VAL
7	E	164	ASP
8	F	1	PRO
10	H	1	LYS
10	H	59	ASN
10	H	61	LEU
10	H	72	VAL
10	H	73	GLN
10	H	82	LYS
10	H	85	ILE
10	H	86	ARG
10	H	118	PRO
10	H	129	ASN
10	H	142	VAL
10	H	150	LYS
10	H	166	ASN
11	I	46	ILE
11	I	52	GLN
11	I	74	ARG
11	I	79	PHE
11	I	107	ASN
11	I	112	ASP
11	I	120	SER
11	I	125	SER
11	I	127	ILE
12	J	7	ASP
12	J	10	GLN
12	J	98	VAL
13	K	30	ARG
13	K	35	ARG
13	K	80	ASP
13	K	117	GLU
14	L	38	VAL
14	L	46	LEU
14	L	48	ARG
14	L	68	ARG
14	L	81	ARG

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Mol	Chain	Res	Type
14	L	87	MET
14	L	93	ARG
14	L	99	ARG
14	L	164	THR
15	M	26	LEU
15	M	43	VAL
15	M	127	LEU
15	M	128	ASP
15	M	152	GLU
15	M	163	PHE
16	N	3	THR
16	N	28	ASP
17	O	91	LYS
17	O	98	ILE
18	P	11	ARG
18	P	16	ASN
18	P	57	ASP
18	P	95	GLU
19	Q	13	THR
19	Q	39	THR
19	Q	82	GLU
21	S	39	ASN
21	S	48	VAL
21	S	73	HIS
21	S	96	VAL
23	U	43	PRO
24	V	4	LEU
24	V	35	VAL
24	V	52	VAL
24	V	73	LEU
24	V	122	ARG
24	V	142	ASP
24	V	146	ILE
24	V	154	ARG
25	W	15	ARG
25	W	27	ASP
25	W	49	ARG
25	W	72	VAL
26	X	141	THR
26	X	154	ARG
26	X	163	THR
26	X	172	THR

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Mol	Chain	Res	Type
26	X	186	ARG
26	X	189	ASN
26	X	200	THR
26	X	203	VAL
26	X	204	ARG
26	X	231	PRO
27	Y	11	THR
27	Y	44	PHE
27	Y	49	ARG
27	Y	64	ILE
29	1	18	ASN
30	2	14	CYS
30	2	42	ARG
30	2	56	PRO

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

Mol	Chain	Res	Type
3	A	92	ASN
3	A	127	GLN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	318	ASN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
5	C	163	HIS
6	D	103	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	8	ASN
10	H	35	ASN
10	H	55	GLN

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Mol	Chain	Res	Type
10	H	58	HIS
10	H	59	ASN
10	H	69	ASN
10	H	74	ASN
10	H	91	HIS
10	H	129	ASN
10	H	130	HIS
10	H	166	ASN
11	I	52	GLN
11	I	107	ASN
11	I	126	ASN
12	J	10	GLN
13	K	18	HIS
13	K	41	HIS
13	K	42	ASN
13	K	116	HIS
14	L	26	HIS
14	L	58	GLN
14	L	89	ASN
14	L	176	GLN
15	M	21	HIS
15	M	107	ASN
15	M	153	GLN
16	N	53	GLN
17	O	50	GLN
17	O	66	GLN
17	O	73	HIS
17	O	118	GLN
18	P	16	ASN
18	P	40	HIS
19	Q	61	GLN
19	Q	94	ASN
19	Q	98	ASN
19	Q	113	HIS
19	Q	117	HIS
19	Q	122	GLN
20	R	53	ASN
21	S	39	ASN
21	S	73	HIS
22	T	39	ASN
23	U	60	GLN
24	V	27	HIS

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Mol	Chain	Res	Type
24	V	87	HIS
24	V	110	GLN
24	V	119	HIS
24	V	125	HIS
24	V	141	HIS
25	W	23	HIS
26	X	133	HIS
26	X	134	HIS
26	X	149	GLN
26	X	189	ASN
27	Y	33	HIS
27	Y	70	GLN
28	Z	8	GLN
28	Z	16	HIS
28	Z	28	HIS
29	1	16	ASN
29	1	18	ASN
29	1	41	HIS
29	1	45	ASN
30	2	30	GLN
30	2	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	239 (8%)	0
2	9	121/122 (99%)	16 (13%)	0
All	All	2866/3044 (94%)	255 (8%)	0

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G

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Mol	Chain	Res	Type
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G

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Mol	Chain	Res	Type
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	898	G
1	0	905	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U

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Mol	Chain	Res	Type
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1161	A
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G
1	0	1177	A
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1380	U
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1603	A

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Mol	Chain	Res	Type
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1904	A
1	0	1919	A
1	0	1942	A
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1982	C
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G

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Mol	Chain	Res	Type
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2346	C
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2681	A

