



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:56 AM UTC

PDB ID : 1QVF / pdb_00001qvf
Title : Structure of a deacylated tRNA minihelix bound to the E site of the large ribosomal subunit of *Haloarcula marismortui*
Authors : Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

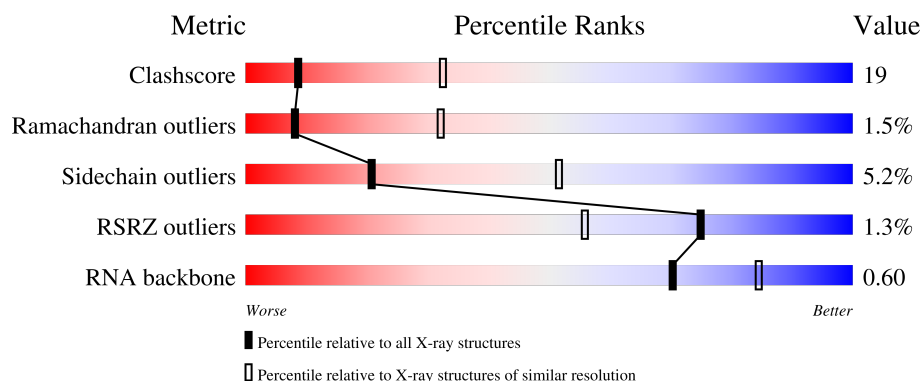
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 56% 30% 7% 6%
2	9	122	3% 45% 37% 15%
3	3	28	18% 14% 11% 57%
4	A	239	% 57% 34% 7%
5	B	337	50% 42% 7%

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

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Mol	Chain	Length	Quality of chain
31	2	92	 61% 36%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8329	-	-	-	X
34	NA	0	8385	-	-	-	X
34	NA	Q	8386	-	-	-	X

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 98648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

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

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

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 RNA chain called Deacylated tRNA minihelix.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	12	Total	C	N	O	P	0	0	0
			257	114	47	84	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	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 6 is a protein called 50S ribosomal protein L4E.

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	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 31 is a protein called 50S ribosomal protein L44E.

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	109	Total Mg 109 109	0	0
32	9	1	Total Mg 1 1	0	0
32	A	2	Total Mg 2 2	0	0
32	B	1	Total Mg 1 1	0	0
32	J	1	Total Mg 1 1	0	0
32	S	1	Total Mg 1 1	0	0
32	X	1	Total Mg 1 1	0	0
32	Y	1	Total Mg 1 1	0	0
32	2	2	Total Mg 2 2	0	0

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	72	Total Na 72 72	0	0
34	9	2	Total Na 2 2	0	0
34	A	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	H	2	Total Na 2 2	0	0
34	I	1	Total Na 1 1	0	0
34	K	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	P	1	Total 1	Na 1	0	0
34	Q	3	Total 3	Na 3	0	0
34	R	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	10	Total 10	Cl 10	0	0
35	A	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	0	0
35	K	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	X	1	Total 1	Cl 1	0	0
35	2	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	N	1	Total 1	Cd 1	0	0
36	T	1	Total 1	Cd 1	0	0
36	Y	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Z	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5836	Total 5836	O 5836	0	0
37	9	138	Total 138	O 138	0	0
37	3	3	Total 3	O 3	0	0
37	A	124	Total 124	O 124	0	0
37	B	150	Total 150	O 150	0	0
37	C	166	Total 166	O 166	0	0
37	D	49	Total 49	O 49	0	0
37	E	42	Total 42	O 42	0	0
37	F	26	Total 26	O 26	0	0
37	G	21	Total 21	O 21	0	0
37	H	75	Total 75	O 75	0	0
37	I	52	Total 52	O 52	0	0
37	J	56	Total 56	O 56	0	0
37	K	79	Total 79	O 79	0	0
37	L	127	Total 127	O 127	0	0
37	M	67	Total 67	O 67	0	0
37	N	42	Total 42	O 42	0	0

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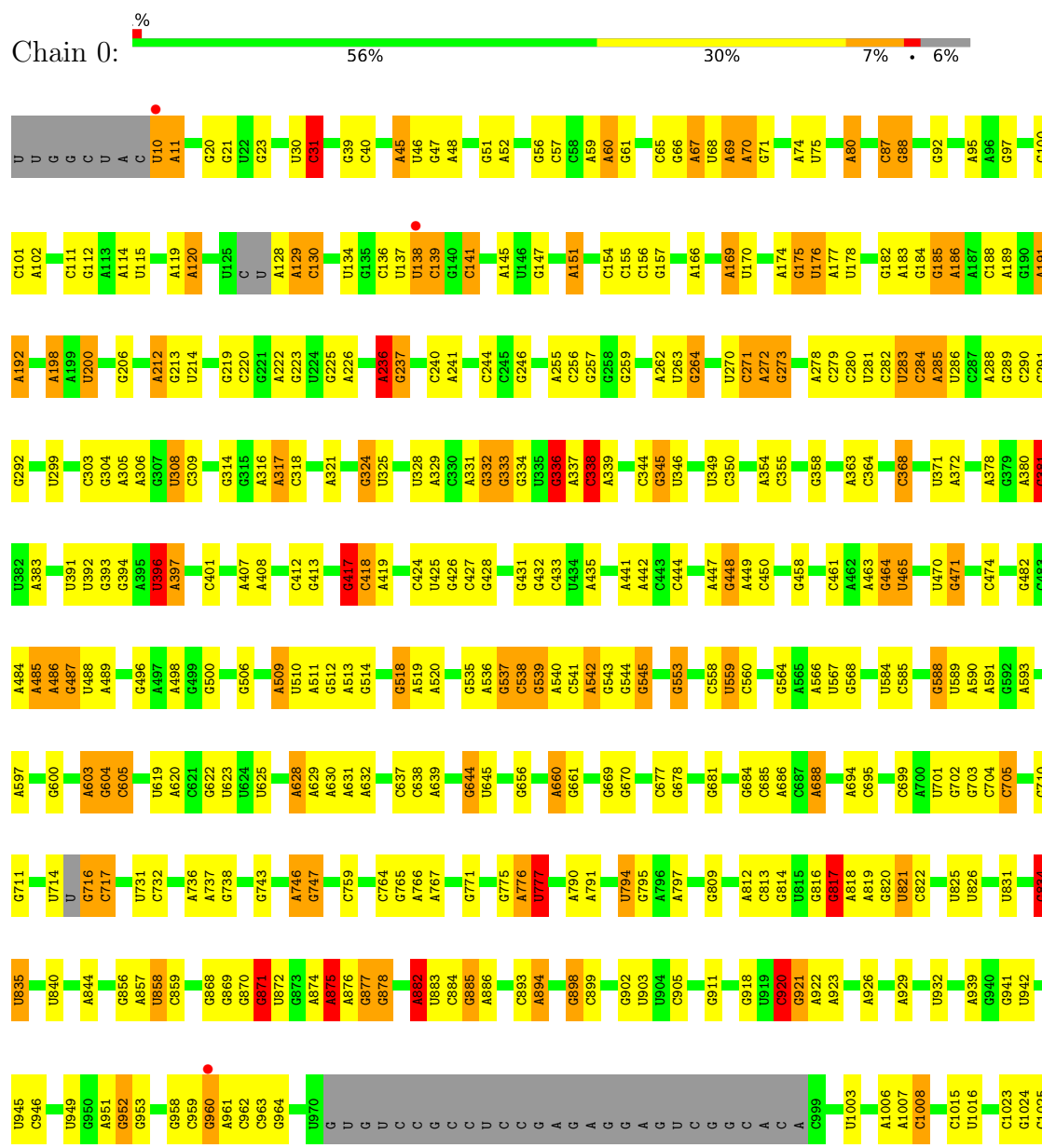
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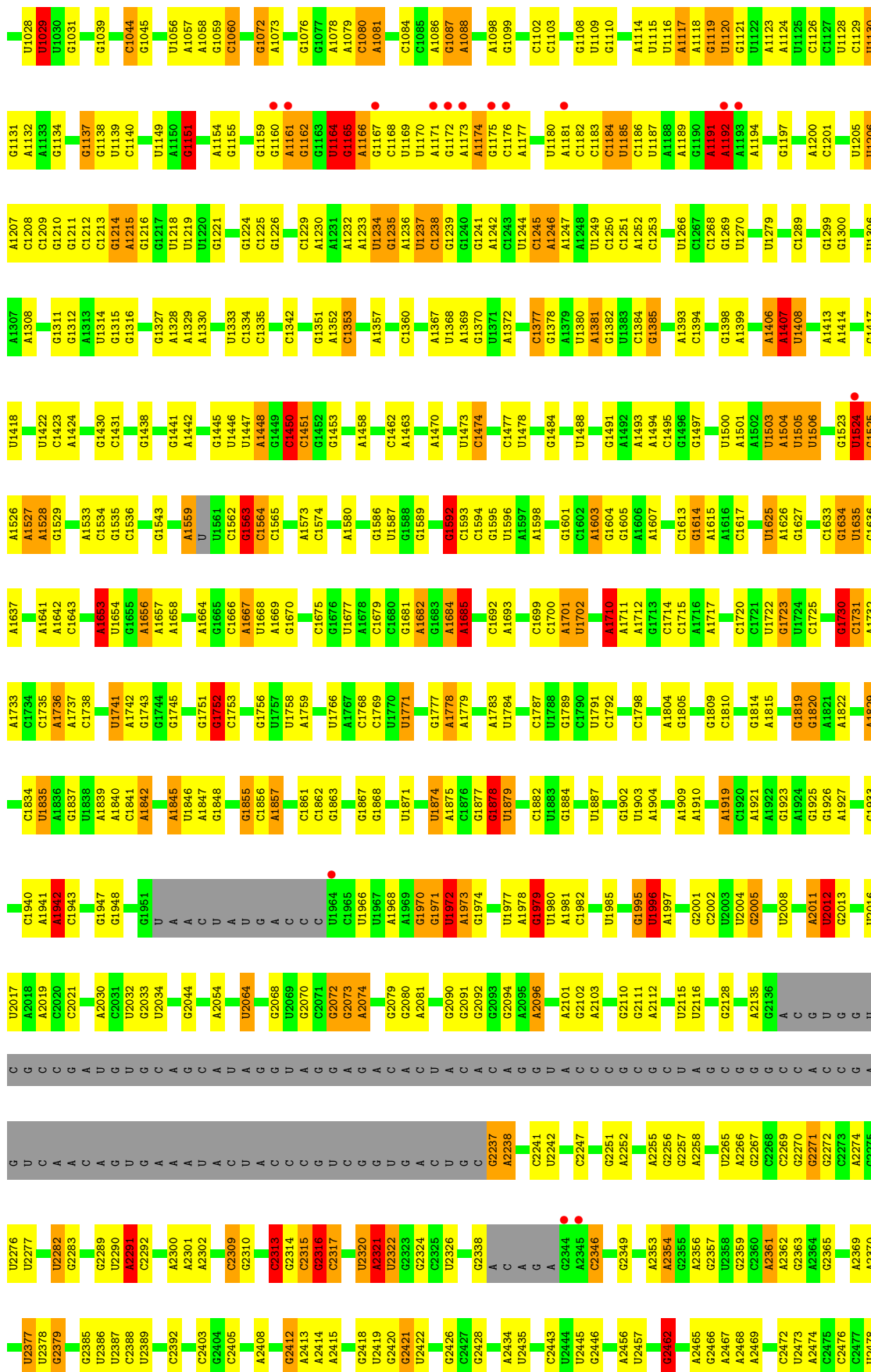
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	62	Total 62	O 62	0	0
37	P	52	Total 52	O 52	0	0
37	Q	82	Total 82	O 82	0	0
37	R	35	Total 35	O 35	0	0
37	S	41	Total 41	O 41	0	0
37	T	23	Total 23	O 23	0	0
37	U	14	Total 14	O 14	0	0
37	V	69	Total 69	O 69	0	0
37	W	29	Total 29	O 29	0	0
37	X	85	Total 85	O 85	0	0
37	Y	38	Total 38	O 38	0	0
37	Z	56	Total 56	O 56	0	0
37	1	42	Total 42	O 42	0	0
37	2	58	Total 58	O 58	0	0

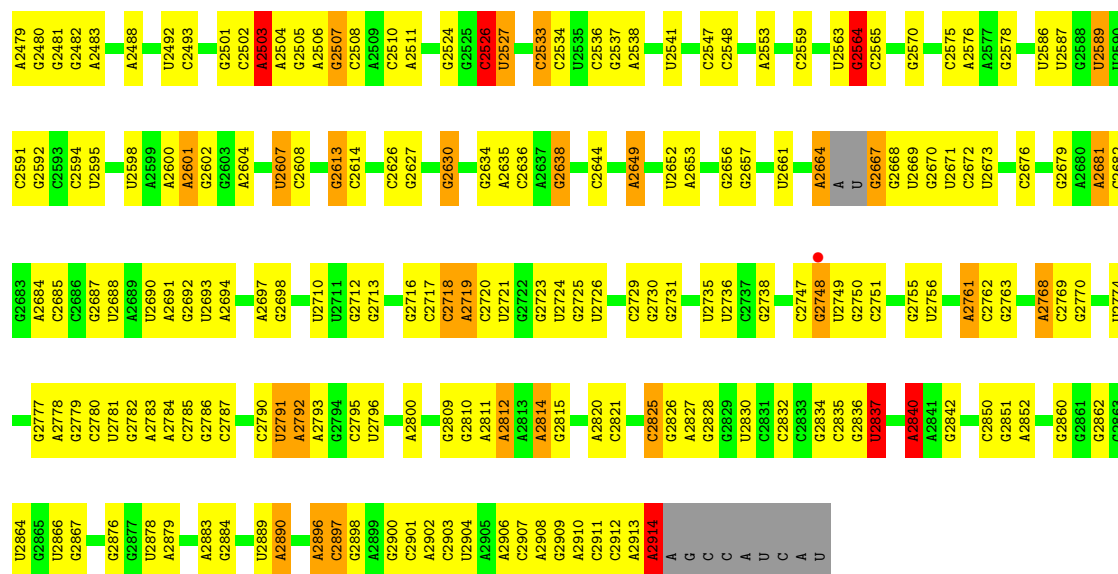
3 Residue-property plots

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

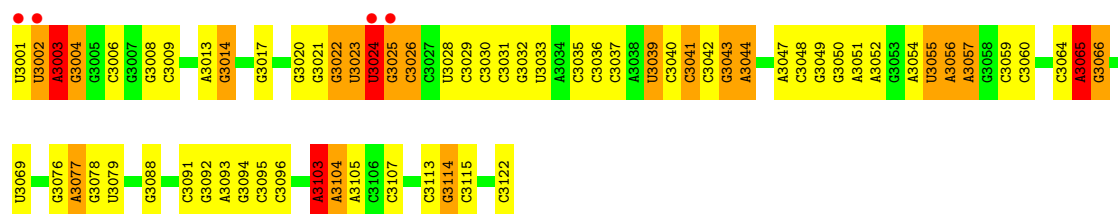
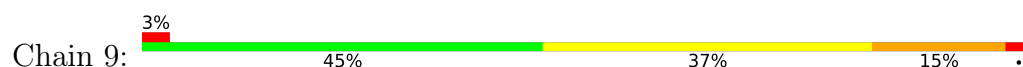
- Molecule 1: 23S ribosomal rna



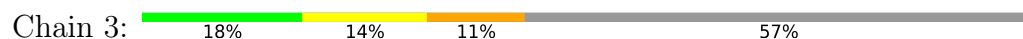




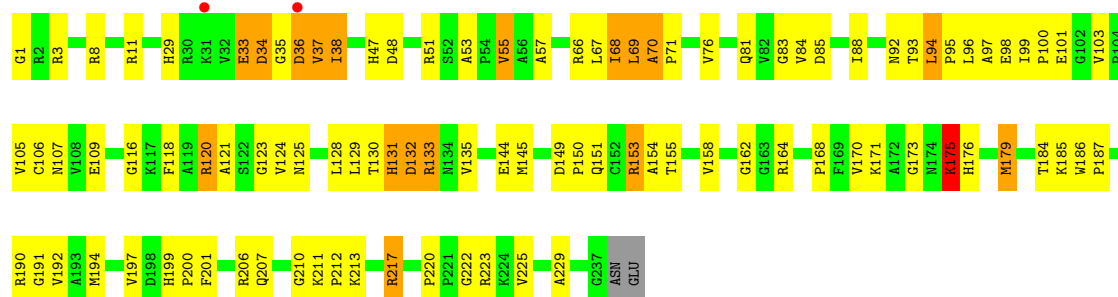
- Molecule 2: 5S ribosomal RNA



- Molecule 3: Deacylated tRNA minihelix

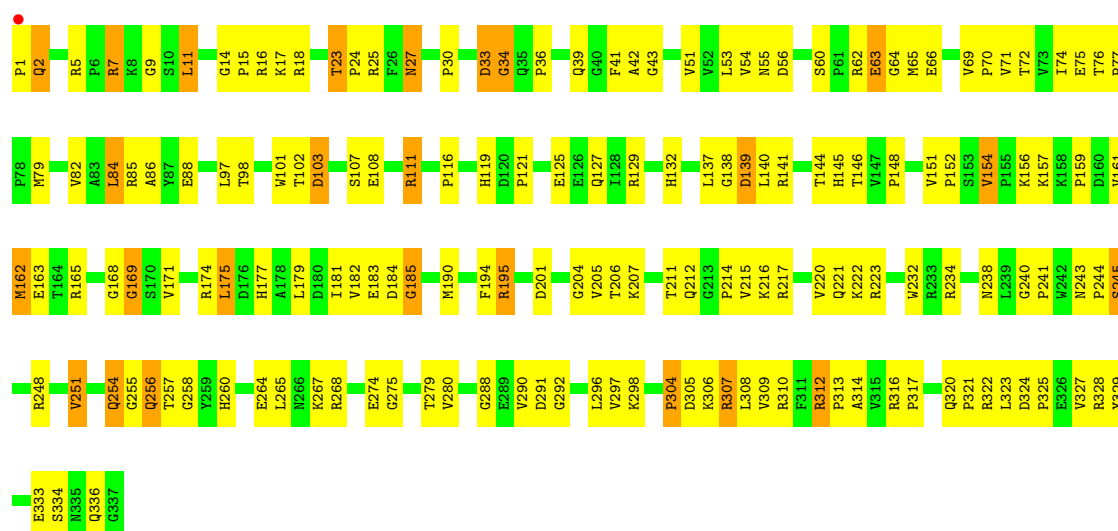


- Molecule 4: 50S ribosomal protein L2P



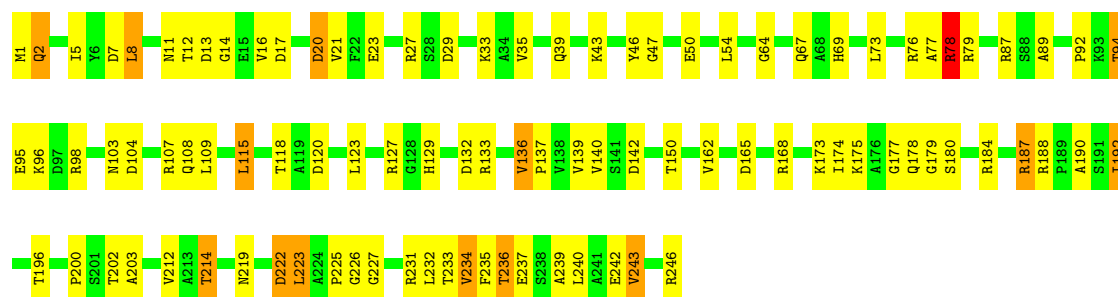
- Molecule 5: 50S ribosomal protein L3P

Chain B: 

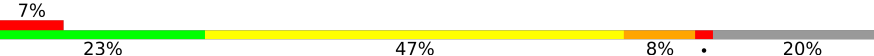


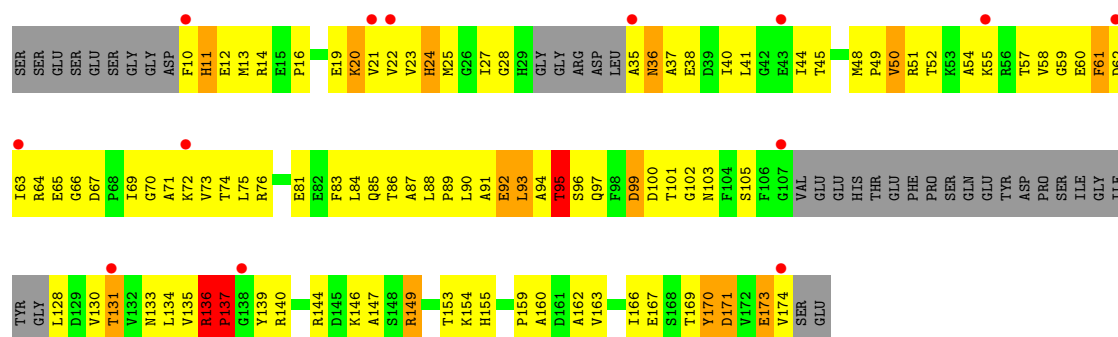
- Molecule 6: 50S ribosomal protein L4E

Chain C: 



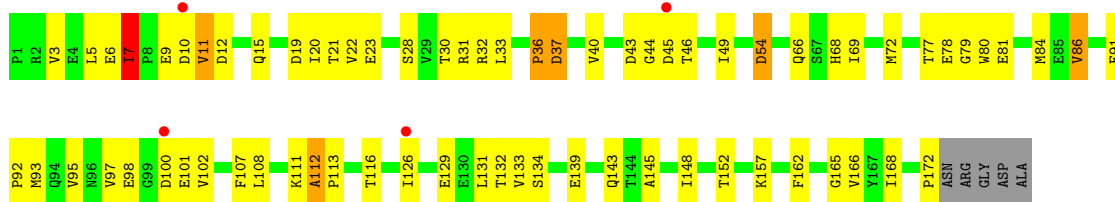
- Molecule 7: 50S ribosomal protein L5P

Chain D: 