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Mol	Chain	Res	Type
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2914	A
2	9	2	U
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	26	C
2	9	41	C
2	9	43	G
2	9	44	A
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.39	60 (2%) 62 59	17, 36, 79, 127	0
2	9	122/122 (100%)	-0.36	6 (4%) 30 29	31, 54, 78, 136	0
3	A	237/239 (99%)	0.38	20 (8%) 12 10	19, 38, 71, 92	0
4	B	337/337 (100%)	0.37	14 (4%) 37 35	21, 45, 71, 82	0
5	C	246/246 (100%)	0.31	9 (3%) 42 41	15, 35, 58, 70	0
6	D	140/176 (79%)	2.55	84 (60%) 0 0	43, 86, 105, 108	0
7	E	172/177 (97%)	0.59	8 (4%) 32 30	37, 59, 77, 81	0
8	F	119/119 (100%)	0.89	21 (17%) 2 1	37, 58, 83, 88	0
9	G	29/348 (8%)	2.56	21 (72%) 0 0	64, 79, 86, 91	0
10	H	156/167 (93%)	0.70	22 (14%) 3 3	30, 47, 75, 79	0
11	I	142/145 (97%)	0.24	5 (3%) 44 43	29, 42, 63, 84	0
12	J	132/132 (100%)	0.16	7 (5%) 27 25	27, 42, 61, 71	0
13	K	145/164 (88%)	0.70	15 (10%) 7 6	18, 54, 90, 102	0
14	L	194/194 (100%)	0.12	6 (3%) 49 47	19, 32, 50, 62	0
15	M	186/186 (100%)	0.60	16 (8%) 11 10	31, 50, 91, 103	0
16	N	115/115 (100%)	-0.04	1 (0%) 84 82	27, 44, 60, 69	0
17	O	143/148 (96%)	0.14	1 (0%) 87 86	30, 44, 57, 64	0
18	P	95/95 (100%)	0.07	1 (1%) 80 79	25, 34, 50, 61	0
19	Q	150/154 (97%)	-0.04	0 100 100	23, 36, 54, 63	0
20	R	81/84 (96%)	0.46	9 (11%) 6 5	31, 47, 68, 72	0
21	S	119/119 (100%)	0.40	3 (2%) 58 55	28, 45, 69, 81	0
22	T	53/66 (80%)	0.34	1 (1%) 67 64	33, 47, 63, 71	0
23	U	65/70 (92%)	1.62	12 (18%) 1 1	39, 59, 97, 101	0
24	V	154/154 (100%)	0.33	5 (3%) 48 46	27, 40, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	82/91 (90%)	0.45	5 (6%) 22 20	35, 48, 73, 91	0
26	X	142/240 (59%)	-0.01	4 (2%) 53 51	22, 35, 59, 74	0
27	Y	73/73 (100%)	0.57	9 (12%) 5 4	36, 49, 63, 77	0
28	Z	56/56 (100%)	0.21	0 100 100	17, 24, 32, 35	0
29	1	46/48 (95%)	0.51	6 (13%) 4 3	27, 49, 77, 86	0
30	2	92/92 (100%)	0.19	2 (2%) 62 59	23, 44, 59, 72	0
All	All	6577/7279 (90%)	0.10	373 (5%) 24 23	15, 41, 80, 136	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	1	THR	13.9
6	D	63	ILE	10.0
23	U	39	ALA	8.7
6	D	57	THR	7.6
23	U	40	PRO	6.7
2	9	1	U	6.7
25	W	88	GLU	6.6
20	R	81	ILE	6.6
3	A	37	VAL	6.5
15	M	186	LEU	6.4
6	D	18	ILE	6.3
15	M	166	ALA	6.3
6	D	10	PHE	6.3
6	D	170	TYR	5.9
23	U	38	GLY	5.9
1	0	1172	G	5.8
25	W	80	GLU	5.7
8	F	106	THR	5.6
4	B	1	PRO	5.4
6	D	69	ILE	5.4
3	A	237	GLY	5.4
6	D	92	GLU	5.4
9	G	23	ILE	5.3
1	0	1198	U	5.3
6	D	66	GLY	5.2
6	D	85	GLN	5.2
6	D	61	PHE	5.2
23	U	43	PRO	5.2
6	D	58	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
6	D	172	VAL	5.0
6	D	166	ILE	5.0
1	0	1200	A	4.9
2	9	25	G	4.9
1	0	282	C	4.8
6	D	75	LEU	4.8
1	0	1177	A	4.7
3	A	36	ASP	4.7
6	D	165	PHE	4.7
1	0	1202	A	4.7
1	0	1174	A	4.7
6	D	88	LEU	4.7
15	M	162	ASP	4.7
2	9	23	U	4.6
3	A	35	GLY	4.6
1	0	1171	A	4.6
6	D	94	ALA	4.5
1	0	284	C	4.5
3	A	85	ASP	4.5
9	G	26	MET	4.4
6	D	50	VAL	4.4
7	E	87	PHE	4.4
26	X	235	GLU	4.4
1	0	1169	U	4.3
6	D	62	ASP	4.2
9	G	12	ILE	4.2
6	D	106	PHE	4.2
6	D	102	GLY	4.2
9	G	70	ALA	4.1
6	D	44	ILE	4.1
6	D	67	ASP	4.1
6	D	95	THR	4.1
1	0	1525	G	4.0
6	D	81	GLU	4.0
1	0	1173	A	4.0
6	D	104	PHE	4.0
1	0	1170	U	4.0
5	C	135	GLU	4.0
1	0	1199	A	4.0
10	H	146	TRP	4.0
1	0	1201	C	3.9
1	0	960	G	3.9

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Mol	Chain	Res	Type	RSRZ
1	0	970	U	3.9
11	I	4	ALA	3.8
6	D	64	ARG	3.8
2	9	24	U	3.8
13	K	81	VAL	3.8
13	K	80	ASP	3.7
1	0	1196	C	3.7
27	Y	80	MET	3.6
6	D	27	ILE	3.6
6	D	56	ARG	3.6
6	D	40	ILE	3.6
6	D	134	LEU	3.6
7	E	45	ASP	3.6
23	U	41	GLU	3.6
9	G	24	VAL	3.6
15	M	163	PHE	3.5
27	Y	22	ILE	3.5
6	D	171	ASP	3.5
1	0	1951	G	3.5
6	D	132	VAL	3.5
6	D	51	ARG	3.5
9	G	73	ASP	3.5
6	D	11	HIS	3.5
8	F	119	ARG	3.5
6	D	17	ARG	3.5
6	D	84	LEU	3.5
6	D	101	THR	3.5
1	0	1192	A	3.5
6	D	68	PRO	3.5
23	U	2	VAL	3.5
10	H	83	PHE	3.5
1	0	1165	G	3.5
1	0	2237	G	3.5
9	G	25	GLU	3.4
6	D	93	LEU	3.4
6	D	73	VAL	3.4
15	M	152	GLU	3.4
13	K	147	GLU	3.4
10	H	163	PRO	3.4
4	B	57	GLU	3.4
1	0	1181	A	3.4
1	0	1179	C	3.4