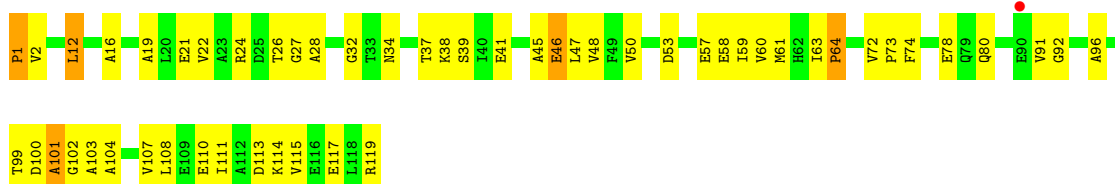


- Molecule 8: 50S ribosomal protein L6P

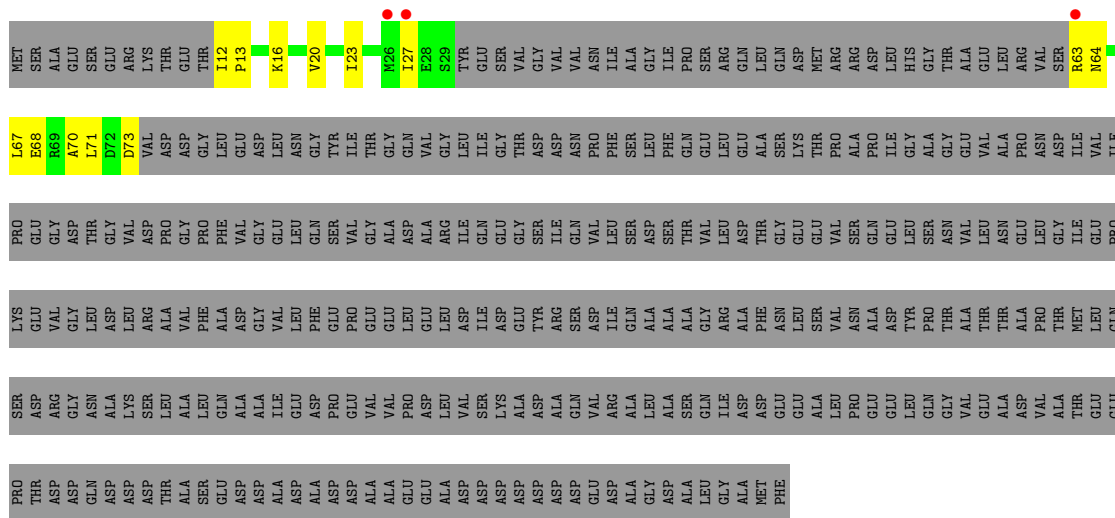
Chain E: 



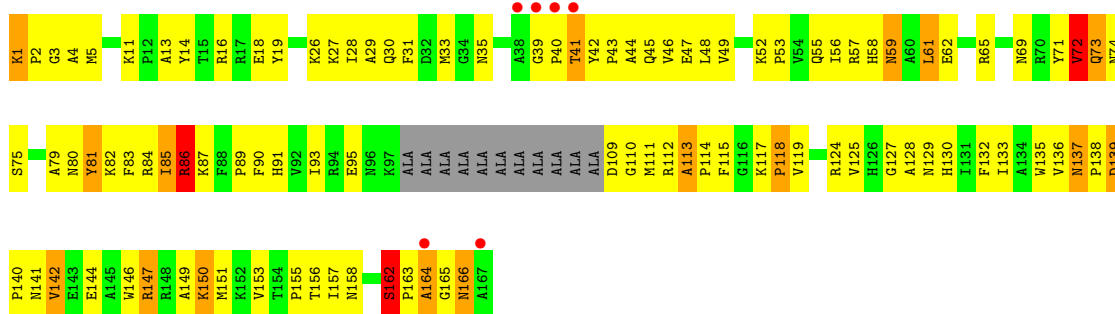
- Molecule 9: 50S ribosomal protein L7Ae



- Molecule 10: 50S RIBOSOMAL PROTEIN L10E



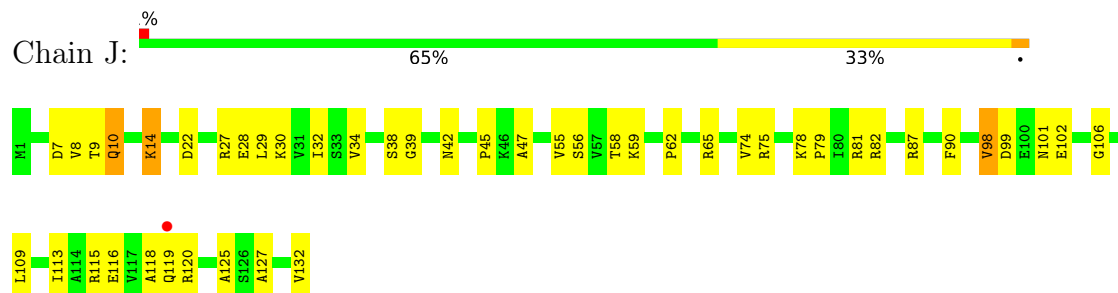
- Molecule 11: L10 Ribosomal Protein



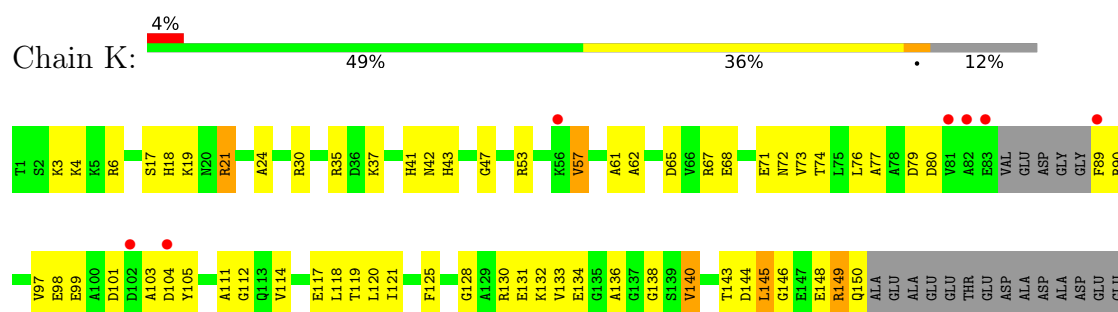
- Molecule 12: 50S ribosomal protein L13P



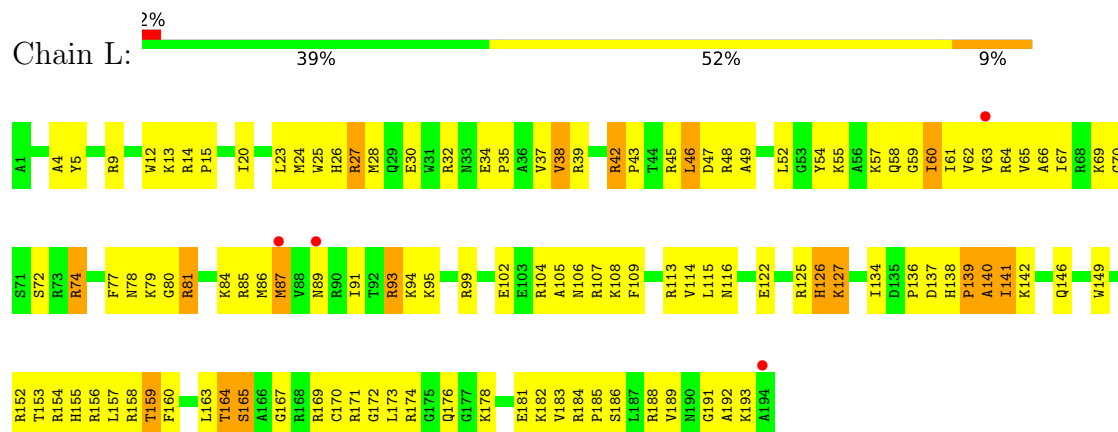
- Molecule 13: 50S ribosomal protein L14P



- Molecule 14: 50S ribosomal protein L15P

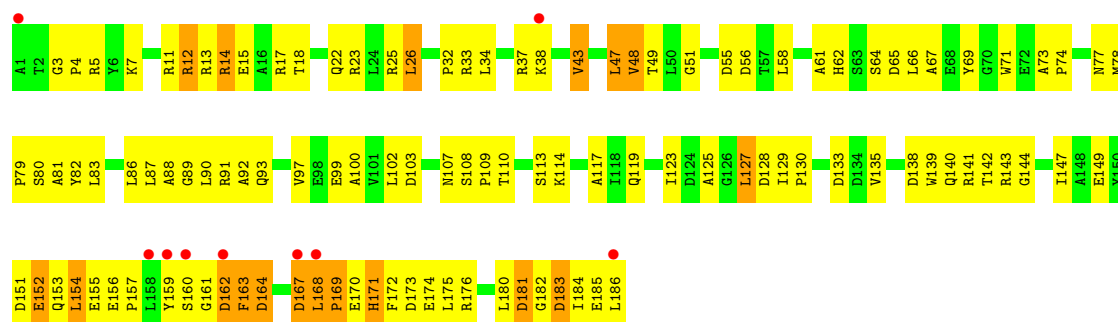


- Molecule 15: L15 Ribosomal Protein



- Molecule 16: 50S ribosomal protein L18P

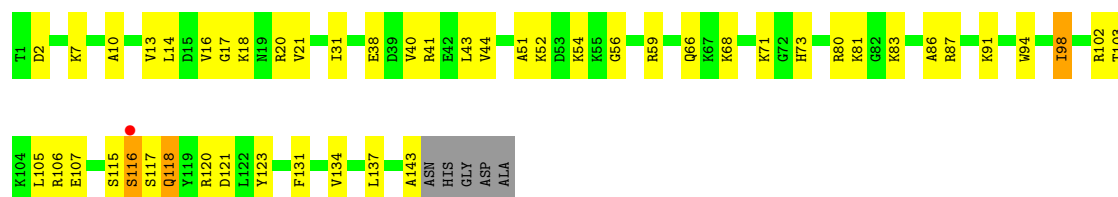




• Molecule 17: 50S ribosomal protein L18e



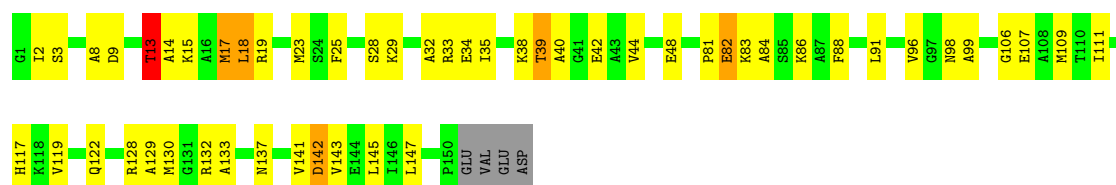
• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P



• Molecule 21: 50S ribosomal protein L23P

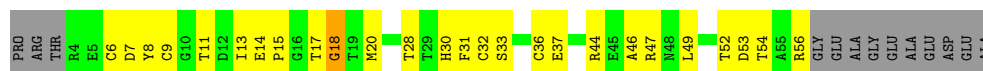




- Molecule 22: 50S ribosomal protein L24P



- Molecule 23: 50S ribosomal protein L24E



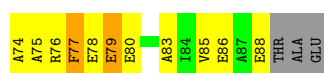
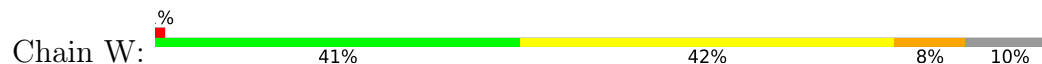
- Molecule 24: 50S ribosomal protein L29P



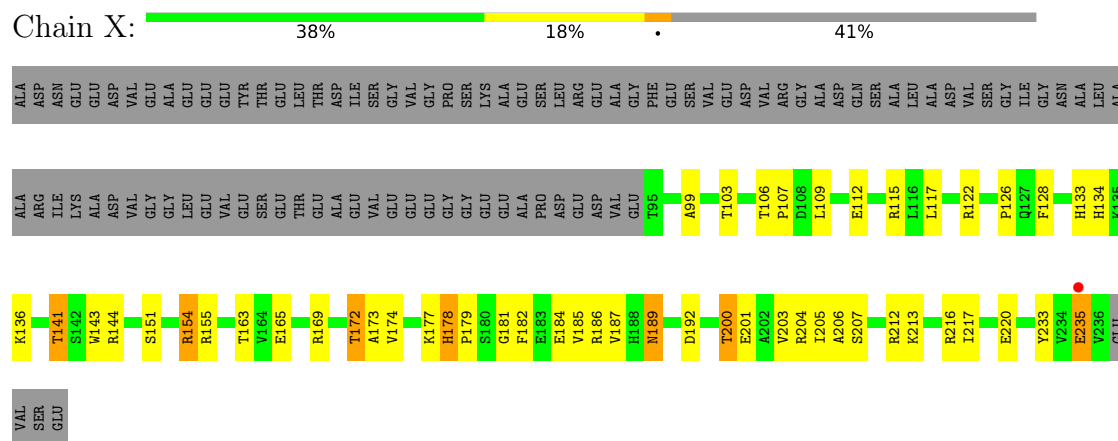
- Molecule 25: 50S ribosomal protein L30P



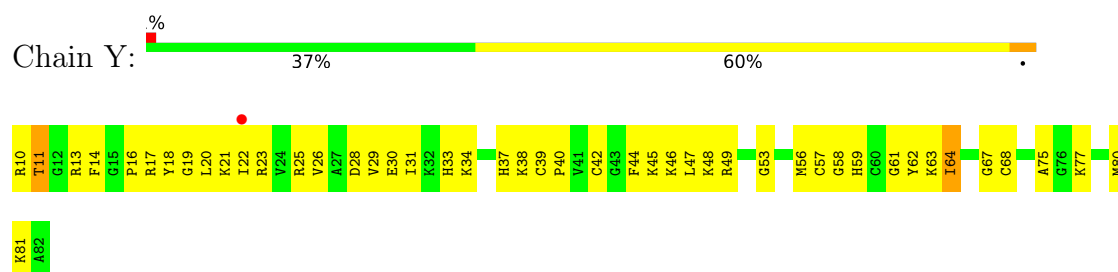
- Molecule 26: 50S ribosomal protein L31e



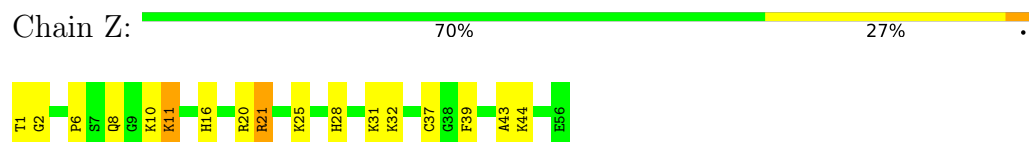
- Molecule 27: 50S ribosomal protein L32E



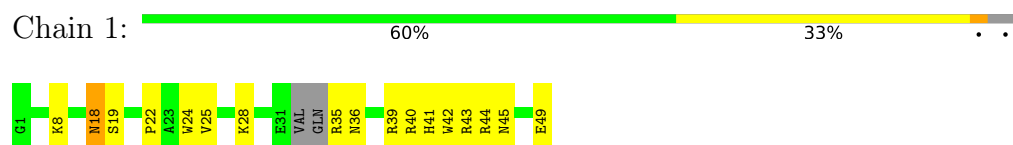
- Molecule 28: L37Ae 50S ribosomal protein



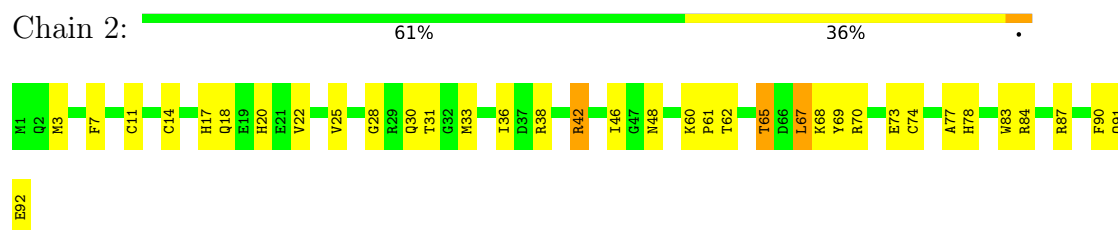
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S 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	213.52Å 300.82Å 574.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 91.3 (50.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.239 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	98648	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

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

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CD, K, NA, 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	0.56	0/66076	0.90	150/103052 (0.1%)
2	9	0.50	0/2905	0.88	9/4528 (0.2%)
3	3	0.75	0/285	1.07	2/438 (0.5%)
4	A	0.68	0/1787	1.11	9/2409 (0.4%)
5	B	0.71	0/2689	1.09	12/3652 (0.3%)
6	C	0.78	0/1883	1.10	8/2551 (0.3%)
7	D	0.57	0/1111	0.99	4/1498 (0.3%)
8	E	0.70	0/1382	0.99	6/1880 (0.3%)
9	F	0.63	0/896	0.96	0/1219
10	G	0.69	0/241	0.86	0/324
11	H	0.78	1/1246 (0.1%)	1.36	14/1686 (0.8%)
12	I	0.78	0/1135	1.03	5/1530 (0.3%)
13	J	0.68	0/1003	1.11	2/1351 (0.1%)
14	K	0.62	0/1126	1.13	7/1504 (0.5%)
15	L	0.80	1/1633 (0.1%)	1.15	10/2180 (0.5%)
16	M	0.62	0/1473	1.16	16/1999 (0.8%)
17	N	0.74	0/873	1.02	3/1181 (0.3%)
18	O	0.67	0/1143	0.98	2/1521 (0.1%)
19	P	0.76	0/748	1.16	9/1005 (0.9%)
20	Q	0.84	1/1172 (0.1%)	1.08	8/1578 (0.5%)
21	R	0.61	0/648	1.00	3/875 (0.3%)
22	S	0.63	0/957	1.08	6/1289 (0.5%)
23	T	0.72	0/417	0.99	1/562 (0.2%)
24	U	0.60	0/502	1.05	3/675 (0.4%)
25	V	0.78	0/1218	1.08	5/1655 (0.3%)
26	W	0.80	0/664	1.10	3/895 (0.3%)
27	X	0.75	0/1146	1.07	2/1536 (0.1%)
28	Y	0.74	0/575	1.06	0/763
29	Z	0.69	0/437	1.06	3/578 (0.5%)
30	1	0.62	0/398	0.83	0/527
31	2	0.61	0/771	0.95	1/1024 (0.1%)
All	All	0.61	3/98540 (0.0%)	0.95	303/147465 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	83
2	9	0	2
3	3	0	1
11	H	0	1
25	V	0	1
All	All	0	88

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	41	THR	CA-CB	5.29	1.60	1.53
20	Q	17	MET	SD-CE	-5.27	1.66	1.79
15	L	60	ILE	CA-CB	-5.20	1.48	1.54