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Mol	Chain	Res	Type	RSRZ
25	W	85	VAL	3.4
6	D	98	PHE	3.3
10	H	135	TRP	3.3
8	F	118	LEU	3.3
12	J	132	VAL	3.3
14	L	194	ALA	3.3
6	D	103	ASN	3.3
8	F	115	VAL	3.3
10	H	32	ASP	3.3
22	T	47	ARG	3.3
1	0	10	U	3.3
24	V	93	ILE	3.3
10	H	79	ALA	3.3
1	0	1203	G	3.3
6	D	173	GLU	3.2
15	M	68	GLU	3.2
3	A	31	LYS	3.2
12	J	119	GLN	3.2
1	0	1175	G	3.2
21	S	1	SER	3.2
13	K	145	LEU	3.2
15	M	181	ASP	3.2
30	2	92	GLU	3.2
6	D	26	GLY	3.1
8	F	16	ALA	3.1
5	C	132	ASP	3.1
6	D	99	ASP	3.1
1	0	1178	G	3.1
3	A	133	ARG	3.1
14	L	87	MET	3.1
1	0	1163	G	3.1
6	D	74	THR	3.1
1	0	1168	C	3.1
9	G	69	ARG	3.1
6	D	96	SER	3.1
6	D	167	GLU	3.0
20	R	77	VAL	3.0
13	K	102	ASP	3.0
16	N	23	GLY	3.0
1	0	1195	G	3.0
6	D	23	VAL	3.0
4	B	133	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
27	Y	38	LYS	3.0
26	X	108	ASP	3.0
20	R	2	TRP	3.0
8	F	108	LEU	3.0
6	D	22	VAL	3.0
4	B	104	GLU	3.0
1	0	1180	U	2.9
1	0	1950	G	2.9
10	H	81	TYR	2.9
27	Y	44	PHE	2.9
3	A	236	GLY	2.9
6	D	55	LYS	2.9
6	D	157	LEU	2.9
9	G	66	LEU	2.9
6	D	78	GLU	2.9
2	9	2	U	2.9
8	F	107	VAL	2.9
3	A	34	ASP	2.9
9	G	15	TRP	2.9
6	D	49	PRO	2.9
1	0	1206	U	2.9
13	K	150	GLN	2.9
5	C	198	ASP	2.8
11	I	5	GLU	2.8
1	0	1176	C	2.8
6	D	86	THR	2.8
29	1	39	ARG	2.8
1	0	1205	U	2.8
29	1	24	TRP	2.8
8	F	99	THR	2.8
9	G	28	GLU	2.8
6	D	89	PRO	2.8
4	B	117	GLU	2.8
8	F	117	GLU	2.8
20	R	80	ARG	2.8
13	K	148	GLU	2.8
3	A	64	ASP	2.8
6	D	25	MET	2.8
4	B	183	GLU	2.7
7	E	169	THR	2.7
8	F	12	LEU	2.7
9	G	71	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
10	H	157	ILE	2.7
8	F	17	LEU	2.7
6	D	65	GLU	2.7
6	D	80	ALA	2.7
7	E	88	TYR	2.7
29	1	35	ARG	2.7
3	A	97	ALA	2.7
24	V	38	THR	2.7
27	Y	11	THR	2.7
9	G	21	ASP	2.7
15	M	164	ASP	2.7
3	A	32	VAL	2.7
5	C	14	GLY	2.7
9	G	14	GLU	2.6
9	G	72	ASP	2.6
1	0	1197	G	2.6
9	G	20	VAL	2.6
6	D	45	THR	2.6
6	D	133	ASN	2.6
4	B	180	ASP	2.6
14	L	165	SER	2.6
10	H	66	VAL	2.6
12	J	108	GLU	2.6
15	M	154	LEU	2.6
7	E	10	ASP	2.6
6	D	158	ASN	2.6
10	H	72	VAL	2.6
4	B	184	ASP	2.6
13	K	75	LEU	2.6
7	E	170	ARG	2.6
30	2	56	PRO	2.6
10	H	41	THR	2.6
25	W	71	ARG	2.6
9	G	27	ILE	2.6
1	0	1167	G	2.6
20	R	76	GLU	2.6
6	D	77	ASP	2.6
14	L	152	ARG	2.6
10	H	35	ASN	2.6
7	E	100	ASP	2.6
27	Y	21	LYS	2.5
4	B	120	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	1162	G	2.5
5	C	143	ASP	2.5
20	R	1	SER	2.5
8	F	110	GLU	2.5
10	H	162	SER	2.5
14	L	140	ALA	2.5
6	D	53	LYS	2.5
13	K	91	VAL	2.5
1	0	735	C	2.5
6	D	156	ARG	2.5
13	K	130	ARG	2.5
12	J	125	ALA	2.5
1	0	2238	A	2.5
4	B	181	ILE	2.5
6	D	47	GLN	2.5
1	0	1948	G	2.5
4	B	123	ALA	2.5
6	D	128	LEU	2.5
1	0	1967	U	2.5
1	0	1208	C	2.5
6	D	48	MET	2.5
8	F	22	VAL	2.4
6	D	130	VAL	2.4
1	0	1625	U	2.4
7	E	129	GLU	2.4
8	F	15	ASP	2.4
9	G	18	GLU	2.4
29	1	49	GLU	2.4
23	U	37	GLY	2.4
8	F	10	ALA	2.4
21	S	82	THR	2.4
1	0	1204	C	2.4
23	U	6	GLN	2.4
6	D	90	LEU	2.4
6	D	70	GLY	2.4
13	K	104	ASP	2.4
15	M	138	ASP	2.4
10	H	142	VAL	2.4
15	M	139	TRP	2.4
26	X	236	VAL	2.3
1	0	2769	C	2.3
6	D	54	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	C	13	ASP	2.3
1	0	283	U	2.3
6	D	139	TYR	2.3
8	F	28	ALA	2.3
9	G	17	GLN	2.3
4	B	115	VAL	2.3
5	C	61	PHE	2.3
5	C	162	VAL	2.3
15	M	177	GLU	2.3