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	74	ASN	N-CA-C	-15.61	91.75	114.39
1	0	1164	U	OP1-P-O3'	-13.46	67.61	108.00
1	0	1164	U	OP2-P-O3'	-12.99	69.02	108.00
1	0	1448	A	C2'-C3'-O3'	-12.57	90.65	109.50
1	0	1979	G	C2'-C3'-O3'	11.94	127.40	109.50
11	H	141	ASN	N-CA-C	-11.84	98.94	113.50
15	L	141	ILE	N-CA-C	-11.69	102.43	111.90
1	0	1563	G	C2'-C3'-O3'	11.45	126.67	109.50
1	0	1029	U	C2'-C3'-O3'	-11.02	92.97	109.50
16	M	135	VAL	N-CA-C	-9.88	103.49	113.47
1	0	1942	A	C5'-C4'-C3'	9.62	130.43	116.00
7	D	136	ARG	CA-C-N	9.24	131.39	119.84
7	D	136	ARG	C-N-CA	9.24	131.39	119.84
15	L	139	PRO	N-CA-C	-8.65	98.97	111.33
1	0	1165	G	O5'-P-OP1	-8.59	82.23	108.00
11	H	156	THR	N-CA-C	-8.54	97.83	110.48
8	E	11	VAL	N-CA-C	8.48	122.34	109.20
19	P	17	LYS	N-CA-C	-8.45	98.42	110.08
1	0	644	G	C4'-C3'-O3'	-8.43	96.76	109.40
2	9	3024	U	C2'-C3'-O3'	8.21	121.82	109.50
11	H	1	LYS	CA-C-N	8.17	128.11	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	1	LYS	C-N-CA	8.17	128.11	119.85
1	0	185	G	C2'-C3'-O3'	-8.05	97.43	109.50
1	0	2718	C	C4'-C3'-O3'	-8.05	97.33	109.40
14	K	57	VAL	N-CA-C	-7.99	105.08	112.43
4	A	222	GLY	N-CA-C	-7.98	104.45	113.79
16	M	169	PRO	N-CA-C	-7.97	103.50	114.27
26	W	22	ASN	N-CA-C	7.96	120.96	111.33
5	B	157	LYS	N-CA-C	-7.93	104.20	114.04
16	M	133	ASP	N-CA-C	7.88	120.86	111.33
1	0	212	A	C4'-C3'-O3'	-7.87	97.59	109.40
7	D	100	ASP	N-CA-C	-7.84	103.71	113.28
22	S	52	ARG	N-CA-C	7.72	123.45	113.18
1	0	1192	A	C4'-C3'-O3'	-7.70	101.45	113.00
4	A	70	ALA	N-CA-C	7.70	119.35	109.65
3	3	3	G	C3'-C2'-O2'	7.66	122.19	110.70
11	H	147	ARG	N-CA-C	-7.65	102.91	111.71
1	0	1523	G	C4'-C3'-O3'	-7.59	101.61	113.00
1	0	834	G	C2'-C3'-O3'	-7.58	102.33	113.70
1	0	2321	A	C2'-C3'-O3'	-7.51	98.24	109.50
1	0	2378	U	C2'-C3'-O3'	-7.45	98.33	109.50
1	0	317	A	C2'-C3'-O3'	-7.40	98.39	109.50
1	0	1108	G	C2'-C3'-O3'	-7.39	98.41	109.50
4	A	213	LYS	N-CA-C	7.33	121.48	112.54
1	0	1814	G	C2'-C3'-O3'	-7.21	98.68	109.50
21	R	57	THR	N-CA-C	7.21	120.28	110.55
16	M	51	GLY	CA-C-N	7.19	127.03	119.05
16	M	51	GLY	C-N-CA	7.19	127.03	119.05
14	K	145	LEU	N-CA-C	-7.15	103.56	111.36
4	A	38	ILE	N-CA-C	7.14	118.57	108.93
29	Z	21	ARG	N-CA-C	7.12	120.09	111.40
1	0	2290	U	C2'-C3'-O3'	-7.03	98.96	109.50
1	0	1819	G	C5'-C4'-C3'	7.03	126.54	116.00
11	H	155	PRO	N-CA-C	7.02	121.95	111.41
1	0	1559	A	C2'-C3'-O3'	7.02	124.23	113.70
2	9	3039	U	C4'-C3'-O3'	-7.01	102.49	113.00
22	S	54	ASP	N-CA-C	-6.95	104.27	112.89
24	U	42	ASN	CA-C-N	6.93	128.51	119.84
24	U	42	ASN	C-N-CA	6.93	128.51	119.84
3	3	2	C	C3'-C2'-O2'	6.93	121.10	110.70
1	0	1730	G	C2'-C3'-O3'	-6.91	99.13	109.50
21	R	27	ALA	N-CA-C	-6.91	97.47	108.73
12	I	71	TYR	CA-C-N	6.88	126.85	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	71	TYR	C-N-CA	6.88	126.85	119.76
1	0	236	A	C5'-C4'-C3'	-6.86	104.91	115.20
20	Q	34	GLU	N-CA-C	6.85	118.82	111.36
1	0	1446	U	C2'-C3'-O3'	-6.75	99.37	109.50
1	0	1491	G	C2'-C3'-O3'	-6.72	99.41	109.50
1	0	2667	G	O5'-C5'-C4'	6.71	121.56	111.50
15	L	89	ASN	N-CA-C	6.70	118.66	111.36
25	V	75	GLY	N-CA-C	6.63	120.35	112.33
1	0	206	G	C5'-C4'-C3'	-6.62	106.07	116.00
6	C	78	ARG	N-CA-C	6.57	118.75	108.96
1	0	2785	C	C2'-C3'-O3'	-6.50	99.74	109.50
6	C	175	LYS	N-CA-C	6.50	118.69	110.24
6	C	64	GLY	N-CA-C	6.47	120.50	113.58
1	0	271	C	C2'-C3'-O3'	-6.46	99.81	109.50
5	B	265	LEU	N-CA-C	6.46	119.27	110.55
20	Q	137	ASN	N-CA-C	6.44	119.99	110.46
22	S	47	THR	N-CA-C	-6.43	99.72	109.95
1	0	746	A	C2'-C3'-O3'	-6.42	99.87	109.50
1	0	2466	G	C4'-C3'-O3'	-6.41	103.38	113.00
19	P	51	ARG	N-CA-C	6.38	118.25	110.41
2	9	3039	U	N1-C1'-C2'	6.38	121.56	112.00
1	0	1164	U	O3'-P-O5'	6.37	113.56	104.00
1	0	80	A	C2'-C3'-O3'	-6.37	99.95	109.50
1	0	1407	A	C2'-C3'-O3'	-6.37	99.95	109.50
20	Q	122	GLN	N-CA-C	-6.34	98.84	108.67
20	Q	142	ASP	N-CA-C	-6.34	100.32	110.14
19	P	47	VAL	CA-C-N	6.33	125.55	118.97
19	P	47	VAL	C-N-CA	6.33	125.55	118.97
31	2	67	LEU	N-CA-C	6.33	119.85	109.85
1	0	1378	G	C2'-C3'-O3'	-6.31	100.03	109.50
1	0	1357	A	C2'-C3'-O3'	-6.29	100.06	109.50
19	P	68	GLY	N-CA-C	-6.27	100.68	111.47
21	R	59	ASP	N-CA-C	-6.27	105.57	113.72
1	0	2291	A	C4'-C3'-O3'	-6.25	103.62	113.00
1	0	688	A	C2'-C3'-O3'	-6.25	100.13	109.50
1	0	198	A	C2'-C3'-O3'	-6.23	100.16	109.50
17	N	69	VAL	N-CA-C	6.22	117.44	108.48
1	0	70	A	C2'-C3'-O3'	-6.22	100.17	109.50
1	0	920	C	C2'-C3'-O3'	-6.20	104.41	113.70
1	0	30	U	C2'-C3'-O3'	-6.19	100.21	109.50
15	L	74	ARG	N-CA-C	6.16	119.51	109.59
2	9	3043	G	C4'-C3'-O3'	-6.16	100.17	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	179	GLY	N-CA-C	-6.15	105.09	113.27
1	0	1447	U	C2'-C3'-O3'	-6.14	100.29	109.50
1	0	1693	A	C2'-C3'-O3'	-6.13	100.30	109.50
1	0	1996	U	C2'-C3'-O3'	-6.13	100.30	109.50
1	0	1235	G	C2'-C3'-O3'	-6.13	100.31	109.50
11	H	162	SER	CA-C-N	-6.12	112.19	119.84
11	H	162	SER	C-N-CA	-6.12	112.19	119.84
1	0	875	A	C2'-C3'-O3'	-6.09	100.37	109.50
1	0	1191	A	C2'-C3'-O3'	-6.07	104.59	113.70
1	0	2649	A	C2'-C3'-O3'	-6.07	100.40	109.50
11	H	110	GLY	N-CA-C	-6.04	98.86	113.18
5	B	222	LYS	N-CA-C	-6.02	101.08	110.42
16	M	153	GLN	N-CA-C	-6.02	104.53	112.72
15	L	70	GLY	N-CA-C	6.01	119.40	111.70
23	T	18	GLY	N-CA-C	6.01	121.71	112.81
1	0	1165	G	O5'-P-OP2	-6.01	89.97	108.00
1	0	1524	U	C2'-C3'-O3'	6.01	118.51	109.50
17	N	2	LYS	N-CA-C	-6.01	102.44	110.55
29	Z	43	ALA	N-CA-C	-6.00	104.31	111.69
1	0	448	G	C2'-C3'-O3'	-5.98	100.53	109.50
4	A	220	PRO	CA-C-N	-5.98	113.78	119.76
4	A	220	PRO	C-N-CA	-5.98	113.78	119.76
1	0	681	G	C2'-C3'-O3'	-5.98	100.53	109.50
1	0	2761	A	C2'-C3'-O3'	-5.97	100.54	109.50
27	X	143	TRP	N-CA-C	5.97	118.91	109.96
1	0	2338	G	C2'-C3'-O3'	5.96	122.64	113.70
16	M	117	ALA	N-CA-C	-5.93	104.90	111.36
14	K	43	HIS	N-CA-C	-5.92	99.34	109.24
1	0	1677	U	C2'-C3'-O3'	-5.92	100.61	109.50
1	0	509	A	C4'-C3'-O3'	-5.92	100.52	109.40
8	E	37	ASP	N-CA-C	5.92	119.82	112.24
1	0	777	U	C5'-C4'-C3'	-5.92	106.33	115.20
1	0	1087	G	C2'-C3'-O3'	-5.91	100.64	109.50
20	Q	18	LEU	N-CA-C	-5.91	100.55	109.95
1	0	1504	A	N9-C1'-C2'	5.89	120.84	112.00
13	J	8	VAL	N-CA-C	5.89	116.97	108.48
1	0	2271	G	C5'-C4'-C3'	-5.88	106.38	115.20
5	B	151	VAL	CA-C-N	5.87	125.08	118.97
5	B	151	VAL	C-N-CA	5.87	125.08	118.97
1	0	1120	U	C5'-C4'-C3'	-5.87	107.20	116.00
1	0	1819	G	C2'-C3'-O3'	-5.86	104.91	113.70
1	0	138	U	C2'-C3'-O3'	-5.84	104.94	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2607	U	C4'-C3'-O3'	-5.84	100.64	109.40
15	L	126	HIS	CB-CA-C	-5.84	99.97	110.36
1	0	1884	G	C2'-C3'-O3'	-5.83	100.75	109.50
1	0	1592	G	N9-C1'-C2'	5.83	120.75	112.00
1	0	2313	C	C5'-C4'-C3'	5.83	124.75	116.00
11	H	113	ALA	CA-C-N	5.82	126.69	120.47
11	H	113	ALA	C-N-CA	5.82	126.69	120.47
13	J	14	LYS	N-CA-C	-5.81	101.44	110.10
1	0	2291	A	N9-C1'-C2'	5.81	120.71	112.00
19	P	13	LYS	N-CA-C	5.81	119.47	112.38
1	0	1438	G	C2'-C3'-O3'	-5.80	100.80	109.50
1	0	1615	A	C5'-C4'-C3'	5.80	124.70	116.00
1	0	2300	A	N9-C1'-C2'	5.79	122.68	114.00
1	0	1981	A	C2'-C3'-O3'	-5.78	100.84	109.50
25	V	143	THR	N-CA-C	-5.77	105.07	111.71
1	0	1664	A	C4'-C3'-O3'	-5.77	100.75	109.40
16	M	102	LEU	N-CA-C	5.76	117.60	108.67
18	O	118	GLN	N-CA-C	-5.76	104.92	111.14
26	W	79	GLU	N-CA-C	5.75	120.14	113.18
1	0	1710	A	C2'-C3'-O3'	-5.75	100.88	109.50
1	0	1738	C	C5'-C4'-C3'	5.74	124.61	116.00
15	L	42	ARG	CA-C-N	5.73	126.02	119.83
15	L	42	ARG	C-N-CA	5.73	126.02	119.83
14	K	47	GLY	N-CA-C	5.72	117.91	111.85
1	0	1871	U	C2'-C3'-O3'	-5.71	100.93	109.50
20	Q	3	SER	N-CA-C	-5.71	100.67	109.52
24	U	64	GLY	N-CA-C	-5.70	107.11	115.72
1	0	1151	G	C4'-C3'-O3'	-5.69	100.87	109.40
1	0	1369	A	C4'-C3'-O3'	-5.68	100.88	109.40
1	0	463	A	C2'-C3'-O3'	-5.68	100.98	109.50
1	0	485	A	C2'-C3'-O3'	-5.67	100.99	109.50
1	0	1534	C	C2'-C3'-O3'	-5.67	101.00	109.50
16	M	14	ARG	N-CA-C	-5.66	105.03	111.14
1	0	381	G	N9-C1'-C2'	5.64	122.47	114.00
1	0	509	A	O4'-C1'-C2'	5.64	111.44	105.80
1	0	537	G	N9-C1'-C2'	5.64	122.46	114.00
1	0	1330	A	C2'-C3'-O3'	-5.62	105.26	113.70
16	M	48	VAL	N-CA-C	5.62	116.69	108.53
1	0	141	C	N1-C1'-C2'	5.62	122.42	114.00
1	0	817	G	C4'-C3'-O3'	-5.61	100.98	109.40
12	I	112	ASP	N-CA-C	-5.61	100.15	109.46
25	V	17	ILE	N-CA-C	-5.61	105.64	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1315	G	C2'-C3'-O3'	-5.61	101.09	109.50
1	0	644	G	N9-C1'-C2'	5.60	122.40	114.00
1	0	174	A	C2'-C3'-O3'	-5.59	101.11	109.50
11	H	137	ASN	N-CA-C	-5.58	101.92	110.07
1	0	2282	U	C5'-C4'-C3'	-5.56	106.86	115.20
6	C	192	ILE	N-CA-C	5.56	116.77	109.21
1	0	31	C	C2'-C3'-O3'	-5.55	101.17	109.50
1	0	2607	U	N1-C1'-C2'	5.55	122.33	114.00
16	M	168	LEU	N-CA-C	5.55	120.75	108.64
1	0	2322	U	C2'-C3'-O3'	-5.55	101.17	109.50
16	M	91	ARG	N-CA-C	-5.54	105.24	111.28
1	0	2538	A	C2'-C3'-O3'	-5.54	101.20	109.50
20	Q	13	THR	N-CA-C	5.53	118.46	109.06
1	0	1985	U	C2'-C3'-O3'	-5.53	101.21	109.50
1	0	1685	A	C2'-C3'-O3'	-5.52	101.21	109.50
1	0	1653	A	N9-C1'-C2'	5.50	122.25	114.00
1	0	1450	C	C2'-C3'-O3'	-5.50	105.45	113.70
7	D	137	PRO	N-CA-C	5.49	123.78	112.47
20	Q	141	VAL	N-CA-C	5.48	116.38	108.48
1	0	220	C	N1-C1'-C2'	5.48	122.22	114.00
1	0	45	A	C4'-C3'-O3'	-5.47	101.19	109.40
1	0	264	G	O4'-C1'-C2'	5.45	111.25	105.80
1	0	535	G	N9-C1'-C2'	5.44	122.16	114.00
15	L	127	LYS	N-CA-C	-5.44	98.69	108.48
25	V	69	ARG	N-CA-C	5.43	119.46	112.41
18	O	56	GLY	N-CA-C	-5.42	102.61	110.90
19	P	25	PRO	CA-C-N	5.42	124.93	119.19
19	P	25	PRO	C-N-CA	5.42	124.93	119.19
1	0	1855	G	C2'-C3'-O3'	-5.42	101.38	109.50
1	0	1117	A	C2'-C3'-O3'	-5.41	101.39	109.50
19	P	49	ASN	N-CA-C	5.41	118.43	110.59
8	E	7	ILE	CA-C-N	5.41	125.33	119.76
8	E	7	ILE	C-N-CA	5.41	125.33	119.76
1	0	874	A	C4'-C3'-O3'	-5.40	104.90	113.00
6	C	177	GLY	N-CA-C	5.40	117.55	112.04
2	9	3103	A	C4'-C3'-C2'	-5.40	97.20	102.60
17	N	82	SER	N-CA-C	-5.40	103.77	110.41
1	0	2837	U	C2'-C3'-O3'	-5.38	101.44	109.50
27	X	178	HIS	N-CA-C	-5.37	102.37	109.84
5	B	154	VAL	CA-C-N	5.37	125.44	119.32
5	B	154	VAL	C-N-CA	5.37	125.44	119.32
5	B	23	THR	CA-C-N	5.36	125.65	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	23	THR	C-N-CA	5.36	125.65	119.92
5	B	111	ARG	N-CA-C	-5.36	106.75	113.28
12	I	68	GLY	N-CA-C	5.35	119.35	112.18
1	0	2814	A	C2'-C3'-O3'	-5.35	101.48	109.50
22	S	3	GLN	CA-C-N	5.33	125.39	119.32
22	S	3	GLN	C-N-CA	5.33	125.39	119.32
4	A	133	ARG	N-CA-C	-5.33	106.62	113.23
1	0	939	A	C2'-C3'-O3'	-5.33	101.51	109.50
1	0	714	U	C2'-C3'-O3'	-5.32	101.52	109.50
1	0	1505	U	C2'-C3'-O3'	-5.30	101.55	109.50
14	K	149	ARG	N-CA-C	5.30	116.02	108.54
16	M	3	GLY	CA-C-N	5.29	125.09	119.28
16	M	3	GLY	C-N-CA	5.29	125.09	119.28
1	0	1819	G	C4'-C3'-C2'	-5.29	97.31	102.60
4	A	118	PHE	N-CA-C	5.28	118.72	110.32
1	0	1942	A	C4'-C3'-C2'	-5.28	97.32	102.60
2	9	3003	A	C5'-C4'-C3'	-5.27	107.29	115.20
1	0	2313	C	C4'-C3'-C2'	-5.27	97.33	102.60
1	0	496	G	C2'-C3'-O3'	-5.26	101.61	109.50
1	0	87	C	C2'-C3'-O3'	-5.26	101.61	109.50
6	C	89	ALA	N-CA-C	5.26	117.43	111.02
2	9	3065	A	C4'-C3'-O3'	-5.25	105.12	113.00
1	0	1246	A	C2'-C3'-O3'	-5.23	101.65	109.50
2	9	3043	G	O4'-C1'-C2'	5.23	111.03	105.80
16	M	171	HIS	N-CA-C	-5.23	105.70	111.71
1	0	2462	G	C2'-C3'-O3'	-5.23	101.66	109.50
1	0	46	U	C2'-C3'-O3'	-5.22	101.66	109.50
6	C	20	ASP	N-CA-C	5.22	116.97	111.28
25	V	9	GLY	N-CA-C	5.22	119.25	112.25
14	K	42	ASN	N-CA-C	5.21	118.78	111.74
29	Z	11	LYS	N-CA-C	5.21	117.59	108.52
14	K	37	LYS	N-CA-C	5.20	116.42	108.30
1	0	338	C	C2'-C3'-O3'	-5.20	101.70	109.50
2	9	3065	A	N9-C1'-C2'	5.20	119.80	112.00
4	A	175	LYS	N-CA-C	-5.20	105.61	111.28
1	0	2914	A	C2'-C3'-O3'	5.20	121.49	113.70
1	0	1214	G	O4'-C1'-C2'	5.19	110.99	105.80
1	0	2096	A	C4'-C3'-O3'	-5.18	105.23	113.00
1	0	2889	U	C4'-C3'-O3'	-5.16	101.66	109.40
5	B	161	VAL	N-CA-C	5.16	115.73	108.36
1	0	831	U	C2'-C3'-O3'	-5.15	101.78	109.50
1	0	2316	G	C5'-C4'-C3'	-5.14	107.48	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1737	A	C5'-C4'-C3'	-5.14	108.30	116.00
1	0	1752	G	C4'-C3'-O3'	-5.14	101.69	109.40
1	0	1563	G	C5'-C4'-C3'	-5.13	107.51	115.20
1	0	1234	U	C4'-C3'-O3'	-5.13	101.71	109.40
1	0	705	C	C5'-C4'-C3'	-5.12	108.31	116.00
8	E	112	ALA	CA-C-N	5.12	124.88	119.76
8	E	112	ALA	C-N-CA	5.12	124.88	119.76
1	0	2835	C	C4'-C3'-O3'	-5.12	105.33	113.00
1	0	1533	A	C2'-C3'-O3'	-5.11	101.83	109.50
1	0	1408	U	C2'-C3'-O3'	-5.11	101.83	109.50
1	0	1837	G	C4'-C3'-O3'	-5.11	101.74	109.40
1	0	1504	A	C4'-C3'-O3'	-5.09	105.36	113.00
1	0	1044	C	C2'-C3'-O3'	-5.09	101.87	109.50
5	B	175	LEU	N-CA-C	-5.08	105.64	111.07
1	0	2864	U	C4'-C3'-O3'	-5.07	105.39	113.00
22	S	78	THR	N-CA-C	5.07	117.12	109.41
11	H	86	ARG	N-CA-C	5.07	119.31	113.18
1	0	2021	C	C2'-C3'-O3'	-5.06	101.91	109.50
1	0	264	G	C5'-C4'-C3'	-5.05	107.62	115.20
1	0	441	A	O4'-C1'-C2'	5.05	110.85	105.80
15	L	27	ARG	N-CA-C	5.05	117.18	111.02
1	0	1752	G	O4'-C1'-C2'	5.04	110.84	105.80
1	0	922	A	C2'-C3'-O3'	-5.04	106.14	113.70
1	0	871	G	C5'-C4'-O4'	-5.04	102.25	109.80
1	0	1408	U	C5'-C4'-C3'	-5.03	107.65	115.20
1	0	1504	A	C1'-O4'-C4'	-5.03	104.87	109.90
26	W	80	GLU	N-CA-C	-5.03	107.13	114.12
16	M	13	ARG	N-CA-C	-5.03	106.31	112.90
1	0	2649	A	O4'-C1'-C2'	5.01	110.81	105.80
12	I	36	VAL	N-CA-C	5.00	116.49	108.89

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1191	A	Sidechain
1	0	1226	G	Sidechain
1	0	1230	A	Sidechain
1	0	1300	G	Sidechain
1	0	1327	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1385	G	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1445	G	Sidechain
1	0	1458	A	Sidechain
1	0	1501	A	Sidechain
1	0	1503	U	Sidechain
1	0	1614	G	Sidechain
1	0	1635	U	Sidechain
1	0	1653	A	Sidechain
1	0	1710	A	Sidechain
1	0	1720	C	Sidechain
1	0	1736	A	Sidechain
1	0	1741	U	Sidechain
1	0	1758	U	Sidechain
1	0	1771	U	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1839	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1933	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	2012	U	Sidechain
1	0	2112	A	Sidechain
1	0	2313	C	Sidechain
1	0	2315	C	Sidechain
1	0	2377	U	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2492	U	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2526	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2664	A	Sidechain
1	0	2673	U	Sidechain
1	0	2774	U	Sidechain
1	0	2790	C	Sidechain
1	0	2793	A	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	308	U	Sidechain
1	0	324	G	Sidechain
1	0	332	G	Sidechain
1	0	333	G	Sidechain
1	0	336	G	Sidechain
1	0	391	U	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	435	A	Sidechain
1	0	458	G	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	743	G	Sidechain
1	0	771	G	Sidechain
1	0	794	U	Sidechain
1	0	817	G	Sidechain
1	0	882	A	Sidechain
1	0	898	G	Sidechain
1	0	903	U	Sidechain
1	0	918	G	Sidechain
3	3	3	G	Sidechain
2	9	3065	A	Sidechain
2	9	3094	G	Sidechain
11	H	81	TYR	Sidechain
25	V	90	TYR	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	29799	945	0
2	9	2600	0	1326	91	0
3	3	257	0	133	3	0
4	A	1754	0	1763	125	0
5	B	2624	0	2533	188	0
6	C	1858	0	1816	120	0
7	D	1094	0	1085	144	0
8	E	1357	0	1266	86	0
9	F	885	0	854	65	0
10	G	240	0	231	23	0
11	H	1215	0	1215	152	0
12	I	1119	0	1098	65	0
13	J	993	0	1027	56	0
14	K	1114	0	1072	63	0
15	L	1605	0	1676	157	0
16	M	1444	0	1401	130	0
17	N	864	0	873	29	0
18	O	1133	0	1127	51	0
19	P	734	0	728	19	0
20	Q	1149	0	1122	55	0
21	R	641	0	605	25	0
22	S	949	0	923	59	0
23	T	410	0	364	37	0
24	U	499	0	511	34	0
25	V	1195	0	1137	104	0
26	W	654	0	653	46	0
27	X	1130	0	1133	66	0
28	Y	563	0	597	60	0
29	Z	430	0	426	25	0
30	1	393	0	406	25	0
31	2	755	0	728	35	0
32	0	109	0	0	0	0
32	2	2	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	S	1	0	0	0	0
32	X	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	2	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	3	0	0	0	0
34	R	1	0	0	0	0
35	0	10	0	0	0	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	1	0
35	K	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	Q	1	0	0	0	0
35	X	1	0	0	0	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5836	0	0	198	0
37	1	42	0	0	5	0
37	2	58	0	0	6	0
37	3	3	0	0	0	0
37	9	138	0	0	16	0
37	A	124	0	0	19	0
37	B	150	0	0	28	0
37	C	166	0	0	31	0
37	D	49	0	0	20	0
37	E	42	0	0	16	0
37	F	26	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	21	0	0	7	0
37	H	75	0	0	20	0
37	I	52	0	0	6	0
37	J	56	0	0	11	0
37	K	79	0	0	18	0
37	L	127	0	0	23	0
37	M	67	0	0	15	0
37	N	42	0	0	6	0
37	O	62	0	0	4	0
37	P	52	0	0	3	0
37	Q	82	0	0	7	0
37	R	35	0	0	6	0
37	S	41	0	0	10	0
37	T	23	0	0	6	0
37	U	14	0	0	2	0
37	V	69	0	0	10	0
37	W	29	0	0	5	0
37	X	85	0	0	18	0
37	Y	38	0	0	13	0
37	Z	56	0	0	5	0
All	All	98648	0	59628	2825	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 19.