23	U	45	ARG	2.3
29	1	44	ARG	2.3
6	D	71	ALA	2.3
8	F	100	ASP	2.3
1	0	2004	U	2.3
13	K	149	ARG	2.3
10	H	36	ASN	2.3
6	D	59	GLY	2.3
12	J	126	SER	2.3
15	M	184	ILE	2.3
27	Y	40	PRO	2.2
10	H	158	ASN	2.2
1	0	1279	U	2.2
3	A	38	ILE	2.2
6	D	162	ALA	2.2
10	H	59	ASN	2.2
6	D	43	GLU	2.2
1	0	281	U	2.2
1	0	1207	A	2.2
6	D	29	HIS	2.2
25	W	73	ARG	2.2
12	J	129	THR	2.2
8	F	18	GLU	2.2
20	R	46	ASP	2.2
1	0	2508	C	2.2
9	G	68	GLU	2.2
10	H	139	ASP	2.2
4	B	92	TYR	2.2
6	D	83	PHE	2.2
13	K	144	ASP	2.2
20	R	45	TYR	2.2
10	H	33	MET	2.2
8	F	114	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
11	I	39	VAL	2.2
6	D	169	THR	2.2
3	A	66	ARG	2.2
6	D	135	VAL	2.1
8	F	26	THR	2.1
1	0	1965	C	2.1
6	D	41	LEU	2.1
15	M	134	ASP	2.1
24	V	91	ASP	2.1
14	L	63	VAL	2.1
26	X	95	THR	2.1
15	M	179	LEU	2.1
1	0	2825	C	2.1
1	0	1166	A	2.1
24	V	61	THR	2.1
3	A	99	ILE	2.1
1	0	1949	G	2.1
8	F	11	ASP	2.1
13	K	90	ARG	2.1
12	J	101	ASN	2.1
15	M	175	LEU	2.1
23	U	49	LEU	2.1
24	V	86	GLU	2.1
11	I	7	ASP	2.1
13	K	89	PHE	2.1
1	0	1164	U	2.1
20	R	79	SER	2.1
10	H	80	ASN	2.1
29	1	36	ASN	2.1
1	0	999	C	2.0
4	B	61	PRO	2.0
27	Y	75	ALA	2.0
10	H	136	VAL	2.0
11	I	47	THR	2.0
3	A	94	LEU	2.0
23	U	28	LEU	2.0
3	A	89	ALA	2.0
6	D	164	ALA	2.0
3	A	134	ASN	2.0
3	A	63	GLY	2.0
27	Y	47	LEU	2.0
1	0	2250	G	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	60	PHE	2.0
18	P	95	GLU	2.0
10	H	128	ALA	2.0
5	C	141	SER	2.0
2	9	122	C	2.0
17	O	76	GLY	2.0
9	G	67	LEU	2.0
21	S	59	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	NA	0	8320	1/1	0.99	0.29	31.60	38,38,38,38	0
33	NA	0	8350	1/1	0.93	0.35	29.76	36,36,36,36	0
33	NA	0	8371	1/1	0.76	0.36	23.72	49,49,49,49	0
33	NA	0	8372	1/1	0.92	0.43	23.09	54,54,54,54	0
33	NA	0	8362	1/1	0.94	0.34	18.39	51,51,51,51	0
33	NA	0	8327	1/1	0.92	0.27	17.22	38,38,38,38	0
33	NA	0	8340	1/1	0.90	0.26	15.56	47,47,47,47	0
33	NA	Q	8386	1/1	0.62	0.44	12.93	74,74,74,74	0
33	NA	0	8366	1/1	0.96	0.26	12.64	54,54,54,54	0
33	NA	0	8331	1/1	0.98	0.27	11.15	39,39,39,39	0
33	NA	0	8376	1/1	0.91	0.28	10.71	39,39,39,39	0
33	NA	0	8302	1/1	0.93	0.24	9.87	44,44,44,44	0
33	NA	0	8364	1/1	0.97	0.26	8.74	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	0	8314	1/1	0.93	0.32	8.45	40,40,40,40	0
33	NA	0	8374	1/1	0.96	0.20	6.89	44,44,44,44	0
33	NA	0	8325	1/1	0.94	0.23	4.93	47,47,47,47	0
33	NA	0	8361	1/1	0.93	0.23	4.34	38,38,38,38	0
33	NA	K	8380	1/1	0.97	0.26	4.24	42,42,42,42	0
33	NA	0	8305	1/1	0.98	0.22	4.09	32,32,32,32	0
31	MG	0	8060	1/1	0.99	0.21	3.89	31,31,31,31	0
33	NA	0	8321	1/1	0.94	0.24	2.81	40,40,40,40	0
33	NA	0	8303	1/1	0.98	0.17	2.58	32,32,32,32	0
33	NA	9	8383	1/1	0.89	0.21	1.79	43,43,43,43	0
33	NA	0	8356	1/1	0.93	0.20	1.33	37,37,37,37	0
33	NA	0	8368	1/1	0.94	0.14	1.04	48,48,48,48	0
33	NA	0	8335	1/1	0.96	0.18	0.92	31,31,31,31	0
33	NA	0	8339	1/1	0.98	0.19	0.87	20,20,20,20	0
31	MG	0	8012	1/1	0.95	0.14	0.51	32,32,32,32	0
33	NA	0	8373	1/1	0.90	0.12	0.27	43,43,43,43	0
33	NA	C	8304	1/1	0.85	0.18	-0.09	30,30,30,30	0
33	NA	0	8365	1/1	0.96	0.18	-0.20	28,28,28,28	0
31	MG	0	8067	1/1	0.91	0.14	-0.24	34,34,34,34	0
33	NA	0	8324	1/1	0.95	0.13	-0.25	48,48,48,48	0