All (2825) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.59	1.17
1:0:1160:G:H5'	1:0:1161:A:H5'	1.29	1.15
1:0:1134:G:H4'	11:H:151:MET:HE1	1.32	1.12
2:9:3024:U:O2'	2:9:3025:G:H4'	1.50	1.11
6:C:236:THR:HG22	6:C:239:ALA:H	1.02	1.11
1:0:960:G:H4'	37:0:6875:HOH:O	1.47	1.11
20:Q:99:ALA:HB1	20:Q:109:MET:HE1	1.25	1.09
2:9:3023:U:H4'	2:9:3024:U:OP2	1.49	1.09
22:S:71:VAL:HG11	22:S:90:PRO:HB3	1.34	1.07
13:J:10:GLN:NE2	13:J:10:GLN:H	1.52	1.07
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.36	1.07
7:D:25:MET:HE2	7:D:41:LEU:HG	1.37	1.06
15:L:164:THR:HG22	15:L:167:GLY:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:156:C:H5''	15:L:171:ARG:HD3	1.38	1.05
28:Y:10:ARG:HA	37:Y:8415:HOH:O	1.55	1.05
15:L:52:LEU:HD11	37:L:8616:HOH:O	1.55	1.04
12:I:19:MET:HE3	12:I:132:LEU:HD11	1.34	1.04
11:H:45:GLN:HB3	11:H:163:PRO:HD2	1.33	1.03
11:H:162:SER:HB2	11:H:163:PRO:HD3	1.37	1.03
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.39	1.02
26:W:37:LEU:HD13	26:W:85:VAL:HG21	1.38	1.02
11:H:26:LYS:HD2	11:H:28:ILE:HD12	1.42	1.02
2:9:3023:U:H3'	37:9:8478:HOH:O	1.60	1.01
11:H:86:ARG:HH11	11:H:133:ILE:CG1	1.73	1.01
1:0:1835:U:H5	1:0:1840:A:N7	1.59	1.01
16:M:47:LEU:HD11	16:M:127:LEU:HD21	1.42	1.01
1:0:506:G:H22	1:0:509:A:H5'	1.24	1.00
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.42	1.00
15:L:102:GLU:OE1	15:L:164:THR:HG21	1.59	1.00
11:H:165:GLY:HA3	37:H:8395:HOH:O	1.61	0.99
25:V:88:THR:HB	37:V:6679:HOH:O	1.63	0.99
25:V:149:LEU:HG	25:V:153:MET:HE2	1.44	0.98
12:I:76:ASP:HA	37:I:5907:HOH:O	1.63	0.98
1:0:856:G:H2'	37:0:4887:HOH:O	1.64	0.97
5:B:162:MET:HE1	5:B:308:LEU:HD21	1.43	0.97
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.45	0.97
1:0:1242:A:H5'	12:I:82:THR:HG23	1.46	0.97
1:0:1751:G:H2'	1:0:1752:G:H5''	1.47	0.97
14:K:79:ASP:HB3	37:K:8557:HOH:O	1.65	0.97
27:X:200:THR:HG22	27:X:201:GLU:HG3	1.47	0.96
1:0:542:A:H5'	1:0:542:A:H8	1.31	0.96
2:9:3056:A:H2'	2:9:3057:A:H5''	1.47	0.96
3:3:4:G:H1	3:3:69:U:H3	0.96	0.96
13:J:10:GLN:HE21	13:J:10:GLN:N	1.63	0.95
5:B:238:ASN:HD22	5:B:240:GLY:H	1.14	0.95
1:0:1474:C:H6	1:0:1474:C:H5'	1.32	0.94
13:J:29:LEU:HB3	13:J:55:VAL:HG11	1.45	0.94
15:L:87:MET:HB3	31:2:46:ILE:HD13	1.48	0.94
37:0:6224:HOH:O	16:M:4:PRO:HD2	1.68	0.94
15:L:35:PRO:HG2	15:L:38:VAL:HG23	1.46	0.94
6:C:236:THR:HG21	37:C:8375:HOH:O	1.68	0.94
37:0:4332:HOH:O	15:L:14:ARG:HG2	1.67	0.94
30:1:39:ARG:HG2	37:1:3143:HOH:O	1.68	0.94
15:L:24:MET:HE3	15:L:28:MET:HE3	1.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:140:LEU:HA	37:B:8578:HOH:O	1.65	0.93
11:H:139:ASP:HA	37:H:8370:HOH:O	1.68	0.93
13:J:81:ARG:HB2	13:J:87:ARG:HH11	1.30	0.93
1:O:236:A:H4'	1:O:237:G:H5'	1.50	0.93
2:9:3006:C:H5''	16:M:37:ARG:NH1	1.84	0.92
5:B:321:PRO:HA	37:B:8661:HOH:O	1.70	0.92
7:D:105:SER:HB2	7:D:131:THR:HG23	1.51	0.92
18:O:115:SER:H	18:O:118:GLN:NE2	1.68	0.92
1:O:1372:A:H3'	37:O:6638:HOH:O	1.69	0.91
1:O:1116:U:O2'	1:O:1118:A:H2	1.54	0.91
11:H:86:ARG:HH11	11:H:133:ILE:HG13	0.80	0.91
1:O:21:G:H5'	20:Q:2:ILE:HA	1.53	0.91
1:O:1524:U:H4'	1:O:1525:G:O4'	1.71	0.90
37:O:6325:HOH:O	15:L:178:LYS:HB2	1.69	0.90
6:C:2:GLN:HB3	37:C:8336:HOH:O	1.71	0.90
1:O:871:G:C8	1:O:871:G:H5'	2.05	0.90
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.85	0.90
6:C:236:THR:HG22	6:C:239:ALA:N	1.86	0.90
1:O:2426:G:H1'	37:O:5554:HOH:O	1.70	0.90
5:B:86:ALA:HA	37:B:8578:HOH:O	1.71	0.90
26:W:30:MET:HE1	26:W:58:ALA:HB3	1.53	0.90
1:O:1118:A:H8	1:O:1119:G:H5''	1.35	0.90
15:L:94:LYS:HE3	37:L:8580:HOH:O	1.71	0.90
37:O:3224:HOH:O	15:L:157:LEU:HD11	1.72	0.90
7:D:64:ARG:HG2	7:D:67:ASP:HB3	1.54	0.89
17:N:47:ARG:HG3	17:N:47:ARG:HH11	1.37	0.89
1:O:962:C:H1'	16:M:5:ARG:NH1	1.88	0.89
28:Y:58:GLY:HA3	37:Y:8439:HOH:O	1.73	0.88
1:O:871:G:H5'	1:O:871:G:H8	1.37	0.88
11:H:29:ALA:HB3	11:H:65:ARG:HH12	1.39	0.88
11:H:162:SER:HB2	11:H:163:PRO:CD	2.03	0.88
28:Y:46:LYS:HD3	28:Y:59:HIS:HB2	1.55	0.88
11:H:55:GLN:HE21	11:H:124:ARG:HE	1.20	0.88
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.56	0.88
18:O:115:SER:N	18:O:118:GLN:HE21	1.71	0.88
1:O:1184:C:H1'	37:O:6911:HOH:O	1.74	0.87
7:D:154:LYS:H	7:D:154:LYS:HD2	1.39	0.87
28:Y:38:LYS:HE2	28:Y:45:LYS:HE2	1.54	0.87
11:H:4:ALA:HB3	37:H:8365:HOH:O	1.74	0.86
25:V:88:THR:HG22	25:V:89:ASP:H	1.37	0.86
21:R:57:THR:HG22	21:R:59:ASP:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.58	0.86
1:0:1625:U:H4'	37:0:4143:HOH:O	1.75	0.86
15:L:35:PRO:CG	15:L:38:VAL:HG23	2.05	0.86
1:0:1116:U:H3	1:0:1246:A:H62	1.20	0.86
7:D:146:LYS:NZ	16:M:107:ASN:HD21	1.74	0.86
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.56	0.85
26:W:78:GLU:HG2	26:W:79:GLU:H	1.41	0.85
8:E:97:VAL:HG12	37:E:4191:HOH:O	1.76	0.85
30:1:41:HIS:H	30:1:45:ASN:HD22	1.25	0.85
5:B:62:ARG:HA	5:B:65:MET:HE3	1.57	0.85
25:V:137:GLN:HE21	25:V:141:HIS:HE1	1.24	0.85
11:H:27:LYS:H	11:H:58:HIS:HD2	1.22	0.84
25:V:88:THR:HG23	25:V:110:GLN:NE2	1.92	0.84
13:J:10:GLN:H	13:J:10:GLN:HE21	0.85	0.84
16:M:7:LYS:HE3	19:P:21:ARG:O	1.76	0.84
1:0:2508:C:H2'	37:0:6206:HOH:O	1.78	0.83
37:0:3282:HOH:O	15:L:189:VAL:HG21	1.78	0.83
14:K:68:GLU:HA	37:K:8544:HOH:O	1.77	0.83
1:0:381:G:H5''	37:0:3805:HOH:O	1.78	0.83
1:0:645:U:OP2	14:K:4:LYS:HE2	1.79	0.83
1:0:2812:A:H2	1:0:2814:A:H62	1.25	0.83
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.60	0.83
1:0:2274:A:N3	15:L:86:MET:HE1	1.94	0.83
11:H:2:PRO:HB2	37:H:8365:HOH:O	1.79	0.83
16:M:23:ARG:HD3	37:M:8547:HOH:O	1.78	0.83
2:9:3025:G:H3'	2:9:3026:C:H5'	1.59	0.83
15:L:106:ASN:HD22	15:L:114:VAL:HG23	1.43	0.83
37:0:5755:HOH:O	7:D:99:ASP:HA	1.78	0.83
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.61	0.83
6:C:132:ASP:HB3	37:C:8364:HOH:O	1.78	0.83
18:O:115:SER:H	18:O:118:GLN:HE21	0.86	0.83
1:0:1878:G:HO2'	1:0:1879:U:H6	1.20	0.83
11:H:14:TYR:H	11:H:91:HIS:CE1	1.97	0.83
16:M:49:THR:HG22	16:M:56:ASP:HB2	1.61	0.83
1:0:1118:A:C8	1:0:1119:G:H5''	2.13	0.82
14:K:133:VAL:HA	37:K:8571:HOH:O	1.77	0.82
16:M:87:LEU:HD12	16:M:186:LEU:HD21	1.60	0.82
4:A:192:VAL:HB	37:A:8594:HOH:O	1.79	0.82
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.61	0.82
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.14	0.82
1:0:870:G:H2'	1:0:871:G:H5''	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:144:GLY:O	16:M:147:ILE:HG22	1.78	0.82
1:O:1209:C:H4'	37:O:4744:HOH:O	1.80	0.82
1:O:214:U:H5'	37:O:5602:HOH:O	1.79	0.82
16:M:83:LEU:HD13	16:M:175:LEU:HD23	1.61	0.82
25:V:6:GLN:HB2	25:V:26:ILE:HD12	1.61	0.82
37:O:5254:HOH:O	15:L:170:CYS:SG	2.37	0.82
4:A:199:HIS:HD2	4:A:201:PHE:H	1.28	0.82
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.62	0.82
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.43	0.82
37:O:3058:HOH:O	15:L:152:ARG:HG3	1.79	0.81
1:O:1329:A:H2	37:O:4158:HOH:O	1.63	0.81
5:B:221:GLN:HE22	13:J:42:ASN:HD22	1.27	0.81
6:C:242:GLU:HG3	37:C:8383:HOH:O	1.78	0.81
15:L:164:THR:HG23	15:L:165:SER:N	1.95	0.81
27:X:187:VAL:HG23	27:X:192:ASP:HB2	1.62	0.81
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.60	0.81
20:Q:8:ALA:HB1	20:Q:13:THR:HG21	1.63	0.81
20:Q:17:MET:HE1	20:Q:19:ARG:NH2	1.94	0.81
16:M:164:ASP:CG	16:M:167:ASP:HA	2.05	0.81
1:O:1118:A:C8	1:O:1118:A:H3'	2.15	0.81
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.10	0.81
7:D:20:LYS:HA	7:D:75:LEU:O	1.81	0.81
2:9:3076:G:H3'	2:9:3077:A:H5''	1.63	0.80
25:V:88:THR:HG23	25:V:110:GLN:HE21	1.44	0.80
1:O:1667:A:H8	1:O:1667:A:H5'	1.45	0.80
11:H:49:VAL:O	11:H:157:ILE:HG23	1.81	0.80
1:O:2586:U:H3	1:O:2592:G:H22	1.27	0.80
2:9:3025:G:H3'	2:9:3026:C:C5'	2.11	0.80
9:F:96:ALA:HA	37:F:3111:HOH:O	1.80	0.80
1:O:346:U:H4'	37:O:6294:HOH:O	1.81	0.80
1:O:545:G:H5'	1:O:545:G:H8	1.47	0.80
1:O:711:G:H1'	37:O:6547:HOH:O	1.80	0.80
15:L:87:MET:HB3	31:2:46:ILE:HG21	1.62	0.80
11:H:26:LYS:HG2	11:H:28:ILE:H	1.46	0.80
25:V:154:ARG:C	37:V:4276:HOH:O	2.24	0.80
1:O:272:A:H3'	37:O:6974:HOH:O	1.80	0.80
15:L:172:GLY:O	15:L:183:VAL:HG11	1.81	0.80
26:W:71:ARG:HB3	26:W:88:GLU:OE1	1.82	0.80
13:J:81:ARG:HB2	13:J:87:ARG:NH1	1.97	0.79
1:O:871:G:H8	1:O:871:G:C5'	1.95	0.79
1:O:2316:G:H5'	37:O:5554:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.62	0.79
7:D:146:LYS:HZ3	16:M:107:ASN:HD21	1.28	0.79
1:0:1118:A:H8	1:0:1118:A:H3'	1.46	0.79
15:L:139:PRO:O	15:L:140:ALA:HB3	1.83	0.79
13:J:39:GLY:HA2	37:J:4183:HOH:O	1.83	0.79
31:2:70:ARG:HD3	37:2:8534:HOH:O	1.82	0.79
1:0:1474:C:H5'	1:0:1474:C:C6	2.18	0.78
25:V:122:ARG:HH21	25:V:154:ARG:HD2	1.46	0.78
6:C:139:VAL:HG13	37:C:8444:HOH:O	1.83	0.78
27:X:133:HIS:HD2	37:X:8573:HOH:O	1.66	0.78
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.48	0.78
5:B:175:LEU:C	5:B:175:LEU:HD23	2.08	0.78
11:H:142:VAL:HG13	37:H:8378:HOH:O	1.82	0.78
14:K:67:ARG:O	14:K:71:GLU:HG3	1.83	0.78
22:S:9:LYS:HB2	37:S:7242:HOH:O	1.83	0.78
1:0:2004:U:H4'	37:0:4771:HOH:O	1.82	0.78
27:X:186:ARG:HH11	27:X:186:ARG:HG2	1.48	0.78
28:Y:49:ARG:HD2	37:Y:8430:HOH:O	1.84	0.77
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.67	0.77
24:U:42:ASN:HB3	37:U:7247:HOH:O	1.85	0.77
2:9:3014:G:H5'	2:9:3014:G:H8	1.49	0.77
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.66	0.77
7:D:64:ARG:CG	7:D:67:ASP:HB3	2.14	0.77
1:0:560:C:H42	1:0:597:A:H61	1.32	0.77
37:0:3180:HOH:O	15:L:79:LYS:HD3	1.83	0.77
11:H:47:GLU:HB3	11:H:133:ILE:CD1	2.14	0.77
15:L:64:ARG:HD2	37:L:8584:HOH:O	1.84	0.77
1:0:289:G:H22	1:0:363:A:H2	1.32	0.77
22:S:61:GLU:HG3	37:S:3851:HOH:O	1.83	0.77
31:2:60:LYS:HG3	31:2:61:PRO:HD2	1.66	0.77
1:0:1878:G:O2'	1:0:1879:U:C6	2.38	0.77
12:I:131:THR:HG22	12:I:134:GLU:H	1.48	0.77
18:O:59:ARG:NH2	18:O:66:GLN:HE22	1.82	0.77
25:V:68:THR:HG23	25:V:69:ARG:HG2	1.64	0.77
11:H:47:GLU:HB3	11:H:133:ILE:HD13	1.67	0.77
1:0:1878:G:O2'	1:0:1879:U:H6	1.68	0.76
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.15	0.76
9:F:91:VAL:HG12	9:F:92:GLY:H	1.50	0.76
23:T:14:GLU:O	23:T:17:THR:HB	1.85	0.76
15:L:164:THR:HG22	15:L:167:GLY:N	1.99	0.76
1:0:1603:A:H5'	1:0:1605:G:O4'	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:O2'	1:0:1667:A:H5''	1.85	0.76
17:N:42:GLU:HB2	37:N:2176:HOH:O	1.83	0.76
27:X:187:VAL:HG23	27:X:192:ASP:CB	2.16	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.84	0.76
6:C:140:VAL:HB	37:C:8447:HOH:O	1.85	0.76
7:D:27:ILE:HG22	7:D:28:GLY:H	1.50	0.76
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.65	0.76
14:K:148:GLU:HA	37:K:8570:HOH:O	1.84	0.76
16:M:113:SER:HB2	37:M:8558:HOH:O	1.84	0.76
16:M:164:ASP:OD2	16:M:167:ASP:HA	1.85	0.76
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.68	0.76
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.21	0.75
8:E:84:MET:HE2	8:E:133:VAL:CG2	2.17	0.75
6:C:214:THR:HG21	37:C:8403:HOH:O	1.86	0.75
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.69	0.75
25:V:65:VAL:HA	25:V:68:THR:HG22	1.68	0.75
1:0:1701:A:H5''	1:0:1702:U:H3'	1.69	0.75
15:L:84:LYS:HE2	37:L:8574:HOH:O	1.85	0.75
1:0:1771:U:H4'	28:Y:20:LEU:HD21	1.68	0.75
25:V:88:THR:HG22	25:V:89:ASP:N	2.02	0.75
1:0:541:C:H2'	1:0:542:A:H5''	1.68	0.75
1:0:1730:G:H5'	1:0:1731:C:C6	2.22	0.75
1:0:1119:G:H22	1:0:1246:A:H2	1.29	0.75
1:0:1835:U:C5	1:0:1840:A:N7	2.50	0.75
12:I:74:ARG:HB3	12:I:74:ARG:HH11	1.50	0.75
11:H:150:LYS:HE2	37:H:8380:HOH:O	1.84	0.75
13:J:81:ARG:HD3	13:J:87:ARG:NH1	2.01	0.75
24:U:12:THR:HG22	24:U:15:GLU:CG	2.15	0.75
11:H:26:LYS:HD2	11:H:28:ILE:CD1	2.16	0.75
1:0:2346:C:O2'	7:D:52:THR:HG21	1.87	0.74
37:O:4420:HOH:O	2:9:3103:A:H4'	1.86	0.74
2:9:3056:A:C2'	2:9:3057:A:H5''	2.17	0.74
13:J:14:LYS:HB2	13:J:45:PRO:HG2	1.67	0.74
1:0:1995:G:O2'	1:0:1997:A:N7	2.20	0.74
37:O:6901:HOH:O	5:B:211:THR:HG21	1.85	0.74
18:O:115:SER:OG	18:O:118:GLN:HG3	1.86	0.74
1:0:541:C:C2'	1:0:542:A:H5''	2.17	0.74
1:0:962:C:H1'	16:M:5:ARG:HH12	1.53	0.74
1:0:1160:G:H5'	1:0:1161:A:C5'	2.15	0.74
25:V:122:ARG:HG2	25:V:122:ARG:HH11	1.52	0.74
1:0:282:C:H1'	1:0:368:C:N4	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:H5'	1:0:542:A:C8	2.21	0.74
11:H:139:ASP:N	11:H:140:PRO:HD3	2.03	0.74
25:V:72:PRO:HG2	25:V:77:ALA:HB3	1.68	0.74
6:C:236:THR:HA	37:C:8447:HOH:O	1.87	0.74
15:L:106:ASN:ND2	35:L:8518:CL:CL	2.58	0.74
11:H:75:SER:O	11:H:79:ALA:HB2	1.86	0.74
27:X:220:GLU:HG2	37:X:8543:HOH:O	1.88	0.74
30:1:41:HIS:N	30:1:45:ASN:HD22	1.86	0.74
13:J:74:VAL:HG11	13:J:113:ILE:HG12	1.68	0.74
1:0:1160:G:C5'	1:0:1161:A:H5'	2.15	0.73
1:0:1834:C:H2'	1:0:1840:A:N6	2.03	0.73
1:0:2054:A:N3	20:Q:128:ARG:NH2	2.36	0.73
6:C:1:MET:HG2	6:C:2:GLN:H	1.51	0.73
16:M:86:LEU:HD12	16:M:125:ALA:HB2	1.68	0.73
20:Q:9:ASP:O	20:Q:13:THR:HB	1.88	0.73
11:H:55:GLN:NE2	11:H:124:ARG:HE	1.85	0.73
26:W:72:VAL:HG22	26:W:85:VAL:HG12	1.70	0.73
28:Y:40:PRO:HD3	28:Y:47:LEU:HD11	1.71	0.73
4:A:199:HIS:CD2	4:A:201:PHE:H	2.06	0.73
1:0:1666:C:H2'	1:0:1667:A:H5'	1.69	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
16:M:71:TRP:CE3	16:M:175:LEU:HD22	2.24	0.73
21:R:51:GLN:HE21	21:R:53:ASN:HD21	1.36	0.73
1:0:2533:C:H5'	1:0:2533:C:H6	1.54	0.73
4:A:131:HIS:O	4:A:132:ASP:HB2	1.87	0.73
12:I:45:VAL:HG23	12:I:130:VAL:O	1.89	0.73
16:M:48:VAL:CG1	16:M:55:ASP:HB3	2.18	0.73
1:0:1080:C:H4'	1:0:1081:A:OP1	1.88	0.73
1:0:2710:U:H1'	37:0:7064:HOH:O	1.89	0.73
11:H:41:THR:HA	37:H:8392:HOH:O	1.87	0.73
13:J:22:ASP:HB2	37:J:5264:HOH:O	1.88	0.73
28:Y:37:HIS:HB2	28:Y:47:LEU:HB2	1.71	0.73
1:0:182:G:H5'	37:0:4625:HOH:O	1.89	0.73
25:V:13:MET:HE2	25:V:18:GLN:HA	1.71	0.73
28:Y:38:LYS:HG2	28:Y:45:LYS:HG2	1.69	0.73
1:0:1172:G:H1'	37:0:4443:HOH:O	1.88	0.73
1:0:2851:G:O2'	1:0:2852:A:H5'	1.89	0.73
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.70	0.72
11:H:59:ASN:H	11:H:59:ASN:HD22	1.34	0.72
1:0:2414:A:H2'	1:0:2415:A:C8	2.24	0.72
20:Q:39:THR:HG22	20:Q:42:GLU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:316:A:N3	1:0:336:G:O2'	2.22	0.72
14:K:143:THR:HG22	14:K:144:ASP:N	2.04	0.72
1:0:288:A:H61	1:0:364:C:H42	1.37	0.72
15:L:87:MET:CB	31:2:46:ILE:HD13	2.20	0.72
25:V:149:LEU:CG	25:V:153:MET:HE2	2.19	0.72
1:0:544:G:H2'	1:0:545:G:H5''	1.71	0.72
37:0:3946:HOH:O	15:L:146:GLN:HG2	1.87	0.72
6:C:236:THR:CG2	6:C:239:ALA:H	1.93	0.72
12:I:93:ARG:HB3	12:I:93:ARG:HH11	1.51	0.72
24:U:1:THR:HG23	24:U:2:VAL:H	1.54	0.72
31:2:73:GLU:HB3	37:2:8549:HOH:O	1.89	0.72
11:H:139:ASP:H	11:H:140:PRO:HD3	1.54	0.72
31:2:70:ARG:HG2	31:2:77:ALA:HB2	1.70	0.72
1:0:396:U:H1'	37:0:7071:HOH:O	1.89	0.72
1:0:871:G:C8	1:0:871:G:C5'	2.72	0.72
11:H:46:VAL:HG12	11:H:146:TRP:HZ3	1.54	0.72
23:T:9:CYS:HA	23:T:52:THR:HG23	1.71	0.72
10:G:12:ILE:HA	37:G:4499:HOH:O	1.87	0.72
1:0:2717:C:O2'	1:0:2718:C:H5''	1.90	0.72
5:B:204:GLY:HA3	37:B:8657:HOH:O	1.88	0.72
27:X:189:ASN:HA	27:X:217:ILE:HD11	1.71	0.71
1:0:2676:C:H4'	12:I:70:PHE:CE1	2.25	0.71
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.72	0.71
10:G:12:ILE:N	10:G:13:PRO:HD3	2.04	0.71
15:L:139:PRO:O	15:L:140:ALA:CB	2.36	0.71
2:9:3024:U:O2'	2:9:3025:G:C4'	2.36	0.71
6:C:237:GLU:HB2	37:C:8429:HOH:O	1.89	0.71
28:Y:61:GLY:HA3	37:Y:8427:HOH:O	1.89	0.71
37:0:9209:HOH:O	5:B:254:GLN:HG3	1.90	0.71
2:9:3006:C:H5''	16:M:37:ARG:HH12	1.52	0.71
12:I:107:ASN:ND2	12:I:109:TYR:H	1.88	0.71
5:B:62:ARG:HA	5:B:65:MET:CE	2.20	0.71
12:I:99:GLU:HA	37:I:7377:HOH:O	1.90	0.71
21:R:57:THR:HG22	21:R:59:ASP:N	2.05	0.71
1:0:669:G:O2'	1:0:670:G:H5'	1.90	0.71
1:0:1450:C:O2'	1:0:1493:A:H2'	1.89	0.71
1:0:2717:C:C2'	1:0:2718:C:H5''	2.20	0.71
1:0:2768:A:H2'	1:0:2769:C:O4'	1.89	0.71
15:L:74:ARG:HH11	15:L:74:ARG:HG3	1.56	0.71
4:A:69:LEU:HD21	4:A:120:ARG:HB3	1.71	0.71
11:H:59:ASN:HD22	11:H:59:ASN:N	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:216:ARG:HD3	37:X:8561:HOH:O	1.89	0.70
7:D:55:LYS:HA	37:D:6752:HOH:O	1.91	0.70
27:X:141:THR:HG23	37:X:8579:HOH:O	1.91	0.70
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.70	0.70
14:K:53:ARG:NH2	14:K:57:VAL:HG12	2.06	0.70
25:V:4:LEU:HD22	25:V:52:VAL:HG21	1.73	0.70
29:Z:10:LYS:HG3	37:Z:8432:HOH:O	1.90	0.70
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.20	0.70
4:A:121:ALA:O	4:A:124:VAL:HG22	1.92	0.70
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.72	0.70
5:B:258:GLY:H	5:B:260:HIS:CE1	2.09	0.70
1:O:777:U:O2'	29:Z:11:LYS:HG2	1.91	0.70
1:O:1328:A:OP1	27:X:169:ARG:HD2	1.91	0.70
1:O:1192:A:N1	37:O:5509:HOH:O	2.25	0.70
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.73	0.70
11:H:33:MET:HB2	11:H:83:PHE:HB3	1.74	0.70
13:J:62:PRO:HG3	13:J:65:ARG:HH21	1.57	0.70
1:O:1134:G:C4'	11:H:151:MET:HE1	2.17	0.69
1:O:603:A:H5''	1:O:604:G:OP1	1.92	0.69
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.56	0.69
5:B:238:ASN:HD22	5:B:240:GLY:N	1.90	0.69
6:C:115:LEU:O	6:C:118:THR:HB	1.91	0.69
1:O:2672:C:H1'	37:B:8637:HOH:O	1.92	0.69
1:O:2716:G:H5''	5:B:206:THR:HG21	1.75	0.69
2:9:3024:U:H4'	2:9:3025:G:OP1	1.92	0.69
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.26	0.69
8:E:7:ILE:HD11	8:E:11:VAL:C	2.18	0.69
11:H:84:ARG:NH2	11:H:135:TRP:HH2	1.89	0.69
1:O:1166:A:H1'	1:O:1192:A:C2	2.28	0.69
5:B:175:LEU:HD23	5:B:175:LEU:O	1.92	0.69
7:D:95:THR:O	7:D:97:GLN:N	2.22	0.69
27:X:235:GLU:H	27:X:235:GLU:CD	2.01	0.69
4:A:175:LYS:HE2	37:A:8576:HOH:O	1.93	0.69
15:L:30:GLU:O	15:L:34:GLU:HG3	1.92	0.69
1:O:417:G:P	37:O:6865:HOH:O	2.50	0.69
1:O:1594:C:OP2	18:O:120:ARG:HD2	1.92	0.69
1:O:2768:A:O2'	1:O:2769:C:H5'	1.93	0.69
5:B:145:HIS:HD2	5:B:146:THR:O	1.75	0.69
12:I:103:VAL:HG12	37:I:5907:HOH:O	1.92	0.69
24:U:39:ALA:N	24:U:40:PRO:HD2	2.08	0.69
31:2:31:THR:HB	31:2:33:MET:HE3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:281:U:H2'	1:0:282:C:O4'	1.93	0.69
1:0:1191:A:N1	1:0:1206:U:O4	2.26	0.69
1:0:2468:A:H61	31:2:48:ASN:HD21	1.41	0.69
6:C:236:THR:H	6:C:239:ALA:HB3	1.58	0.69
37:C:8358:HOH:O	17:N:3:THR:HG21	1.93	0.69
12:I:107:ASN:HD21	12:I:109:TYR:HB2	1.58	0.69
23:T:14:GLU:OE1	23:T:15:PRO:HD2	1.92	0.69
7:D:23:VAL:HG23	7:D:23:VAL:O	1.93	0.69
25:V:21:LEU:HD22	25:V:26:ILE:HD11	1.75	0.69
26:W:76:ARG:HH11	26:W:76:ARG:HG3	1.58	0.69
5:B:62:ARG:CA	5:B:65:MET:HE3	2.24	0.68
13:J:75:ARG:CZ	37:J:4172:HOH:O	2.40	0.68
15:L:34:GLU:HB3	15:L:35:PRO:HD2	1.75	0.68
37:O:4307:HOH:O	12:I:47:THR:HB	1.93	0.68
7:D:136:ARG:HD2	7:D:155:HIS:O	1.93	0.68
16:M:71:TRP:HE3	16:M:175:LEU:HD22	1.56	0.68
26:W:25:ARG:HD2	37:W:3861:HOH:O	1.92	0.68
1:0:31:C:H2'	37:O:7130:HOH:O	1.93	0.68
23:T:37:GLU:HB3	37:T:408:HOH:O	1.93	0.68
24:U:4:HIS:HB3	37:U:6622:HOH:O	1.94	0.68
29:Z:25:LYS:HE2	37:Z:8457:HOH:O	1.92	0.68
11:H:71:TYR:C	11:H:73:GLN:H	2.02	0.68
17:N:32:ARG:O	17:N:32:ARG:HD3	1.92	0.68
20:Q:99:ALA:CB	20:Q:109:MET:HE1	2.14	0.68
1:0:21:G:C5'	20:Q:2:ILE:HA	2.22	0.68
1:0:2310:G:OP2	11:H:114:PRO:HD2	1.94	0.68
7:D:97:GLN:HG2	7:D:97:GLN:O	1.94	0.68
20:Q:33:ARG:NH1	37:Q:8542:HOH:O	2.26	0.68
1:0:447:A:OP1	22:S:2:LYS:HG2	1.94	0.68
1:0:2690:U:O2'	8:E:111:LYS:HE3	1.94	0.68
13:J:82:ARG:NH2	13:J:115:ARG:HG2	2.08	0.68
25:V:13:MET:HE2	25:V:18:GLN:CA	2.24	0.68
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.68
1:0:2890:A:H1'	23:T:56:ARG:NH2	2.09	0.68
1:0:380:A:H5''	15:L:48:ARG:NH2	2.09	0.67
1:0:1192:A:C2	37:O:5509:HOH:O	2.47	0.67
1:0:282:C:O2'	1:0:283:U:H5'	1.94	0.67
1:0:338:C:H4'	6:C:174:ILE:CD1	2.23	0.67
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.57	0.67
18:O:71:LYS:HG3	18:O:71:LYS:O	1.93	0.67
1:0:2587:U:H2'	1:0:2589:U:H5''	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:57:THR:HG23	7:D:63:ILE:HG22	1.76	0.67
8:E:15:GLN:NE2	8:E:40:VAL:O	2.28	0.67
2:9:3048:C:H4'	16:M:141:ARG:HH21	1.59	0.67
15:L:87:MET:CB	31:2:46:ILE:HG21	2.24	0.67
1:0:470:U:O2'	29:Z:16:HIS:HD2	1.76	0.67
1:0:1751:G:C2'	1:0:1752:G:H5''	2.22	0.67
13:J:62:PRO:HG3	13:J:65:ARG:NH2	2.10	0.67
27:X:200:THR:HG22	27:X:201:GLU:CG	2.24	0.67
1:0:506:G:N2	1:0:509:A:H5'	2.06	0.67
1:0:2908:A:H2'	1:0:2909:G:O4'	1.94	0.67
8:E:7:ILE:HD11	8:E:11:VAL:O	1.94	0.67
10:G:12:ILE:HD12	37:G:692:HOH:O	1.93	0.67
25:V:122:ARG:NH2	25:V:154:ARG:HD2	2.09	0.67
1:0:558:C:O2'	1:0:559:U:H5''	1.95	0.67
1:0:2346:C:H6	1:0:2346:C:O5'	1.77	0.67
2:9:3006:C:OP1	16:M:37:ARG:NH1	2.27	0.67
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.77	0.67
16:M:159:TYR:HB3	16:M:162:ASP:HB2	1.77	0.67
2:9:3002:U:OP2	2:9:3003:A:H5'	1.95	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.43	0.66
12:I:19:MET:HE2	12:I:79:PHE:HA	1.76	0.66
15:L:61:ILE:HG13	37:L:8623:HOH:O	1.95	0.66
5:B:162:MET:HE2	5:B:310:ARG:CD	2.25	0.66
20:Q:106:GLY:HA2	20:Q:109:MET:HE3	1.77	0.66
1:0:1187:U:H2'	37:0:6348:HOH:O	1.96	0.66
1:0:1730:G:H5'	1:0:1731:C:C5	2.30	0.66
1:0:2783:A:H3'	37:0:4697:HOH:O	1.95	0.66
37:0:7025:HOH:O	28:Y:31:ILE:HG13	1.93	0.66
2:9:3003:A:N6	2:9:3022:G:H1'	2.09	0.66
15:L:24:MET:HE3	15:L:28:MET:CE	2.25	0.66
1:0:1878:G:H1'	37:0:5583:HOH:O	1.94	0.66
37:0:8908:HOH:O	15:L:94:LYS:HE2	1.96	0.66
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.77	0.66
20:Q:18:LEU:HB2	20:Q:143:VAL:HG12	1.76	0.66
27:X:185:VAL:HG12	37:X:8562:HOH:O	1.95	0.66
4:A:36:ASP:OD2	4:A:85:ASP:HB2	1.94	0.66
17:N:47:ARG:HG3	17:N:47:ARG:NH1	2.09	0.66
17:N:87:THR:O	17:N:91:GLN:HG3	1.96	0.66
2:9:3029:C:H2'	2:9:3030:C:H5'	1.78	0.66
7:D:69:ILE:HG22	7:D:69:ILE:O	1.94	0.66
15:L:164:THR:CG2	15:L:165:SER:N	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:14:LEU:HD23	17:N:102:ILE:HD11	1.78	0.66
25:V:21:LEU:HD21	25:V:48:VAL:HG11	1.76	0.66
1:O:1407:A:O2'	1:O:1408:U:H3'	1.96	0.66
1:O:1441:G:O2'	1:O:1442:A:H5'	1.95	0.66
6:C:214:THR:HG23	37:C:8434:HOH:O	1.95	0.66
8:E:23:GLU:HG2	8:E:28:SER:CB	2.26	0.66
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.31	0.66
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.76	0.66
35:I:8501:CL:CL	37:I:4038:HOH:O	2.51	0.66
30:1:24:TRP:CD1	37:1:6863:HOH:O	2.49	0.66
1:O:281:U:H3'	37:O:6656:HOH:O	1.96	0.65
1:O:485:A:O2'	1:O:487:G:H5'	1.96	0.65
1:O:870:G:C2'	1:O:871:G:H5''	2.26	0.65
1:O:2506:A:N3	37:O:5425:HOH:O	2.28	0.65
2:9:3014:G:H5'	2:9:3014:G:C8	2.30	0.65
8:E:100:ASP:HB2	37:E:2789:HOH:O	1.95	0.65
13:J:32:ILE:HD11	13:J:56:SER:HB3	1.79	0.65
16:M:80:SER:HB2	37:M:8536:HOH:O	1.95	0.65
30:1:41:HIS:H	30:1:45:ASN:ND2	1.94	0.65
1:O:299:U:H5'	37:O:6781:HOH:O	1.97	0.65
1:O:2548:C:OP2	5:B:5:ARG:NH2	2.29	0.65
4:A:194:MET:HE3	4:A:199:HIS:CB	2.27	0.65
7:D:19:GLU:O	7:D:20:LYS:HG2	1.97	0.65
7:D:135:VAL:HG22	7:D:136:ARG:H	1.61	0.65
9:F:99:THR:HA	37:F:3461:HOH:O	1.97	0.65
26:W:15:ARG:HB3	26:W:15:ARG:HH11	1.61	0.65
1:O:2638:G:H1'	37:O:7200:HOH:O	1.96	0.65
5:B:103:ASP:HB2	37:B:8591:HOH:O	1.96	0.65
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.26	0.65
27:X:126:PRO:HG2	27:X:128:PHE:CE1	2.32	0.65
7:D:38:GLU:HB3	7:D:49:PRO:HG2	1.77	0.65
1:O:1205:U:C2'	1:O:1206:U:H5''	2.26	0.65
7:D:95:THR:C	7:D:97:GLN:H	2.05	0.65
15:L:80:GLY:O	15:L:81:ARG:HD3	1.97	0.65
1:O:541:C:H2'	1:O:542:A:C5'	2.26	0.65
1:O:559:U:H6	1:O:559:U:H5'	1.60	0.65
1:O:1130:U:H5'	37:O:7113:HOH:O	1.96	0.65
29:Z:8:GLN:HE22	29:Z:11:LYS:NZ	1.95	0.65
1:O:2791:U:H1'	1:O:2792:A:H5''	1.78	0.65
1:O:2878:U:H2'	1:O:2879:A:O4'	1.97	0.65
2:9:3051:A:H5'	16:M:160:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:64:GLY:O	24:U:65:ASP:HB2	1.95	0.65
15:L:87:MET:HG2	31:2:46:ILE:HG21	1.79	0.65
25:V:5:VAL:HG11	25:V:153:MET:HE1	1.78	0.65
1:0:191:A:N1	1:0:236:A:O2'	2.29	0.64
25:V:81:ASP:OD1	25:V:92:ASP:HB2	1.97	0.64
1:0:2676:C:H4'	12:I:70:PHE:HE1	1.61	0.64
9:F:46:GLU:O	9:F:73:PRO:HD2	1.97	0.64
1:0:183:A:H5'	15:L:157:LEU:HD12	1.79	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
1:0:2756:U:H3	1:0:2896:A:H2	1.42	0.64
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.79	0.64
7:D:65:GLU:HG3	37:D:6752:HOH:O	1.96	0.64
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.98	0.64
1:0:31:C:H4'	37:S:7242:HOH:O	1.97	0.64
1:0:2005:G:H3'	1:0:2005:G:OP2	1.98	0.64
7:D:25:MET:CE	7:D:37:ALA:HB1	2.27	0.64
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.98	0.64
13:J:55:VAL:HG12	13:J:56:SER:N	2.12	0.64
19:P:11:ARG:HD3	37:P:5620:HOH:O	1.98	0.64
22:S:47:THR:HB	22:S:100:ASP:HB3	1.78	0.64
8:E:11:VAL:HG12	8:E:12:ASP:N	2.11	0.64
12:I:19:MET:HE1	12:I:78:ILE:HG22	1.79	0.64
27:X:187:VAL:CG2	27:X:192:ASP:HB2	2.27	0.64
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.79	0.64
20:Q:18:LEU:HD12	20:Q:143:VAL:HG11	1.78	0.64
20:Q:119:VAL:O	20:Q:119:VAL:HG12	1.96	0.64
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.12	0.64
11:H:130:HIS:CD2	11:H:133:ILE:HD11	2.32	0.64
6:C:246:ARG:HB3	6:C:246:ARG:NH1	2.12	0.64
11:H:27:LYS:N	11:H:58:HIS:HD2	1.93	0.64
25:V:4:LEU:O	25:V:32:CYS:HA	1.98	0.64
1:0:1209:C:H2'	1:0:1210:G:H8	1.62	0.64
1:0:1741:U:H5'	1:0:1742:A:OP1	1.98	0.64
1:0:2321:A:O2'	1:0:2322:U:H3'	1.98	0.64
1:0:2830:U:H3'	37:0:4693:HOH:O	1.97	0.64
2:9:3039:U:H1'	2:9:3044:A:H61	1.63	0.64
5:B:140:LEU:HD23	37:B:8578:HOH:O	1.98	0.64
11:H:75:SER:C	11:H:79:ALA:HB2	2.23	0.64
1:0:185:G:H4'	1:0:186:A:H4'	1.80	0.64
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.64
1:0:631:A:N3	1:0:2073:G:O2'	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:33:GLU:O	4:A:34:ASP:HB2	1.97	0.64
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.27	0.64
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.63	0.64
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.28	0.64
9:F:110:GLU:HG2	37:F:6926:HOH:O	1.98	0.64
15:L:87:MET:HB2	15:L:91:ILE:HD11	1.80	0.64
1:O:111:C:O2'	29:Z:20:ARG:HG2	1.99	0.63
5:B:82:VAL:O	5:B:82:VAL:HG12	1.97	0.63
14:K:143:THR:HG22	14:K:145:LEU:H	1.62	0.63
28:Y:62:TYR:CE2	28:Y:64:ILE:HG23	2.33	0.63
31:2:65:THR:HG23	31:2:67:LEU:HG	1.80	0.63
1:O:485:A:N3	1:O:487:G:H5''	2.13	0.63
1:O:553:G:P	27:X:204:ARG:HH22	2.21	0.63
1:O:1028:U:H1'	37:O:3148:HOH:O	1.98	0.63
1:O:1184:C:O2'	1:O:1185:U:P	2.55	0.63
1:O:1314:U:H5''	1:O:1316:G:O4'	1.98	0.63
5:B:195:ARG:HD2	5:B:324:ASP:OD1	1.97	0.63
1:O:1246:A:O2'	1:O:1247:A:H3'	1.99	0.63
1:O:2001:G:O2'	1:O:2002:C:H5'	1.99	0.63
7:D:174:VAL:HG13	37:D:6555:HOH:O	1.98	0.63
11:H:46:VAL:O	11:H:146:TRP:HH2	1.80	0.63
12:I:133:GLY:O	12:I:137:GLU:HG3	1.98	0.63
20:Q:39:THR:HB	20:Q:42:GLU:HG3	1.78	0.63
24:U:39:ALA:C	24:U:41:GLU:H	2.07	0.63
24:U:49:LEU:O	24:U:53:ILE:HG13	1.97	0.63
11:H:35:ASN:ND2	11:H:80:ASN:HA	2.13	0.63
11:H:166:ASN:HD22	11:H:166:ASN:N	1.95	0.63
18:O:38:GLU:HA	18:O:41:ARG:NH1	2.14	0.63
6:C:16:VAL:HG12	6:C:17:ASP:N	2.13	0.63
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.79	0.63
8:E:93:MET:HE1	8:E:165:GLY:N	2.14	0.63
14:K:133:VAL:HB	37:K:8556:HOH:O	1.97	0.63
14:K:145:LEU:O	14:K:148:GLU:HG3	1.98	0.63
24:U:44:GLY:O	24:U:48:GLU:HG2	1.98	0.63
1:O:2237:G:O2'	1:O:2238:A:C8	2.51	0.63
1:O:2503:A:OP1	11:H:147:ARG:NH2	2.28	0.63
1:O:2779:G:H21	8:E:143:GLN:NE2	1.96	0.63
13:J:115:ARG:HG3	13:J:116:GLU:N	2.14	0.63
14:K:136:ALA:HB3	37:K:8571:HOH:O	1.99	0.63
24:U:58:THR:O	24:U:62:GLU:HG3	1.99	0.63
29:Z:28:HIS:CD2	29:Z:31:LYS:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1008:C:H5''	11:H:16:ARG:HH12	1.61	0.63
21:R:23:LYS:HE2	37:R:8330:HOH:O	1.99	0.63
28:Y:58:GLY:CA	37:Y:8439:HOH:O	2.41	0.63
1:O:797:A:C4'	28:Y:10:ARG:N	2.62	0.63
8:E:37:ASP:OD1	12:I:125:SER:HB3	1.99	0.63
8:E:101:GLU:HB2	8:E:116:THR:O	1.98	0.63
10:G:63:ARG:N	37:G:2569:HOH:O	2.32	0.63
1:O:1450:C:H4'	1:O:1451:C:OP2	1.96	0.63
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.64	0.63
4:A:101:GLU:OE2	4:A:131:HIS:HB2	1.99	0.63
5:B:125:GLU:O	5:B:129:ARG:HG3	1.98	0.63
8:E:172:PRO:HB3	37:E:6931:HOH:O	1.99	0.63
15:L:104:ARG:O	15:L:108:LYS:HE2	1.99	0.63
15:L:138:HIS:ND1	15:L:139:PRO:O	2.23	0.63
16:M:33:ARG:NH1	16:M:103:ASP:OD2	2.28	0.63