31	MG	0	8010	1/1	0.97	0.17	-0.35	24,24,24,24	0
31	MG	0	8007	1/1	0.98	0.17	-0.39	21,21,21,21	0
34	CL	I	8521	1/1	0.94	0.17	-0.39	47,47,47,47	0
34	CL	0	8516	1/1	0.99	0.14	-0.47	42,42,42,42	0
34	CL	L	8518	1/1	0.98	0.15	-0.50	32,32,32,32	0
33	NA	0	8381	1/1	0.98	0.12	-0.54	41,41,41,41	0
35	CD	Y	8403	1/1	0.99	0.14	-0.67	49,49,49,49	0
31	MG	0	8064	1/1	0.94	0.15	-0.72	26,26,26,26	0
33	NA	0	8378	1/1	0.97	0.17	-0.73	39,39,39,39	0
31	MG	0	8013	1/1	0.95	0.15	-0.75	22,22,22,22	0
33	NA	L	8347	1/1	0.97	0.14	-0.82	18,18,18,18	0
31	MG	0	8086	1/1	0.99	0.09	-0.90	33,33,33,33	0
31	MG	0	8015	1/1	0.98	0.18	-1.03	26,26,26,26	0
33	NA	0	8344	1/1	0.97	0.11	-1.11	24,24,24,24	0
33	NA	0	8382	1/1	0.94	0.10	-1.31	64,64,64,64	0
31	MG	0	8038	1/1	0.98	0.13	-1.38	22,22,22,22	0
33	NA	H	8309	1/1	0.99	0.10	-1.47	28,28,28,28	0
34	CL	0	8515	1/1	0.99	0.11	-1.54	48,48,48,48	0
33	NA	0	8332	1/1	0.97	0.12	-1.54	33,33,33,33	0
35	CD	T	8401	1/1	0.99	0.10	-1.62	49,49,49,49	0
33	NA	0	8310	1/1	0.94	0.11	-1.74	27,27,27,27	0
34	CL	B	8519	1/1	0.99	0.14	-1.78	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CD	2	8404	1/1	0.99	0.09	-1.86	47,47,47,47	0
34	CL	0	8512	1/1	0.99	0.11	-1.86	34,34,34,34	0
31	MG	0	8054	1/1	0.98	0.16	-1.94	18,18,18,18	0
33	NA	I	8346	1/1	0.98	0.09	-2.02	34,34,34,34	0
33	NA	0	8353	1/1	0.99	0.14	-2.14	18,18,18,18	0
33	NA	0	8333	1/1	0.95	0.09	-2.19	23,23,23,23	0
31	MG	0	8004	1/1	0.99	0.13	-2.28	21,21,21,21	0
31	MG	0	8027	1/1	0.98	0.06	-2.39	37,37,37,37	0
33	NA	0	8317	1/1	0.96	0.10	-2.53	27,27,27,27	0
33	NA	0	8334	1/1	0.95	0.09	-2.54	33,33,33,33	0
34	CL	0	8505	1/1	0.98	0.11	-2.66	41,41,41,41	0
32	K	0	8201	1/1	0.95	0.14	-2.72	62,62,62,62	0
34	CL	N	8508	1/1	0.97	0.07	-2.75	52,52,52,52	0
31	MG	2	8078	1/1	0.98	0.10	-2.77	39,39,39,39	0
33	NA	P	8348	1/1	0.95	0.07	-2.80	32,32,32,32	0
31	MG	S	8073	1/1	0.98	0.06	-3.07	39,39,39,39	0
33	NA	A	8345	1/1	0.93	0.09	-3.18	46,46,46,46	0
31	MG	0	8091	1/1	0.96	0.10	-3.21	41,41,41,41	0
33	NA	S	8343	1/1	0.97	0.06	-3.27	29,29,29,29	0
31	MG	0	8003	1/1	0.98	0.11	-3.28	21,21,21,21	0
31	MG	0	8077	1/1	0.92	0.14	-3.29	23,23,23,23	0
31	MG	0	8057	1/1	0.98	0.12	-3.32	35,35,35,35	0
31	MG	0	8074	1/1	0.97	0.06	-3.40	36,36,36,36	0
31	MG	0	8096	1/1	0.97	0.10	-3.50	37,37,37,37	0
31	MG	0	8017	1/1	1.00	0.13	-3.61	12,12,12,12	0
31	MG	0	8112	1/1	0.98	0.10	-3.93	23,23,23,23	0
31	MG	0	8033	1/1	0.97	0.09	-4.00	20,20,20,20	0
35	CD	Z	8402	1/1	0.99	0.04	-4.10	37,37,37,37	0
31	MG	0	8008	1/1	0.99	0.10	-4.16	22,22,22,22	0
31	MG	X	8109	1/1	0.98	0.08	-4.18	25,25,25,25	0
31	MG	0	8080	1/1	0.94	0.07	-4.33	41,41,41,41	0
31	MG	0	8020	1/1	0.97	0.09	-4.47	24,24,24,24	0
31	MG	0	8110	1/1	0.99	0.10	-4.65	24,24,24,24	0
31	MG	B	8055	1/1	0.91	0.07	-4.80	40,40,40,40	0
31	MG	0	8084	1/1	0.98	0.07	-5.01	39,39,39,39	0
33	NA	Q	8337	1/1	0.96	0.07	-5.14	33,33,33,33	0
33	NA	0	8323	1/1	0.99	0.12	-5.40	31,31,31,31	0
31	MG	0	8056	1/1	0.98	0.04	-5.49	31,31,31,31	0
31	MG	A	8065	1/1	0.97	0.07	-5.63	24,24,24,24	0
31	MG	0	8108	1/1	0.97	0.07	-5.64	62,62,62,62	0
33	NA	0	8313	1/1	0.94	0.09	-5.93	48,48,48,48	0