16:M:151:ASP:O	16:M:154:LEU:HB2	1.99	0.63
1:O:200:U:H2'	37:O:9948:HOH:O	1.99	0.62
1:O:2827:A:H2'	1:O:2828:G:O4'	1.98	0.62
7:D:37:ALA:O	7:D:40:ILE:HG12	1.99	0.62
11:H:162:SER:CB	11:H:163:PRO:HD3	2.19	0.62
22:S:63:ILE:HD11	22:S:75:GLU:HB2	1.80	0.62
26:W:78:GLU:CG	26:W:79:GLU:H	2.11	0.62
1:O:338:C:H5''	37:C:8420:HOH:O	1.99	0.62
7:D:105:SER:CB	7:D:131:THR:HG23	2.26	0.62
11:H:75:SER:HB3	11:H:79:ALA:HB1	1.82	0.62
15:L:52:LEU:HD21	37:L:8616:HOH:O	1.99	0.62
25:V:21:LEU:HD22	25:V:26:ILE:CD1	2.29	0.62
27:X:172:THR:HG22	27:X:173:ALA:N	2.12	0.62
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.64	0.62
4:A:191:GLY:HA2	4:A:194:MET:CE	2.29	0.62
8:E:6:GLU:HA	8:E:46:THR:HG22	1.80	0.62
15:L:12:TRP:CE2	15:L:20:ILE:HD11	2.35	0.62
25:V:21:LEU:HD21	25:V:48:VAL:CG1	2.30	0.62
5:B:36:PRO:HA	5:B:168:GLY:CA	2.29	0.62
8:E:166:VAL:HG12	37:E:3134:HOH:O	1.99	0.62
1:O:431:G:P	15:L:48:ARG:HH12	2.22	0.62
1:O:1118:A:C8	1:O:1118:A:C3'	2.80	0.62
1:O:2570:G:H5''	37:O:4382:HOH:O	1.99	0.62
6:C:180:SER:HB2	37:C:8441:HOH:O	1.99	0.62
1:O:1701:A:H5'	37:O:5744:HOH:O	1.98	0.62
6:C:27:ARG:HD2	6:C:29:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:48:VAL:HG11	16:M:55:ASP:HB3	1.82	0.62
16:M:154:LEU:O	16:M:155:GLU:HB3	1.98	0.62
26:W:41:PHE:O	26:W:43:VAL:HG23	1.99	0.62
1:O:2004:U:H2'	1:O:2005:G:OP1	2.00	0.62
1:O:2316:G:C5'	37:O:5554:HOH:O	2.42	0.62
14:K:53:ARG:HH22	14:K:57:VAL:HG12	1.63	0.62
14:K:114:VAL:HG11	37:K:8571:HOH:O	2.00	0.62
26:W:78:GLU:HG2	26:W:79:GLU:N	2.13	0.62
28:Y:53:GLY:HA2	28:Y:67:GLY:O	2.00	0.62
11:H:81:TYR:CD1	11:H:81:TYR:C	2.77	0.62
29:Z:25:LYS:O	29:Z:25:LYS:HG2	1.99	0.62
1:O:1119:G:H8	12:I:52:GLN:HE22	1.48	0.61
1:O:1185:U:H2'	1:O:1186:C:C6	2.35	0.61
2:9:3049:G:H5''	37:9:8464:HOH:O	1.98	0.61
13:J:74:VAL:CG1	13:J:113:ILE:HG12	2.30	0.61
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.16	0.61
10:G:12:ILE:N	10:G:13:PRO:CD	2.63	0.61
10:G:64:ASN:HD22	10:G:64:ASN:N	1.97	0.61
11:H:3:GLY:HA2	11:H:57:ARG:HH12	1.63	0.61
16:M:37:ARG:NE	37:M:8534:HOH:O	2.33	0.61
16:M:78:MET:HB2	16:M:79:PRO:HD3	1.81	0.61
16:M:169:PRO:O	16:M:172:PHE:HB3	2.00	0.61
23:T:20:MET:HE2	23:T:30:HIS:NE2	2.15	0.61
25:V:4:LEU:HD22	25:V:52:VAL:CG2	2.30	0.61
11:H:139:ASP:HB2	37:H:8346:HOH:O	2.00	0.61
20:Q:39:THR:HB	20:Q:42:GLU:CD	2.25	0.61
20:Q:44:VAL:O	20:Q:48:GLU:HG3	2.00	0.61
20:Q:111:ILE:HG23	20:Q:145:LEU:HD11	1.82	0.61
1:O:175:G:H2'	15:L:192:ALA:HB3	1.81	0.61
1:O:1164:U:O4	1:O:1192:A:H2	1.84	0.61
1:O:1249:U:H2'	1:O:1250:C:C6	2.35	0.61
1:O:2428:G:N7	31:2:60:LYS:NZ	2.44	0.61
1:O:2526:C:O2'	1:O:2527:U:H5'	2.00	0.61
4:A:210:GLY:HA3	37:A:8587:HOH:O	2.00	0.61
7:D:38:GLU:OE2	7:D:51:ARG:CZ	2.49	0.61
8:E:79:GLY:HA3	37:E:7046:HOH:O	2.00	0.61
1:O:545:G:H5'	1:O:545:G:C8	2.33	0.61
1:O:960:G:N3	1:O:960:G:H2'	2.16	0.61
2:9:3055:U:H4'	2:9:3056:A:C8	2.35	0.61
25:V:137:GLN:HE21	25:V:141:HIS:CE1	2.13	0.61
1:O:2044:G:OP1	26:W:23:HIS:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.35	0.61
1:0:289:G:N2	1:0:363:A:H2	1.97	0.61
4:A:173:GLY:O	4:A:176:HIS:HB3	2.00	0.61
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.83	0.61
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.69	0.61
15:L:60:ILE:C	15:L:61:ILE:HD12	2.26	0.61
15:L:74:ARG:HG3	15:L:74:ARG:NH1	2.15	0.61
18:O:80:ARG:HG2	18:O:87:ARG:CZ	2.31	0.61
1:0:604:G:H4'	1:0:605:C:O5'	2.01	0.61
1:0:1874:U:H2'	4:A:120:ARG:HG3	1.81	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	2.01	0.61
18:O:10:ALA:HA	18:O:13:VAL:HG12	1.81	0.61
27:X:112:GLU:CD	27:X:115:ARG:NH1	2.58	0.61
27:X:144:ARG:CZ	37:X:8601:HOH:O	2.48	0.61
1:0:371:U:H2'	1:0:372:A:H8	1.64	0.61
12:I:130:VAL:HG12	12:I:131:THR:N	2.16	0.61
1:0:263:U:O4'	9:F:59:ILE:HD13	2.01	0.61
1:0:660:A:H4'	1:0:661:G:O5'	1.99	0.61
1:0:1667:A:H5'	1:0:1667:A:C8	2.34	0.61
5:B:329:TYR:CE2	23:T:15:PRO:HG2	2.36	0.61
7:D:93:LEU:HB3	7:D:97:GLN:OE1	2.01	0.61
16:M:61:ALA:HB3	16:M:88:ALA:HB2	1.83	0.61
20:Q:132:ARG:CZ	37:Q:8580:HOH:O	2.49	0.61
1:0:1679:C:H5'	37:0:8837:HOH:O	2.01	0.60
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.83	0.60
8:E:69:ILE:HA	8:E:72:MET:CE	2.31	0.60
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.82	0.60
16:M:43:VAL:HG11	16:M:81:ALA:HA	1.82	0.60
16:M:183:ASP:OD2	16:M:186:LEU:HD12	2.00	0.60
22:S:9:LYS:HE3	22:S:13:ARG:NH1	2.16	0.60
25:V:4:LEU:HD23	25:V:54:PHE:HB3	1.82	0.60
1:0:1878:G:O2'	1:0:1879:U:P	2.59	0.60
1:0:2265:U:H2'	1:0:2266:A:C8	2.36	0.60
1:0:2630:G:O6	4:A:206:ARG:NH2	2.34	0.60
1:0:2862:G:H4'	5:B:336:GLN:O	2.00	0.60
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.01	0.60
1:0:1819:G:H2'	1:0:1820:G:H4'	1.83	0.60
1:0:2787:C:H5	37:0:4108:HOH:O	1.84	0.60
5:B:119:HIS:O	5:B:121:PRO:HD3	2.01	0.60
9:F:58:GLU:OE1	15:L:27:ARG:NH2	2.28	0.60
12:I:107:ASN:HD22	12:I:107:ASN:C	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:5:VAL:HG22	25:V:32:CYS:HB2	1.83	0.60
1:O:2420:G:O2'	1:O:2421:G:H5'	2.01	0.60
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.83	0.60
5:B:307:ARG:HH11	5:B:307:ARG:HB2	1.66	0.60
7:D:99:ASP:CB	7:D:103:ASN:H	2.15	0.60
11:H:44:ALA:HA	11:H:163:PRO:O	2.02	0.60
12:I:52:GLN:HG3	12:I:53:ILE:N	2.16	0.60
1:O:1058:A:H2'	1:O:1060:C:H5''	1.83	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HB3	1.83	0.60
6:C:103:ASN:HB3	37:C:8309:HOH:O	2.01	0.60
8:E:132:THR:HB	37:E:2227:HOH:O	2.00	0.60
13:J:74:VAL:HG12	13:J:75:ARG:HG3	1.82	0.60
16:M:47:LEU:HD13	16:M:97:VAL:HG11	1.84	0.60
25:V:6:GLN:HB2	25:V:26:ILE:CD1	2.31	0.60
30:1:22:PRO:HB2	30:1:24:TRP:CD1	2.36	0.60
1:O:2363:G:O3'	19:P:11:ARG:NH1	2.35	0.60
4:A:76:VAL:HG23	28:Y:63:LYS:HB3	1.84	0.60
1:O:182:G:O3'	15:L:157:LEU:CD1	2.50	0.60
1:O:184:G:H5''	15:L:153:THR:HG22	1.83	0.60
1:O:536:A:H3'	37:O:4517:HOH:O	2.01	0.60
1:O:790:A:H1'	1:O:1710:A:H2'	1.82	0.60
1:O:1168:C:H2'	1:O:1169:U:O4'	2.00	0.60
37:O:3681:HOH:O	27:X:186:ARG:HD2	2.02	0.60
2:9:3025:G:C3'	2:9:3026:C:H5'	2.29	0.60
8:E:69:ILE:HA	8:E:72:MET:HE2	1.82	0.60
28:Y:42:CYS:SG	28:Y:44:PHE:HB2	2.41	0.60
1:O:1214:G:HO2'	1:O:1215:A:H8	1.49	0.60
1:O:2578:G:H5'	1:O:2578:G:H8	1.66	0.60
14:K:104:ASP:O	14:K:105:TYR:HB3	2.00	0.60
15:L:38:VAL:C	15:L:63:VAL:HG13	2.26	0.60
28:Y:29:VAL:O	28:Y:33:HIS:HB2	2.02	0.60
1:O:282:C:H1'	1:O:368:C:H42	1.64	0.60
1:O:284:C:H4'	1:O:285:A:O5'	2.00	0.60
1:O:2717:C:H2'	1:O:2718:C:C5'	2.32	0.60
11:H:27:LYS:H	11:H:58:HIS:CD2	2.13	0.60
11:H:150:LYS:HB2	11:H:157:ILE:HD12	1.83	0.60
12:I:19:MET:HE3	12:I:132:LEU:CD1	2.21	0.60
4:A:37:VAL:HG22	37:A:8597:HOH:O	2.02	0.60
5:B:179:LEU:O	5:B:183:GLU:HG2	2.02	0.60
11:H:48:LEU:HG	11:H:157:ILE:HG21	1.83	0.60
11:H:140:PRO:HB3	37:H:8378:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:39:THR:HG23	20:Q:107:GLU:O	2.02	0.60
22:S:32:ARG:NH1	22:S:38:ARG:HH12	1.99	0.60
1:O:2694:A:H4'	8:E:91:PHE:HE1	1.66	0.59
2:9:3002:U:H4'	37:9:8477:HOH:O	2.01	0.59
37:9:8464:HOH:O	16:M:147:ILE:HB	2.02	0.59
4:A:170:VAL:HG13	28:Y:22:ILE:HG21	1.84	0.59
6:C:246:ARG:NE	37:C:8423:HOH:O	2.35	0.59
6:C:246:ARG:NH2	37:C:8423:HOH:O	2.35	0.59
15:L:48:ARG:NH2	37:L:8559:HOH:O	2.35	0.59
16:M:155:GLU:O	16:M:156:GLU:HG3	2.02	0.59
37:O:3556:HOH:O	5:B:27:ASN:HB2	2.02	0.59
4:A:211:LYS:NZ	37:A:8573:HOH:O	2.34	0.59
6:C:133:ARG:HD2	37:C:8410:HOH:O	2.02	0.59
11:H:118:PRO:HD2	37:H:8338:HOH:O	2.01	0.59
12:I:74:ARG:HH11	12:I:74:ARG:CB	2.14	0.59
25:V:80:ASP:O	25:V:84:VAL:HG23	2.01	0.59
27:X:155:ARG:NH1	37:X:8551:HOH:O	2.35	0.59
1:O:182:G:O3'	15:L:157:LEU:HD13	2.03	0.59
1:O:2256:G:H2'	1:O:2257:G:H5'	1.84	0.59
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.84	0.59
8:E:43:ASP:HA	37:E:5864:HOH:O	2.02	0.59
18:O:38:GLU:HA	18:O:41:ARG:HH11	1.68	0.59
1:O:1559:A:H1'	37:O:5329:HOH:O	2.02	0.59
1:O:1771:U:O2'	28:Y:23:ARG:NH2	2.34	0.59
11:H:56:ILE:HG22	11:H:61:LEU:HD22	1.83	0.59
1:O:95:A:H5''	1:O:97:G:O4'	2.02	0.59
1:O:285:A:H2'	1:O:286:U:O4'	2.02	0.59
1:O:1172:G:N3	37:O:6786:HOH:O	2.32	0.59
1:O:1636:G:O2'	1:O:1637:A:H5'	2.01	0.59
8:E:84:MET:HE2	8:E:133:VAL:HG21	1.82	0.59
11:H:47:GLU:CB	11:H:133:ILE:HD13	2.32	0.59
20:Q:39:THR:HB	20:Q:42:GLU:CG	2.32	0.59
1:O:1634:G:H3'	37:O:3388:HOH:O	2.02	0.59
1:O:1641:A:H2'	1:O:1642:A:H5'	1.84	0.59
1:O:2547:C:OP2	5:B:5:ARG:NH1	2.36	0.59
27:X:165:GLU:HB3	37:X:8583:HOH:O	2.01	0.59
27:X:186:ARG:HG2	27:X:186:ARG:NH1	2.15	0.59
1:O:558:C:H5'	37:O:4722:HOH:O	2.02	0.59
1:O:797:A:H4'	28:Y:10:ARG:N	2.17	0.59
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.32	0.59
6:C:233:THR:HG22	6:C:234:VAL:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:12:THR:CG2	24:U:15:GLU:HG3	2.22	0.59
25:V:108:ARG:HE	25:V:114:PRO:HG3	1.66	0.59
1:0:259:G:H21	15:L:58:GLN:NE2	2.00	0.59
1:0:1044:C:H5''	37:0:8541:HOH:O	2.02	0.59
7:D:166:ILE:HD12	37:D:6326:HOH:O	2.02	0.59
1:0:1182:C:H1'	1:0:1192:A:H8	1.67	0.59
1:0:1189:A:H1'	1:0:1209:C:C1'	2.33	0.59
1:0:2821:C:H4'	5:B:116:PRO:HB3	1.84	0.59
9:F:19:ALA:O	9:F:22:VAL:HG22	2.03	0.59
9:F:58:GLU:HG3	9:F:61:MET:HE2	1.85	0.59
14:K:143:THR:HG22	14:K:144:ASP:H	1.68	0.59
15:L:149:TRP:O	15:L:152:ARG:HG2	2.01	0.59
29:Z:21:ARG:HD2	29:Z:37:CYS:SG	2.43	0.59
1:0:281:U:O2'	1:0:282:C:H5'	2.03	0.59
1:0:544:G:C2'	1:0:545:G:H5''	2.32	0.59
1:0:2769:C:H2'	1:0:2770:G:O4'	2.03	0.59
5:B:138:GLY:O	5:B:139:ASP:O	2.20	0.59
7:D:101:THR:HG22	37:D:7400:HOH:O	2.03	0.59
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.38	0.59
27:X:189:ASN:HD22	27:X:189:ASN:C	2.11	0.59
1:0:67:A:H5''	1:0:69:A:C8	2.38	0.58
1:0:1159:G:H21	1:0:1189:A:H8	1.49	0.58
1:0:2064:U:H4'	1:0:2653:A:OP1	2.03	0.58
12:I:75:PRO:HG2	12:I:105:LEU:HD21	1.84	0.58
13:J:74:VAL:HG13	13:J:113:ILE:HG23	1.85	0.58
15:L:81:ARG:HG3	15:L:85:ARG:HB2	1.85	0.58
16:M:90:LEU:HB2	16:M:186:LEU:HD22	1.84	0.58
25:V:21:LEU:HB3	25:V:26:ILE:HG12	1.85	0.58
1:0:182:G:H4'	15:L:157:LEU:HD13	1.85	0.58
1:0:902:G:N7	14:K:18:HIS:HD2	2.00	0.58
4:A:105:VAL:HG12	4:A:106:CYS:N	2.18	0.58
7:D:86:THR:O	7:D:90:LEU:HG	2.04	0.58
15:L:173:LEU:HD23	15:L:183:VAL:HG12	1.84	0.58
26:W:18:ARG:NH1	37:W:4132:HOH:O	2.33	0.58
28:Y:19:GLY:O	28:Y:23:ARG:HG2	2.02	0.58
1:0:1329:A:C2	37:0:4158:HOH:O	2.46	0.58
2:9:3041:C:O4'	7:D:50:VAL:HG23	2.04	0.58
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.86	0.58
7:D:36:ASN:HA	37:D:7500:HOH:O	2.02	0.58
8:E:32:ARG:O	8:E:33:LEU:HD23	2.02	0.58
25:V:13:MET:HE3	25:V:17:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:O6	14:K:6:ARG:HD3	2.03	0.58
1:0:2488:A:H61	1:0:2534:C:H42	1.52	0.58
1:0:2604:A:H5'	37:0:5252:HOH:O	2.03	0.58
6:C:12:THR:HB	37:C:8437:HOH:O	2.03	0.58
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.85	0.58
1:0:1441:G:H1'	37:0:7205:HOH:O	2.03	0.58
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.84	0.58
5:B:238:ASN:ND2	5:B:240:GLY:H	1.95	0.58
9:F:58:GLU:HA	9:F:61:MET:HG3	1.86	0.58
20:Q:99:ALA:HB1	20:Q:109:MET:CE	2.16	0.58
26:W:75:ALA:O	26:W:83:ALA:HA	2.03	0.58
1:0:2670:G:O2'	1:0:2671:U:H5'	2.03	0.58
1:0:2825:C:H4'	1:0:2826:G:O5'	2.04	0.58
6:C:79:ARG:O	6:C:87:ARG:HG2	2.03	0.58
16:M:49:THR:CG2	16:M:56:ASP:HB2	2.32	0.58
24:U:8:ILE:HA	24:U:11:MET:HE3	1.84	0.58
25:V:122:ARG:HH22	25:V:154:ARG:C	2.11	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.87	0.58
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.33	0.58
5:B:2:GLN:HA	37:B:8620:HOH:O	2.03	0.58
27:X:126:PRO:HG2	27:X:128:PHE:CZ	2.38	0.58
1:0:188:C:H5''	15:L:163:LEU:HD21	1.85	0.58
1:0:1117:A:N1	1:0:1244:U:O2'	2.32	0.58
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.37	0.58
1:0:2011:A:P	37:0:5422:HOH:O	2.61	0.58
1:0:2092:G:H5'	37:0:8630:HOH:O	2.03	0.58
1:0:2301:A:H5''	1:0:2302:A:H5'	1.85	0.58
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.86	0.58
8:E:31:ARG:HH12	8:E:68:HIS:CE1	2.22	0.58
23:T:52:THR:CG2	23:T:54:THR:HB	2.34	0.58
25:V:13:MET:CE	25:V:17:ILE:HG22	2.33	0.58
1:0:2081:A:H4'	12:I:69:TYR:CE1	2.38	0.58
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.86	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.58
1:0:324:G:O2'	1:0:325:U:H5'	2.04	0.58
1:0:396:U:O2'	1:0:397:A:OP1	2.22	0.58
1:0:450:C:OP1	6:C:184:ARG:NH2	2.29	0.58
1:0:1353:C:P	37:0:4155:HOH:O	2.61	0.58
2:9:3044:A:O4'	7:D:76:ARG:NE	2.37	0.58
6:C:246:ARG:HB3	6:C:246:ARG:HH11	1.67	0.58
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:58:GLU:CD	15:L:27:ARG:HH22	2.12	0.58
23:T:11:THR:HG22	23:T:53:ASP:OD2	2.04	0.58
1:O:777:U:HO2'	29:Z:11:LYS:HG2	1.69	0.57
4:A:94:LEU:HD23	4:A:94:LEU:N	2.19	0.57
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.22	0.57
11:H:5:MET:HG3	37:H:8365:HOH:O	2.02	0.57
16:M:64:SER:C	16:M:66:LEU:H	2.12	0.57
25:V:139:GLY:O	25:V:141:HIS:HD2	1.86	0.57
1:O:1197:G:N2	37:O:5694:HOH:O	2.37	0.57
1:O:1733:A:H4'	5:B:212:GLN:HA	1.84	0.57
2:9:3030:C:OP1	7:D:137:PRO:O	2.21	0.57
14:K:143:THR:CG2	14:K:144:ASP:N	2.66	0.57
16:M:34:LEU:HA	16:M:47:LEU:HD23	1.87	0.57
18:O:103:THR:HA	18:O:106:ARG:NH1	2.19	0.57
27:X:144:ARG:NE	37:X:8601:HOH:O	2.36	0.57
1:O:1244:U:OP1	12:I:18:ILE:HD13	2.05	0.57
4:A:170:VAL:HG22	28:Y:22:ILE:HG23	1.86	0.57
16:M:77:ASN:OD1	16:M:80:SER:HB2	2.05	0.57
21:R:43:GLU:HB3	37:R:8344:HOH:O	2.03	0.57
23:T:52:THR:HG22	23:T:54:THR:H	1.70	0.57
1:O:1003:U:O2	11:H:90:PHE:HZ	1.88	0.57
5:B:168:GLY:N	5:B:174:ARG:HD3	2.19	0.57
11:H:14:TYR:N	11:H:91:HIS:CE1	2.70	0.57
23:T:52:THR:HG22	23:T:54:THR:N	2.19	0.57
30:1:35:ARG:HB2	37:1:2691:HOH:O	2.03	0.57
1:O:1766:U:O2	1:O:1778:A:H5'	2.04	0.57
1:O:2064:U:H5'	1:O:2652:U:O3'	2.05	0.57
37:O:4021:HOH:O	11:H:151:MET:HE2	2.04	0.57
2:9:3092:G:H2'	2:9:3093:A:C8	2.39	0.57
6:C:246:ARG:CZ	37:C:8423:HOH:O	2.52	0.57
15:L:172:GLY:C	15:L:183:VAL:HG11	2.29	0.57
23:T:46:ALA:HB1	23:T:52:THR:HG21	1.86	0.57
1:O:703:G:O2'	1:O:704:C:H5'	2.04	0.57
1:O:1086:A:C6	25:V:11:VAL:HG11	2.38	0.57
1:O:1184:C:HO2'	1:O:1185:U:P	2.26	0.57
1:O:1972:U:H2'	1:O:1973:A:H5'	1.86	0.57
1:O:2501:G:H1'	37:O:4021:HOH:O	2.03	0.57
9:F:28:ALA:HB3	9:F:99:THR:O	2.04	0.57
11:H:46:VAL:HG12	11:H:146:TRP:CZ3	2.38	0.57
11:H:150:LYS:HG2	37:H:8380:HOH:O	2.05	0.57
1:O:485:A:H4'	1:O:486:A:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:55:ASN:HB3	5:B:63:GLU:HA	1.86	0.57
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.04	0.57
5:B:297:VAL:HB	37:B:8604:HOH:O	2.05	0.57
7:D:140:ARG:O	7:D:144:ARG:HG2	2.04	0.57
14:K:57:VAL:HG12	14:K:57:VAL:O	2.04	0.57
15:L:37:VAL:HG21	15:L:108:LYS:HG3	1.87	0.57
16:M:143:ARG:HA	16:M:172:PHE:CD2	2.39	0.57
1:O:449:A:N7	6:C:43:LYS:HG2	2.20	0.57
1:O:1234:U:N3	5:B:244:PRO:HB3	2.20	0.57
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.87	0.57
13:J:34:VAL:HG22	13:J:47:ALA:HB2	1.86	0.57
1:O:1003:U:O2	11:H:90:PHE:CZ	2.58	0.57
1:O:1528:A:H2'	1:O:1529:G:O4'	2.05	0.57
2:9:3006:C:C5'	16:M:37:ARG:NH1	2.64	0.57
5:B:75:GLU:C	5:B:77:PRO:HD3	2.30	0.57
9:F:47:LEU:HB2	9:F:108:LEU:HD11	1.87	0.57
11:H:3:GLY:HA2	11:H:57:ARG:NH1	2.20	0.57
11:H:13:ALA:HA	11:H:91:HIS:CE1	2.40	0.57
14:K:73:VAL:HG23	14:K:74:THR:H	1.70	0.57
26:W:31:ILE:O	26:W:35:GLU:HG3	2.04	0.57
28:Y:11:THR:CG2	28:Y:23:ARG:HB2	2.35	0.57
1:O:661:G:C5	1:O:686:A:C2	2.92	0.57
1:O:1973:A:H5'	1:O:1973:A:H8	1.69	0.57
1:O:2320:U:H4'	1:O:2321:A:O4'	2.05	0.57
1:O:2769:C:C2'	1:O:2770:G:H5'	2.35	0.57
5:B:279:THR:OG1	5:B:290:VAL:HB	2.04	0.57
6:C:77:ALA:O	6:C:78:ARG:HG3	2.05	0.57
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.14	0.57
6:C:118:THR:O	6:C:136:VAL:HG13	2.05	0.57
7:D:146:LYS:NZ	16:M:107:ASN:ND2	2.49	0.57
15:L:59:GLY:HA3	15:L:141:ILE:HD12	1.87	0.57
16:M:37:ARG:NH2	37:M:8534:HOH:O	2.38	0.57
26:W:43:VAL:HG12	26:W:44:ASP:N	2.20	0.57
30:1:18:ASN:HD21	30:1:40:ARG:H	1.52	0.57
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.87	0.56
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.86	0.56
11:H:53:PRO:HG3	11:H:127:GLY:H	1.69	0.56
27:X:107:PRO:HB3	27:X:182:PHE:CD2	2.40	0.56
31:2:17:HIS:O	31:2:18:GLN:HG3	2.05	0.56
4:A:8:ARG:HG2	37:A:8550:HOH:O	2.04	0.56
11:H:31:PHE:HE2	11:H:87:LYS:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:51:GLN:HE21	21:R:53:ASN:ND2	2.03	0.56
22:S:6:LYS:NZ	37:S:644:HOH:O	2.38	0.56
1:0:272:A:H5'	1:0:273:G:OP2	2.04	0.56
1:0:1172:G:N3	37:0:4443:HOH:O	2.33	0.56
1:0:1181:A:H2'	1:0:1182:C:O4'	2.04	0.56
1:0:1484:G:H2'	37:0:8620:HOH:O	2.06	0.56
37:0:4441:HOH:O	11:H:57:ARG:HG3	2.05	0.56
5:B:14:GLY:HA2	5:B:15:PRO:C	2.30	0.56
16:M:152:GLU:C	16:M:154:LEU:H	2.12	0.56
21:R:51:GLN:NE2	21:R:53:ASN:HD21	2.01	0.56
21:R:81:ILE:HG23	37:R:8336:HOH:O	2.04	0.56
23:T:13:ILE:HG12	23:T:32:CYS:HB3	1.87	0.56
1:0:1735:C:O2'	1:0:1736:A:H5'	2.04	0.56
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.35	0.56
12:I:19:MET:CE	12:I:132:LEU:HD11	2.24	0.56
22:S:9:LYS:HE3	22:S:13:ARG:HH11	1.71	0.56
31:2:25:VAL:HG22	31:2:68:LYS:HG3	1.87	0.56
1:0:349:U:O2'	1:0:350:C:H5'	2.05	0.56
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.88	0.56
18:O:16:VAL:HG12	18:O:17:GLY:N	2.20	0.56
18:O:105:LEU:HD21	18:O:137:LEU:HD21	1.88	0.56
25:V:48:VAL:CG1	25:V:48:VAL:O	2.53	0.56
27:X:115:ARG:NE	37:X:8549:HOH:O	2.37	0.56
28:Y:28:ASP:O	28:Y:31:ILE:HG22	2.05	0.56
1:0:1778:A:H2'	1:0:1779:A:H5'	1.87	0.56
1:0:2769:C:O2'	1:0:2770:G:H5'	2.05	0.56
5:B:175:LEU:C	5:B:175:LEU:CD2	2.76	0.56
7:D:50:VAL:O	7:D:71:ALA:HA	2.06	0.56
9:F:110:GLU:O	9:F:114:LYS:HG3	2.05	0.56
15:L:87:MET:HE3	37:L:8592:HOH:O	2.05	0.56
23:T:9:CYS:CA	23:T:52:THR:HG23	2.36	0.56
25:V:149:LEU:HG	25:V:153:MET:CE	2.29	0.56
1:0:1119:G:N2	1:0:1246:A:H2	2.01	0.56
1:0:1183:C:N4	37:0:3884:HOH:O	2.35	0.56
1:0:2456:A:H5'	37:0:5156:HOH:O	2.04	0.56
1:0:2840:A:OP1	5:B:211:THR:HG23	2.04	0.56
37:0:6478:HOH:O	4:A:211:LYS:HG2	2.04	0.56
11:H:58:HIS:HA	11:H:61:LEU:HD23	1.88	0.56
11:H:85:ILE:HB	11:H:132:PHE:CE2	2.40	0.56
1:0:567:U:H5''	37:V:5817:HOH:O	2.05	0.56
1:0:1164:U:O4	1:0:1192:A:C2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:73:VAL:HG23	14:K:74:THR:N	2.20	0.56
17:N:38:ARG:NH1	37:N:7674:HOH:O	2.38	0.56
27:X:187:VAL:HB	37:X:8562:HOH:O	2.05	0.56
8:E:81:GLU:HG2	8:E:134:SER:CB	2.33	0.56
9:F:99:THR:O	9:F:99:THR:HG23	2.05	0.56
16:M:12:ARG:HD3	16:M:18:THR:OG1	2.06	0.56
27:X:99:ALA:HB2	27:X:233:TYR:CZ	2.41	0.56
1:O:506:G:H22	1:O:509:A:C5'	2.09	0.56
4:A:88:ILE:O	4:A:88:ILE:HG22	2.06	0.56
5:B:146:THR:O	5:B:159:PRO:HB3	2.05	0.56
5:B:307:ARG:HH11	5:B:307:ARG:CG	2.18	0.56
6:C:1:MET:HG2	6:C:2:GLN:N	2.20	0.56
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.41	0.56
6:C:235:PHE:HE2	6:C:243:VAL:HG21	1.70	0.56
7:D:44:ILE:HG23	7:D:45:THR:HG23	1.88	0.56
11:H:53:PRO:HA	11:H:125:VAL:O	2.06	0.56
14:K:53:ARG:NH2	14:K:57:VAL:CG1	2.69	0.56
15:L:37:VAL:HG13	15:L:63:VAL:HG11	1.87	0.56
17:N:39:THR:O	17:N:115:ARG:NH2	2.39	0.56
1:O:338:C:H4'	6:C:174:ILE:HD12	1.88	0.55
1:O:542:A:H2'	1:O:543:G:O4'	2.06	0.55
1:O:2004:U:C2'	1:O:2005:G:OP1	2.54	0.55
7:D:10:PHE:CG	7:D:11:HIS:N	2.74	0.55
7:D:91:ALA:HB1	37:D:5198:HOH:O	2.05	0.55
10:G:23:ILE:O	10:G:27:ILE:HG13	2.05	0.55
17:N:14:LEU:CD2	17:N:102:ILE:HD11	2.35	0.55
25:V:48:VAL:O	25:V:48:VAL:HG12	2.05	0.55
28:Y:13:ARG:NH1	28:Y:14:PHE:CE2	2.74	0.55
1:O:1669:A:H2'	1:O:1670:G:C8	2.41	0.55
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.70	0.55
8:E:31:ARG:NH1	37:E:5919:HOH:O	2.38	0.55
11:H:158:ASN:ND2	37:H:8385:HOH:O	2.39	0.55
12:I:74:ARG:O	12:I:78:ILE:HG12	2.06	0.55
20:Q:111:ILE:HG23	20:Q:145:LEU:CD1	2.36	0.55
25:V:106:THR:OG1	25:V:109:GLU:HG3	2.06	0.55
2:9:3035:C:H5''	37:9:8454:HOH:O	2.04	0.55
2:9:3042:C:H2'	37:9:8500:HOH:O	2.05	0.55
13:J:10:GLN:NE2	13:J:10:GLN:N	2.36	0.55
15:L:186:SER:O	15:L:189:VAL:HG12	2.05	0.55
22:S:24:ARG:HH21	22:S:39:ASN:HD22	1.52	0.55
1:O:1730:G:H5'	1:O:1731:C:H6	1.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:O:6140:HOH:O	22:S:38:ARG:NH1	2.39	0.55
5:B:7:ARG:HH11	5:B:7:ARG:CG	2.17	0.55
9:F:37:THR:O	9:F:41:GLU:HG3	2.05	0.55
11:H:26:LYS:CG	11:H:28:ILE:H	2.17	0.55
15:L:37:VAL:HG21	15:L:108:LYS:CG	2.36	0.55
25:V:21:LEU:HD13	25:V:26:ILE:HD11	1.87	0.55
1:O:1120:U:H5''	1:O:1120:U:C6	2.41	0.55
1:O:1393:A:H2'	1:O:1394:C:C6	2.42	0.55
1:O:1667:A:H2'	1:O:1668:U:C6	2.41	0.55
1:O:1730:G:C5'	1:O:1731:C:H6	2.20	0.55
1:O:2314:G:C2'	1:O:2315:C:H5'	2.36	0.55
11:H:26:LYS:HD3	11:H:89:PRO:HG3	1.89	0.55
11:H:45:GLN:HE21	11:H:135:TRP:HE1	1.55	0.55
14:K:149:ARG:O	14:K:150:GLN:HB2	2.07	0.55
1:O:1595:G:O2'	1:O:1596:U:H5'	2.07	0.55
37:O:7121:HOH:O	15:L:154:ARG:HB2	2.07	0.55
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.22	0.55
12:I:80:LYS:HE2	12:I:98:PHE:CZ	2.42	0.55
13:J:109:LEU:HD13	13:J:113:ILE:HD11	1.88	0.55
16:M:89:GLY:O	16:M:92:ALA:HB3	2.07	0.55
26:W:21:PRO:HG2	26:W:24:LYS:HD3	1.88	0.55
1:O:317:A:H5''	22:S:52:ARG:HD2	1.89	0.55
1:O:1167:G:O2'	1:O:1168:C:H5'	2.07	0.55
1:O:1189:A:H1'	1:O:1209:C:H1'	1.89	0.55
1:O:2473:U:O3'	1:O:2474:A:H3'	2.07	0.55
37:O:9073:HOH:O	5:B:267:LYS:HD3	2.04	0.55
7:D:163:VAL:HA	37:D:6326:HOH:O	2.06	0.55
1:O:88:G:N7	30:1:28:LYS:HD2	2.22	0.55
1:O:1213:C:O2'	1:O:1214:G:H5'	2.06	0.55
5:B:280:VAL:HG13	5:B:334:SER:HA	1.89	0.55
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.24	0.55
11:H:166:ASN:N	11:H:166:ASN:ND2	2.54	0.55
25:V:110:GLN:NE2	25:V:110:GLN:HA	2.22	0.55
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.36	0.55
5:B:248:ARG:O	5:B:251:VAL:CG1	2.55	0.55
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.89	0.55
11:H:45:GLN:HE21	11:H:135:TRP:NE1	2.05	0.55
11:H:71:TYR:C	11:H:73:GLN:N	2.64	0.55
15:L:69:LYS:HG2	15:L:127:LYS:HG3	1.89	0.55
18:O:13:VAL:HG21	18:O:41:ARG:HG2	1.88	0.55
25:V:125:HIS:CD2	25:V:127:GLY:H	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:212:ARG:HD2	37:X:8591:HOH:O	2.06	0.55
28:Y:30:GLU:HA	28:Y:33:HIS:HB3	1.88	0.55
1:0:1701:A:H4'	1:0:1702:U:H5''	1.88	0.55
1:0:2717:C:H2'	1:0:2718:C:H5''	1.88	0.55
7:D:11:HIS:O	7:D:12:GLU:HB3	2.07	0.55
29:Z:21:ARG:HD2	29:Z:39:PHE:HB2	1.88	0.55
1:0:738:G:H3'	37:0:6499:HOH:O	2.06	0.54
1:0:2256:G:C2'	1:0:2257:G:H5'	2.37	0.54
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.37	0.54
16:M:157:PRO:HA	37:M:8526:HOH:O	2.07	0.54
1:0:154:C:H2'	1:0:155:C:H6	1.72	0.54
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.22	0.54
37:9:8464:HOH:O	16:M:147:ILE:HD12	2.06	0.54
7:D:11:HIS:C	7:D:13:MET:H	2.15	0.54
11:H:127:GLY:O	11:H:128:ALA:HB3	2.07	0.54
16:M:47:LEU:HD12	16:M:92:ALA:HB1	1.89	0.54
27:X:178:HIS:CG	27:X:179:PRO:HD2	2.43	0.54
1:0:128:A:C8	1:0:128:A:H3'	2.41	0.54
1:0:396:U:OP2	31:2:38:ARG:NH1	2.35	0.54
1:0:629:A:C2	1:0:2074:A:C2	2.96	0.54
1:0:2353:A:O2'	16:M:7:LYS:HB3	2.07	0.54
1:0:2533:C:H5'	1:0:2533:C:C6	2.39	0.54
5:B:7:ARG:CD	5:B:9:GLY:O	2.55	0.54
6:C:236:THR:C	37:C:8444:HOH:O	2.50	0.54
8:E:93:MET:HE1	8:E:165:GLY:H	1.70	0.54
24:U:56:ILE:O	24:U:60:GLN:HG3	2.07	0.54
25:V:65:VAL:HA	25:V:68:THR:CG2	2.37	0.54
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.39	0.54
1:0:1191:A:C2	1:0:1206:U:O4	2.60	0.54
2:9:3069:U:OP1	16:M:4:PRO:HG3	2.07	0.54
5:B:27:ASN:HB3	37:B:8628:HOH:O	2.07	0.54
15:L:155:HIS:CE1	15:L:158:ARG:HE	2.24	0.54
1:0:213:G:N2	1:0:225:G:H2'	2.22	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.08	0.54
1:0:1381:A:H4'	1:0:1382:G:O5'	2.08	0.54
1:0:2004:U:H5''	1:0:2005:G:C8	2.43	0.54
1:0:2717:C:C2'	1:0:2718:C:C5'	2.86	0.54
14:K:143:THR:CG2	14:K:144:ASP:H	2.19	0.54
26:W:43:VAL:CG1	26:W:47:ALA:HB3	2.37	0.54
28:Y:38:LYS:HE2	28:Y:45:LYS:CE	2.32	0.54
2:9:3088:G:OP1	25:V:130:HIS:NE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:26:LYS:HD2	11:H:28:ILE:CG1	2.37	0.54
1:0:380:A:H5''	15:L:48:ARG:HH21	1.73	0.54
1:0:877:G:H5'	1:0:878:G:OP1	2.08	0.54
1:0:1855:G:H8	4:A:144:GLU:OE2	1.91	0.54
5:B:148:PRO:HD2	37:B:8579:HOH:O	2.08	0.54
15:L:113:ARG:NH2	15:L:156:ARG:HG2	2.23	0.54
16:M:171:HIS:CE1	37:M:8566:HOH:O	2.60	0.54
24:U:39:ALA:O	24:U:41:GLU:N	2.41	0.54
1:0:20:G:H21	20:Q:117:HIS:HD2	1.56	0.54
6:C:236:THR:O	6:C:237:GLU:C	2.49	0.54
20:Q:132:ARG:HG2	20:Q:133:ALA:N	2.23	0.54
25:V:41:TYR:O	25:V:45:VAL:HG13	2.08	0.54
1:0:371:U:H2'	1:0:372:A:C8	2.41	0.54
1:0:470:U:O2'	29:Z:16:HIS:CD2	2.59	0.54
1:0:1596:U:H2'	1:0:1598:A:OP2	2.07	0.54
2:9:3028:U:H2'	2:9:3029:C:C6	2.43	0.54
9:F:28:ALA:CB	9:F:99:THR:HG23	2.37	0.54
11:H:75:SER:HB3	11:H:79:ALA:CB	2.37	0.54
15:L:52:LEU:HD13	15:L:116:ASN:HB3	1.90	0.54
15:L:87:MET:CG	31:2:46:ILE:HG21	2.37	0.54
18:O:143:ALA:HA	37:O:5521:HOH:O	2.08	0.54
25:V:88:THR:CG2	25:V:89:ASP:H	2.16	0.54
1:0:1666:C:C2'	1:0:1667:A:H5'	2.36	0.54
22:S:73:HIS:CD2	22:S:88:PRO:HG3	2.43	0.54
30:1:22:PRO:HG2	30:1:25:VAL:HG23	1.89	0.54
1:0:244:C:OP2	9:F:38:LYS:HE3	2.09	0.53
1:0:474:C:O3'	6:C:73:LEU:HD21	2.08	0.53
1:0:694:A:H2'	1:0:695:C:H5'	1.90	0.53
1:0:2361:A:H5''	37:O:8523:HOH:O	2.08	0.53
1:0:2413:A:N7	16:M:109:PRO:HB3	2.23	0.53
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.90	0.53
13:J:132:VAL:C	37:J:3160:HOH:O	2.49	0.53
1:0:88:G:H8	1:0:88:G:H5'	1.73	0.53
1:0:262:A:H5''	1:0:264:G:O4'	2.07	0.53
1:0:875:A:C2	4:A:194:MET:SD	3.01	0.53
1:0:1116:U:O2'	1:0:1118:A:C2	2.39	0.53
1:0:1130:U:H2'	1:0:1131:G:O4'	2.08	0.53
1:0:1333:U:H2'	1:0:1334:C:C6	2.43	0.53
1:0:2472:C:O2'	1:0:2634:G:H4'	2.07	0.53
6:C:16:VAL:HG12	6:C:17:ASP:H	1.71	0.53
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:101:ASP:C	14:K:103:ALA:H	2.15	0.53
16:M:86:LEU:O	16:M:90:LEU:HG	2.09	0.53
16:M:154:LEU:HG	16:M:155:GLU:H	1.72	0.53
23:T:52:THR:HG22	23:T:54:THR:HB	1.90	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.09	0.53
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.53
1:0:2613:G:O2'	1:0:2614:C:H5'	2.09	0.53
37:O:8593:HOH:O	5:B:214:PRO:HD2	2.08	0.53
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.91	0.53
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.90	0.53
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.91	0.53
11:H:69:ASN:O	11:H:72:VAL:HG12	2.09	0.53
12:I:93:ARG:HB3	12:I:93:ARG:NH1	2.22	0.53
19:P:64:GLU:HG3	19:P:74:ASP:OD2	2.08	0.53
22:S:48:VAL:HG22	22:S:97:ARG:C	2.32	0.53
23:T:49:LEU:HD11	37:T:3805:HOH:O	2.09	0.53
24:U:39:ALA:N	24:U:40:PRO:CD	2.70	0.53
25:V:26:ILE:HG13	25:V:26:ILE:O	2.07	0.53
27:X:107:PRO:HB3	27:X:182:PHE:CE2	2.43	0.53
1:0:138:U:H5''	1:0:139:C:OP2	2.09	0.53
1:0:419:A:H1'	1:0:1921:A:C2	2.44	0.53
1:0:2251:G:H2'	1:0:2252:A:C8	2.44	0.53
1:0:2729:C:O2'	1:0:2730:G:H5'	2.09	0.53
2:9:3039:U:H1'	2:9:3044:A:N6	2.22	0.53
2:9:3078:G:N2	2:9:3103:A:OP2	2.40	0.53
5:B:248:ARG:O	5:B:251:VAL:HG13	2.09	0.53
7:D:170:TYR:O	7:D:171:ASP:HB3	2.07	0.53
12:I:107:ASN:HD22	12:I:109:TYR:H	1.55	0.53
24:U:64:GLY:O	24:U:65:ASP:CB	2.57	0.53
26:W:25:ARG:NH1	37:W:3861:HOH:O	2.42	0.53
1:0:1119:G:H8	12:I:52:GLN:NE2	2.07	0.53
1:0:2748:G:H5'	37:O:6985:HOH:O	2.07	0.53
9:F:104:ALA:HA	37:F:6617:HOH:O	2.09	0.53
25:V:122:ARG:CZ	37:V:5817:HOH:O	2.56	0.53
1:0:1500:U:P	18:O:41:ARG:HH22	2.31	0.53
1:0:2326:U:H4'	1:0:2412:G:H4'	1.91	0.53
1:0:2365:G:H4'	19:P:45:PRO:O	2.08	0.53
1:0:2415:A:C2	16:M:25:ARG:HB3	2.44	0.53
5:B:7:ARG:NH1	5:B:11:LEU:HD22	2.23	0.53
5:B:248:ARG:HG2	37:I:3517:HOH:O	2.07	0.53
5:B:280:VAL:CG1	5:B:334:SER:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:59:GLY:HA3	15:L:141:ILE:CD1	2.38	0.53
18:O:143:ALA:HA	37:O:2178:HOH:O	2.09	0.53
20:Q:106:GLY:HA2	20:Q:109:MET:CE	2.39	0.53
1:O:710:G:OP1	17:N:24:ALA:HB3	2.07	0.53
1:O:1060:C:H6	1:O:1060:C:H5'	1.74	0.53
1:O:1126:C:HO2'	1:O:1128:U:H6	1.57	0.53
1:O:1503:U:H2'	1:O:1504:A:O4'	2.09	0.53
1:O:2559:C:H4'	37:O:6706:HOH:O	2.07	0.53
4:A:171:LYS:NZ	37:A:8523:HOH:O	2.41	0.53
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.67	0.53
6:C:95:GLU:CD	6:C:95:GLU:H	2.17	0.53