31	MG	0	8001	1/1	0.98	0.11	-6.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	0	8338	1/1	0.99	0.06	-6.32	36,36,36,36	0
31	MG	0	8107	1/1	0.96	0.03	-6.57	30,30,30,30	0
31	MG	0	8035	1/1	0.98	0.07	-6.62	36,36,36,36	0
31	MG	0	8044	1/1	0.98	0.09	-6.73	32,32,32,32	0
31	MG	0	8058	1/1	0.97	0.06	-6.73	27,27,27,27	0
34	CL	2	8504	1/1	0.98	0.06	-7.08	45,45,45,45	0
31	MG	0	8059	1/1	0.96	0.07	-7.65	25,25,25,25	0
31	MG	0	8053	1/1	0.99	0.07	-8.20	28,28,28,28	0
31	MG	0	8039	1/1	0.97	0.07	-8.73	32,32,32,32	0
31	MG	0	8018	1/1	0.97	0.06	-8.80	27,27,27,27	0
31	MG	0	8032	1/1	0.96	0.06	-8.82	23,23,23,23	0
31	MG	0	8021	1/1	0.99	0.09	-8.96	24,24,24,24	0
31	MG	0	8019	1/1	0.99	0.05	-9.13	23,23,23,23	0
31	MG	0	8006	1/1	0.94	0.07	-10.10	27,27,27,27	0
31	MG	0	8028	1/1	0.96	0.06	-11.38	25,25,25,25	0
31	MG	0	8071	1/1	0.94	0.04	-11.41	62,62,62,62	0
31	MG	0	8002	1/1	0.96	0.08	-12.77	26,26,26,26	0
31	MG	0	8052	1/1	0.98	0.06	-14.41	45,45,45,45	0
32	K	0	8202	1/1	0.99	0.08	-16.18	37,37,37,37	0
33	NA	0	8349	1/1	0.96	0.18	-	37,37,37,37	0
31	MG	0	8087	1/1	0.62	0.28	-	72,72,72,72	0
31	MG	0	8048	1/1	0.98	0.07	-	39,39,39,39	0
34	CL	K	8510	1/1	0.98	0.08	-	36,36,36,36	0
34	CL	I	8502	1/1	0.96	0.11	-	53,53,53,53	0
33	NA	9	8351	1/1	0.90	0.12	-	42,42,42,42	0
31	MG	0	8014	1/1	0.93	0.09	-	25,25,25,25	0
31	MG	0	8102	1/1	0.84	0.11	-	51,51,51,51	0
33	NA	0	8360	1/1	0.93	0.21	-	41,41,41,41	0
34	CL	A	8509	1/1	0.98	0.12	-	50,50,50,50	0
31	MG	0	8016	1/1	0.94	0.09	-	32,32,32,32	0
31	MG	0	8031	1/1	0.97	0.12	-	24,24,24,24	0
31	MG	0	8043	1/1	0.90	0.07	-	33,33,33,33	0
31	MG	0	8116	1/1	0.97	0.09	-	42,42,42,42	0
31	MG	0	8090	1/1	0.90	0.31	-	53,53,53,53	0
34	CL	0	8522	1/1	0.97	0.15	-	44,44,44,44	0
31	MG	0	8066	1/1	0.95	0.49	-	85,85,85,85	0
33	NA	0	8370	1/1	0.77	0.44	-	61,61,61,61	0
31	MG	0	8076	1/1	0.87	0.04	-	46,46,46,46	0
31	MG	A	8105	1/1	0.97	0.16	-	27,27,27,27	0
31	MG	0	8093	1/1	0.94	0.12	-	35,35,35,35	0
34	CL	0	8517	1/1	0.97	0.09	-	50,50,50,50	0
33	NA	0	8306	1/1	0.98	0.13	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	0	8062	1/1	0.91	0.08	-	41,41,41,41	0
31	MG	0	8045	1/1	0.95	0.07	-	51,51,51,51	0
31	MG	0	8024	1/1	0.99	0.15	-	22,22,22,22	0
34	CL	I	8501	1/1	0.98	0.09	-	44,44,44,44	0
31	MG	0	8063	1/1	0.96	0.12	-	62,62,62,62	0
31	MG	0	8022	1/1	0.92	0.12	-	32,32,32,32	0
31	MG	0	8023	1/1	0.97	0.14	-	30,30,30,30	0
31	MG	0	8106	1/1	0.95	0.13	-	42,42,42,42	0
33	NA	0	8330	1/1	0.97	0.07	-	39,39,39,39	0
31	MG	0	8075	1/1	0.98	0.06	-	28,28,28,28	0
31	MG	0	8046	1/1	0.94	0.05	-	38,38,38,38	0
33	NA	0	8307	1/1	0.88	0.13	-	42,42,42,42	0
34	CL	X	8520	1/1	0.96	0.13	-	38,38,38,38	0
31	MG	0	8040	1/1	0.97	0.12	-	38,38,38,38	0
33	NA	0	8355	1/1	0.96	0.38	-	47,47,47,47	0
34	CL	0	8513	1/1	0.99	0.10	-	44,44,44,44	0
31	MG	0	8036	1/1	0.97	0.08	-	35,35,35,35	0
33	NA	0	8326	1/1	0.95	0.21	-	37,37,37,37	0
31	MG	0	8088	1/1	0.99	0.09	-	20,20,20,20	0
34	CL	Q	8506	1/1	0.97	0.12	-	40,40,40,40	0
34	CL	0	8503	1/1	0.98	0.17	-	40,40,40,40	0
31	MG	0	8100	1/1	0.96	0.06	-	64,64,64,64	0
33	NA	0	8358	1/1	0.92	0.35	-	74,74,74,74	0
33	NA	0	8363	1/1	0.88	0.32	-	52,52,52,52	0
31	MG	J	8069	1/1	0.94	0.13	-	46,46,46,46	0
31	MG	0	8083	1/1	0.98	0.07	-	30,30,30,30	0
31	MG	0	8082	1/1	0.94	0.17	-	56,56,56,56	0
31	MG	0	8029	1/1	0.98	0.09	-	35,35,35,35	0
31	MG	0	8047	1/1	0.87	0.10	-	54,54,54,54	0
31	MG	0	8009	1/1	0.97	0.14	-	24,24,24,24	0
33	NA	0	8342	1/1	0.96	0.22	-	33,33,33,33	0
31	MG	0	8030	1/1	0.99	0.07	-	22,22,22,22	0
31	MG	0	8099	1/1	0.93	0.24	-	44,44,44,44	0
31	MG	0	8114	1/1	0.97	0.09	-	35,35,35,35	0
31	MG	0	8049	1/1	0.84	0.12	-	56,56,56,56	0
31	MG	0	8101	1/1	0.88	0.30	-	48,48,48,48	0
33	NA	0	8352	1/1	0.98	0.12	-	40,40,40,40	0
33	NA	0	8316	1/1	0.97	0.22	-	35,35,35,35	0
31	MG	0	8042	1/1	0.97	0.10	-	29,29,29,29	0
33	NA	0	8384	1/1	0.82	0.14	-	52,52,52,52	0
31	MG	0	8113	1/1	0.86	0.13	-	36,36,36,36	0
31	MG	0	8061	1/1	0.97	0.13	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	0	8367	1/1	0.97	0.26	-	45,45,45,45	0
31	MG	0	8041	1/1	0.97	0.10	-	33,33,33,33	0
35	CD	N	8405	1/1	0.98	0.08	-	71,71,71,71	0
33	NA	H	8322	1/1	0.86	0.26	-	52,52,52,52	0
31	MG	0	8092	1/1	0.98	0.10	-	66,66,66,66	0
34	CL	0	8511	1/1	0.98	0.10	-	37,37,37,37	0
31	MG	0	8111	1/1	0.99	0.12	-	32,32,32,32	0
34	CL	0	8514	1/1	0.98	0.20	-	36,36,36,36	0
33	NA	0	8301	1/1	0.97	0.09	-	33,33,33,33	0
31	MG	0	8068	1/1	0.94	0.04	-	44,44,44,44	0
31	MG	0	8115	1/1	0.95	0.07	-	36,36,36,36	0
33	NA	0	8319	1/1	0.96	0.13	-	29,29,29,29	0
31	MG	0	8117	1/1	0.92	0.17	-	36,36,36,36	0
31	MG	9	8095	1/1	0.80	0.15	-	69,69,69,69	0
31	MG	0	8104	1/1	0.94	0.13	-	45,45,45,45	0
33	NA	0	8328	1/1	0.99	0.12	-	28,28,28,28	0
33	NA	0	8336	1/1	0.96	0.06	-	37,37,37,37	0
33	NA	0	8308	1/1	0.89	0.18	-	42,42,42,42	0
33	NA	0	8369	1/1	0.92	0.22	-	40,40,40,40	0
31	MG	0	8070	1/1	0.84	0.15	-	40,40,40,40	0
31	MG	0	8051	1/1	0.94	0.09	-	56,56,56,56	0
31	MG	0	8034	1/1	0.89	0.09	-	31,31,31,31	0
33	NA	0	8341	1/1	0.94	0.11	-	37,37,37,37	0
33	NA	0	8329	1/1	0.80	0.14	-	48,48,48,48	0
31	MG	0	8037	1/1	0.97	0.07	-	35,35,35,35	0
31	MG	0	8005	1/1	0.99	0.12	-	24,24,24,24	0
33	NA	0	8379	1/1	0.97	0.45	-	48,48,48,48	0
31	MG	0	8085	1/1	0.93	0.07	-	35,35,35,35	0
31	MG	0	8081	1/1	0.96	0.11	-	39,39,39,39	0
33	NA	0	8315	1/1	0.95	0.17	-	30,30,30,30	0
33	NA	0	8375	1/1	0.99	0.21	-	39,39,39,39	0
31	MG	0	8025	1/1	0.98	0.10	-	36,36,36,36	0
33	NA	0	8357	1/1	0.94	0.08	-	39,39,39,39	0
33	NA	0	8311	1/1	0.89	0.15	-	48,48,48,48	0
31	MG	0	8050	1/1	0.76	0.12	-	56,56,56,56	0
33	NA	0	8377	1/1	0.94	0.23	-	50,50,50,50	0
31	MG	0	8026	1/1	0.97	0.15	-	26,26,26,26	0
33	NA	0	8385	1/1	0.92	0.40	-	48,48,48,48	0
31	MG	0	8079	1/1	0.95	0.16	-	19,19,19,19	0
33	NA	0	8318	1/1	0.92	0.25	-	49,49,49,49	0
31	MG	0	8103	1/1	0.78	0.23	-	54,54,54,54	0
31	MG	0	8098	1/1	0.95	0.07	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	0	8011	1/1	0.98	0.10	-	23,23,23,23	0
33	NA	0	8359	1/1	0.96	0.26	-	39,39,39,39	0
33	NA	R	8312	1/1	0.93	0.09	-	26,26,26,26	0
34	CL	M	8507	1/1	0.99	0.08	-	45,45,45,45	0
31	MG	0	8094	1/1	0.92	0.09	-	59,59,59,59	0
31	MG	0	8089	1/1	0.91	0.06	-	51,51,51,51	0
31	MG	0	8097	1/1	0.96	0.07	-	30,30,30,30	0
33	NA	0	8354	1/1	0.98	0.16	-	25,25,25,25	0
31	MG	0	8072	1/1	0.81	0.09	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.