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.91	0.53
6:C:234:VAL:O	6:C:234:VAL:HG22	2.09	0.53
7:D:144:ARG:NH2	37:D:3839:HOH:O	2.36	0.53
8:E:84:MET:HE1	8:E:148:ILE:HD13	1.89	0.53
11:H:28:ILE:HA	11:H:62:GLU:OE1	2.08	0.53
16:M:73:ALA:N	37:M:8566:HOH:O	2.41	0.53
17:N:25:VAL:HG23	17:N:26:TRP:N	2.24	0.53
26:W:51:ASP:OD2	26:W:52:PRO:HD2	2.09	0.53
1:O:283:U:H5	1:O:284:C:N4	2.07	0.53
1:O:656:G:OP2	17:N:37:ARG:HD2	2.08	0.53
1:O:926:A:O2'	14:K:41:HIS:HD2	1.91	0.53
1:O:2403:C:H3'	37:O:4677:HOH:O	2.09	0.53
1:O:2815:G:N7	12:I:80:LYS:NZ	2.57	0.53
9:F:101:ALA:HB2	9:F:108:LEU:CD2	2.39	0.53
11:H:26:LYS:HG2	11:H:28:ILE:N	2.19	0.53
27:X:185:VAL:HA	37:X:8556:HOH:O	2.08	0.53
1:O:558:C:H2'	1:O:559:U:C5'	2.39	0.53
2:9:3076:G:C3'	2:9:3077:A:H5''	2.36	0.53
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.91	0.53
20:Q:29:LYS:HB3	37:Q:8531:HOH:O	2.09	0.53
23:T:47:ARG:HG3	37:T:4381:HOH:O	2.08	0.53
25:V:13:MET:HE3	25:V:17:ILE:CG2	2.39	0.53
26:W:72:VAL:HG22	26:W:85:VAL:CG1	2.37	0.53
28:Y:77:LYS:HA	28:Y:80:MET:HE2	1.91	0.53
1:O:2502:C:H4'	11:H:151:MET:HG2	1.91	0.53
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.21	0.53
5:B:307:ARG:HH11	5:B:307:ARG:CB	2.22	0.53
25:V:31:HIS:HB3	37:V:5420:HOH:O	2.08	0.53
25:V:119:HIS:HD2	25:V:120:PRO:O	1.92	0.53
28:Y:26:VAL:O	28:Y:30:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.43	0.52
37:0:5780:HOH:O	7:D:55:LYS:HB2	2.09	0.52
9:F:46:GLU:N	37:F:3461:HOH:O	2.43	0.52
11:H:65:ARG:CZ	37:H:8382:HOH:O	2.57	0.52
16:M:184:ILE:HG22	16:M:185:GLU:HG3	1.90	0.52
20:Q:25:PHE:CE2	20:Q:29:LYS:HE2	2.44	0.52
22:S:53:GLY:HA3	37:S:6384:HOH:O	2.08	0.52
1:0:344:C:H2'	1:0:345:G:O4'	2.09	0.52
37:0:4981:HOH:O	5:B:298:LYS:HD3	2.08	0.52
7:D:154:LYS:H	7:D:154:LYS:CD	2.16	0.52
11:H:35:ASN:HD21	11:H:80:ASN:HA	1.74	0.52
1:0:407:A:H5'	37:0:5488:HOH:O	2.08	0.52
1:0:1840:A:H4'	1:0:1841:C:O5'	2.08	0.52
1:0:2502:C:C2'	1:0:2503:A:H5'	2.39	0.52
1:0:2502:C:C4'	11:H:151:MET:HG2	2.40	0.52
11:H:59:ASN:H	11:H:59:ASN:ND2	2.06	0.52
11:H:163:PRO:O	11:H:164:ALA:HB2	2.10	0.52
16:M:143:ARG:NH1	16:M:173:ASP:OD2	2.34	0.52
18:O:94:TRP:CZ2	18:O:98:ILE:HG13	2.45	0.52
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.52
1:0:638:C:H2'	1:0:639:A:C8	2.44	0.52
1:0:820:G:O2'	1:0:856:G:H4'	2.10	0.52
5:B:162:MET:CE	5:B:308:LEU:HD21	2.28	0.52
7:D:25:MET:HE1	7:D:37:ALA:O	2.09	0.52
7:D:135:VAL:HG22	7:D:136:ARG:N	2.24	0.52
18:O:98:ILE:HD12	18:O:102:ARG:NE	2.24	0.52
25:V:65:VAL:CA	25:V:68:THR:HG22	2.39	0.52
26:W:70:ILE:HG23	26:W:70:ILE:O	2.08	0.52
27:X:106:THR:HG23	27:X:107:PRO:HD2	1.91	0.52
29:Z:8:GLN:HE22	29:Z:11:LYS:HZ1	1.56	0.52
29:Z:25:LYS:HD2	30:1:49:GLU:H	1.74	0.52
1:0:588:G:O6	25:V:154:ARG:NH1	2.43	0.52
1:0:1086:A:N6	25:V:11:VAL:HG11	2.25	0.52
1:0:1120:U:H5'	1:0:1121:G:OP2	2.09	0.52
1:0:1450:C:O2'	1:0:1494:A:H5'	2.10	0.52
1:0:1603:A:H5''	1:0:1604:G:H3'	1.91	0.52
1:0:1996:U:O2'	1:0:1997:A:H5'	2.10	0.52
2:9:3025:G:N2	37:9:8506:HOH:O	2.42	0.52
7:D:59:GLY:C	7:D:61:PHE:H	2.18	0.52
7:D:99:ASP:HB3	7:D:103:ASN:H	1.74	0.52
16:M:11:ARG:HG3	16:M:14:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:105:LEU:CD2	18:O:137:LEU:HD21	2.39	0.52
20:Q:82:GLU:HG3	20:Q:83:LYS:N	2.24	0.52
1:O:1123:A:C6	1:O:1238:C:H5'	2.44	0.52
1:O:2781:U:C2'	1:O:2782:G:H5'	2.39	0.52
37:O:6904:HOH:O	6:C:188:ARG:CD	2.56	0.52
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.52
7:D:84:LEU:C	7:D:86:THR:H	2.17	0.52
11:H:136:VAL:HG22	11:H:137:ASN:O	2.10	0.52
16:M:159:TYR:HE2	16:M:163:PHE:HE2	1.58	0.52
25:V:76:ASP:O	25:V:77:ALA:C	2.53	0.52
27:X:189:ASN:ND2	27:X:192:ASP:H	2.08	0.52
1:O:2090:G:H2'	1:O:2091:G:C8	2.44	0.52
1:O:2251:G:H4'	37:O:6856:HOH:O	2.10	0.52
37:O:3340:HOH:O	11:H:11:LYS:HE2	2.09	0.52
2:9:3022:G:O2'	2:9:3024:U:H5'	2.09	0.52
11:H:129:ASN:HD22	11:H:129:ASN:N	2.07	0.52
14:K:120:LEU:HD12	14:K:133:VAL:HG21	1.91	0.52
18:O:121:ASP:HB2	37:O:5891:HOH:O	2.09	0.52
26:W:74:ALA:CB	26:W:85:VAL:HG22	2.40	0.52
1:O:1189:A:O2'	1:O:1208:C:H2'	2.09	0.52
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.25	0.52
1:O:2896:A:OP1	26:W:15:ARG:NH1	2.43	0.52
1:O:2897:C:H2'	1:O:2898:G:H8	1.72	0.52
2:9:3039:U:H3'	2:9:3040:C:H5''	1.91	0.52
5:B:16:ARG:NH1	37:B:8615:HOH:O	2.42	0.52
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.75	0.52
5:B:254:GLN:HG2	5:B:255:GLY:N	2.25	0.52
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.52
11:H:45:GLN:HG3	11:H:135:TRP:NE1	2.25	0.52
16:M:58:LEU:HD12	16:M:58:LEU:N	2.25	0.52
25:V:5:VAL:O	25:V:52:VAL:HG22	2.10	0.52
25:V:125:HIS:HD2	25:V:127:GLY:H	1.57	0.52
1:O:1149:U:H5''	1:O:1151:G:O4'	2.10	0.52
2:9:3055:U:H4'	2:9:3056:A:H8	1.73	0.52
10:G:12:ILE:O	10:G:12:ILE:HG22	2.09	0.52
11:H:136:VAL:HG23	37:H:8342:HOH:O	2.10	0.52
15:L:104:ARG:O	15:L:108:LYS:HG2	2.09	0.52
1:O:2064:U:H5'	1:O:2652:U:H4'	1.92	0.52
1:O:2324:G:H4'	1:O:2418:G:O2'	2.09	0.52
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.40	0.52
5:B:320:GLN:HG3	5:B:321:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:23:VAL:O	7:D:23:VAL:CG2	2.57	0.52
7:D:86:THR:HG23	37:D:7477:HOH:O	2.10	0.52
8:E:15:GLN:HG2	8:E:19:ASP:O	2.10	0.52
8:E:77:THR:OG1	8:E:78:GLU:N	2.42	0.52
18:O:10:ALA:HA	18:O:13:VAL:CG1	2.39	0.52
25:V:1:MET:HB2	25:V:103:GLU:HG2	1.92	0.52
29:Z:25:LYS:HD2	30:1:49:GLU:N	2.24	0.52
1:O:2777:G:O2'	1:O:2778:A:H5'	2.10	0.51
6:C:76:ARG:HD3	37:C:8368:HOH:O	2.09	0.51
7:D:51:ARG:HD3	37:D:7636:HOH:O	2.10	0.51
9:F:22:VAL:HG21	9:F:104:ALA:HB2	1.91	0.51
22:S:9:LYS:CE	22:S:13:ARG:NH1	2.73	0.51
1:O:834:G:H3'	1:O:835:U:H4'	1.92	0.51
1:O:1497:G:H4'	1:O:1627:G:O2'	2.10	0.51
1:O:1699:C:H4'	37:O:5899:HOH:O	2.11	0.51
1:O:1711:A:O2'	1:O:1712:A:H5'	2.10	0.51
1:O:2377:U:H6	1:O:2377:U:O5'	1.93	0.51
1:O:2474:A:N3	37:O:4136:HOH:O	2.34	0.51
1:O:2661:U:H3	1:O:2812:A:H62	1.59	0.51
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.92	0.51
10:G:12:ILE:HB	37:G:4714:HOH:O	2.09	0.51
1:O:1132:A:N6	1:O:1229:C:H2'	2.25	0.51
1:O:1173:A:H2'	37:O:3833:HOH:O	2.08	0.51
1:O:2291:A:C8	1:O:2309:C:H5'	2.45	0.51
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.10	0.51
18:O:41:ARG:O	18:O:44:VAL:HB	2.10	0.51
18:O:103:THR:O	18:O:107:GLU:HG3	2.10	0.51
31:2:18:GLN:OE1	31:2:73:GLU:HB3	2.09	0.51
1:O:1377:C:H5'	1:O:1377:C:H6	1.75	0.51
1:O:2898:G:H4'	5:B:288:GLY:HA2	1.92	0.51
23:T:47:ARG:CG	37:T:4381:HOH:O	2.58	0.51
25:V:38:THR:HG22	25:V:39:ASP:N	2.25	0.51
1:O:1192:A:C6	37:O:5509:HOH:O	2.63	0.51
1:O:1418:U:OP1	30:1:42:TRP:HB3	2.11	0.51
1:O:2781:U:H1'	8:E:139:GLU:OE2	2.11	0.51
37:O:8731:HOH:O	4:A:11:ARG:HD3	2.10	0.51
5:B:7:ARG:NH1	5:B:11:LEU:CD2	2.74	0.51
7:D:49:PRO:HG3	37:D:5828:HOH:O	2.10	0.51
11:H:57:ARG:O	11:H:61:LEU:HD22	2.10	0.51
11:H:151:MET:HA	11:H:151:MET:HE3	1.92	0.51
12:I:75:PRO:HG2	12:I:105:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
1:0:1205:U:H2'	1:0:1206:U:H5''	1.92	0.51
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.11	0.51
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.51
5:B:168:GLY:O	5:B:169:GLY:O	2.29	0.51
5:B:329:TYR:HE2	23:T:15:PRO:HG2	1.74	0.51
11:H:144:GLU:OE1	11:H:144:GLU:HA	2.10	0.51
14:K:104:ASP:HB3	37:K:8562:HOH:O	2.10	0.51
20:Q:17:MET:HE1	20:Q:19:ARG:CZ	2.40	0.51
25:V:90:TYR:N	25:V:90:TYR:CD1	2.77	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
7:D:86:THR:C	7:D:89:PRO:HD2	2.35	0.51
8:E:10:ASP:HA	37:E:3707:HOH:O	2.09	0.51
15:L:55:LYS:HB2	15:L:60:ILE:CD1	2.41	0.51
16:M:139:TRP:CE3	16:M:139:TRP:HA	2.45	0.51
1:0:1126:C:O2'	1:0:1128:U:H6	1.93	0.51
1:0:1684:A:H1'	30:1:43:ARG:HH22	1.75	0.51
1:0:2435:U:H1'	37:0:4890:HOH:O	2.10	0.51
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.93	0.51
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.75	0.51
7:D:27:ILE:HG22	7:D:28:GLY:N	2.21	0.51
9:F:101:ALA:HB2	9:F:108:LEU:HD22	1.92	0.51
11:H:83:PHE:HZ	11:H:146:TRP:HE1	1.57	0.51
15:L:72:SER:HB2	15:L:93:ARG:HG2	1.93	0.51
1:0:396:U:O2'	1:0:418:C:H4'	2.11	0.51
1:0:2005:G:H3'	1:0:2005:G:P	2.51	0.51
1:0:2502:C:H2'	1:0:2503:A:H5'	1.93	0.51
37:0:4307:HOH:O	12:I:47:THR:CB	2.55	0.51
37:9:8517:HOH:O	16:M:107:ASN:HB3	2.10	0.51
4:A:168:PRO:O	4:A:170:VAL:HG23	2.11	0.51
28:Y:13:ARG:NH1	28:Y:14:PHE:CZ	2.79	0.51
30:1:24:TRP:NE1	37:1:6863:HOH:O	2.44	0.51
1:0:513:A:N3	37:0:3160:HOH:O	2.35	0.51
1:0:1116:U:H3	1:0:1246:A:N6	2.01	0.51
1:0:2419:U:H5''	1:0:2420:G:H5'	1.93	0.51
37:0:3162:HOH:O	15:L:79:LYS:HD2	2.11	0.51
15:L:157:LEU:HB3	15:L:160:PHE:HD1	1.75	0.51
23:T:6:CYS:C	23:T:8:TYR:H	2.19	0.51
30:1:19:SER:HB3	37:1:4479:HOH:O	2.10	0.51
1:0:894:A:C2	6:C:87:ARG:NH2	2.79	0.50
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1398:G:H2'	1:0:1399:A:C8	2.46	0.50
1:0:1789:G:O6	18:O:73:HIS:HE1	1.94	0.50
1:0:2361:A:H2'	1:0:2362:A:C8	2.45	0.50
1:0:2866:U:C2	37:T:7349:HOH:O	2.55	0.50
8:E:22:VAL:O	8:E:28:SER:HA	2.11	0.50
17:N:113:VAL:O	17:N:114:ILE:HD13	2.11	0.50
25:V:88:THR:CG2	25:V:89:ASP:N	2.73	0.50
1:0:157:G:H4'	15:L:95:LYS:HE3	1.94	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.46	0.50
1:0:538:C:H5''	1:0:539:G:C8	2.46	0.50
1:0:1700:C:OP2	37:O:5497:HOH:O	2.20	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.11	0.50
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.38	0.50
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.95	0.50
7:D:57:THR:HG23	7:D:63:ILE:CB	2.41	0.50
15:L:154:ARG:HG3	37:L:8613:HOH:O	2.11	0.50
28:Y:33:HIS:HE1	28:Y:49:ARG:NE	2.09	0.50
30:1:22:PRO:HG2	30:1:25:VAL:CG2	2.41	0.50
1:0:558:C:C2'	1:0:559:U:C5'	2.89	0.50
1:0:1524:U:C4'	1:0:1525:G:O4'	2.52	0.50
1:0:1592:G:O2'	1:0:1593:C:O5'	2.30	0.50
7:D:94:ALA:O	7:D:95:THR:O	2.29	0.50
9:F:28:ALA:HB3	9:F:99:THR:HG23	1.93	0.50
11:H:47:GLU:CB	11:H:133:ILE:CD1	2.86	0.50
13:J:45:PRO:HB2	37:J:7169:HOH:O	2.12	0.50
15:L:63:VAL:HG21	15:L:109:PHE:CE1	2.46	0.50
20:Q:129:ALA:O	20:Q:130:MET:HB2	2.11	0.50
1:0:192:A:H4'	15:L:176:GLN:HE22	1.76	0.50
2:9:3031:C:O2'	2:9:3032:G:H5'	2.11	0.50
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.93	0.50
11:H:84:ARG:CZ	11:H:135:TRP:HH2	2.23	0.50
22:S:48:VAL:HG22	22:S:97:ARG:O	2.12	0.50
25:V:130:HIS:O	25:V:136:GLY:HA3	2.11	0.50
1:0:677:C:H4'	6:C:246:ARG:NH2	2.27	0.50
1:0:797:A:H5'	28:Y:10:ARG:HG2	1.94	0.50
1:0:1162:G:H2'	37:O:6038:HOH:O	2.12	0.50
1:0:1504:A:H5'	37:O:3898:HOH:O	2.12	0.50
7:D:58:VAL:HG12	7:D:59:GLY:N	2.26	0.50
7:D:99:ASP:O	7:D:159:PRO:HG3	2.11	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.21	0.50
11:H:65:ARG:NH1	37:H:8382:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:37:VAL:CG1	15:L:63:VAL:HG11	2.41	0.50
21:R:57:THR:C	21:R:59:ASP:H	2.19	0.50
1:0:566:A:H2'	1:0:567:U:O4'	2.12	0.50
1:0:625:U:H5''	1:0:1044:C:N4	2.26	0.50
1:0:1477:C:H5'	1:0:1868:G:C5'	2.42	0.50
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.50
1:0:2266:A:H2'	1:0:2267:G:C8	2.47	0.50
1:0:2687:G:O2'	1:0:2688:U:H5'	2.11	0.50
7:D:57:THR:HG23	7:D:63:ILE:CG2	2.40	0.50
13:J:106:GLY:HA3	37:J:5264:HOH:O	2.10	0.50
14:K:72:ASN:HB2	37:K:8579:HOH:O	2.11	0.50
15:L:67:ILE:CD1	15:L:104:ARG:HD2	2.42	0.50
15:L:164:THR:HB	37:L:8519:HOH:O	2.12	0.50
16:M:82:TYR:C	16:M:82:TYR:CD2	2.90	0.50
16:M:143:ARG:HH12	16:M:173:ASP:CG	2.18	0.50
16:M:170:GLU:O	16:M:174:GLU:HG3	2.11	0.50
19:P:32:GLU:HA	19:P:71:TYR:OH	2.11	0.50
20:Q:18:LEU:HD12	20:Q:143:VAL:CG1	2.42	0.50
20:Q:29:LYS:HD3	37:Q:8531:HOH:O	2.11	0.50
1:0:321:A:H1'	37:0:6484:HOH:O	2.12	0.50
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.50
4:A:105:VAL:HG13	4:A:155:THR:O	2.11	0.50
10:G:71:LEU:C	10:G:73:ASP:H	2.19	0.50
11:H:147:ARG:HA	11:H:150:LYS:NZ	2.27	0.50
12:I:45:VAL:HG21	12:I:129:PHE:CD1	2.47	0.50
27:X:109:LEU:HA	37:X:8563:HOH:O	2.10	0.50
31:2:65:THR:HB	31:2:83:TRP:H	1.76	0.50
1:0:332:G:O2'	1:0:333:G:H5'	2.12	0.50
1:0:558:C:C2'	1:0:559:U:H5''	2.42	0.50
1:0:603:A:H4'	1:0:604:G:O5'	2.10	0.50
1:0:818:A:O2'	28:Y:13:ARG:HD3	2.12	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.50
1:0:2115:U:H2'	1:0:2116:U:C6	2.47	0.50
1:0:2359:G:N7	37:0:3200:HOH:O	2.35	0.50
4:A:69:LEU:C	4:A:69:LEU:HD12	2.36	0.50
5:B:279:THR:CG2	5:B:280:VAL:N	2.74	0.50
11:H:84:ARG:CZ	11:H:135:TRP:CH2	2.95	0.50
18:O:59:ARG:HH22	18:O:66:GLN:HE22	1.57	0.50
21:R:81:ILE:HG12	37:R:8336:HOH:O	2.11	0.50
22:S:50:VAL:HG12	22:S:56:ALA:HA	1.93	0.50
25:V:38:THR:HG22	37:V:3580:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:136:C:H2'	1:0:137:U:O4'	2.11	0.50
1:0:1182:C:O2	1:0:1192:A:H5''	2.12	0.50
1:0:1189:A:H3'	37:0:7122:HOH:O	2.12	0.50
1:0:1563:G:O2'	1:0:1564:C:OP2	2.29	0.50
1:0:1593:C:OP1	18:O:117:SER:HB3	2.12	0.50
7:D:41:LEU:CA	7:D:44:ILE:HG22	2.41	0.50
11:H:55:GLN:HE22	11:H:91:HIS:CD2	2.30	0.50
13:J:101:ASN:O	13:J:102:GLU:HB2	2.12	0.50
20:Q:18:LEU:HB2	20:Q:143:VAL:CG1	2.41	0.50
31:2:11:CYS:HB2	31:2:20:HIS:CE1	2.47	0.50
31:2:87:ARG:NH1	37:2:8520:HOH:O	2.44	0.50
1:0:1015:C:H2'	1:0:1016:U:C6	2.47	0.49
1:0:1745:G:O2'	1:0:2032:U:O4	2.29	0.49
1:0:2635:A:O2'	1:0:2636:C:H5'	2.11	0.49
5:B:258:GLY:N	5:B:260:HIS:CE1	2.79	0.49
9:F:26:THR:HB	9:F:102:GLY:HA3	1.94	0.49
13:J:27:ARG:HD2	37:J:4747:HOH:O	2.12	0.49
16:M:182:GLY:N	37:M:8570:HOH:O	2.44	0.49
28:Y:30:GLU:HA	28:Y:33:HIS:CB	2.43	0.49
1:0:2314:G:H2'	1:0:2315:C:H5'	1.94	0.49
1:0:2316:G:O2'	1:0:2462:G:O6	2.30	0.49
2:9:3023:U:C4'	2:9:3024:U:OP2	2.41	0.49
2:9:3107:C:H5	37:9:8436:HOH:O	1.91	0.49
3:3:1:G:O2'	3:3:2:C:H5'	2.11	0.49
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.94	0.49
9:F:100:ASP:HB3	37:F:5691:HOH:O	2.12	0.49
12:I:45:VAL:HG22	12:I:46:ILE:N	2.26	0.49
16:M:180:LEU:O	16:M:181:ASP:HB3	2.11	0.49
21:R:33:SER:OG	21:R:36:GLU:HG3	2.12	0.49
1:0:588:G:O2'	1:0:589:U:OP2	2.29	0.49
1:0:1116:U:HO2'	1:0:1118:A:H2	0.71	0.49
1:0:1120:U:H5''	1:0:1120:U:H6	1.77	0.49
1:0:2730:G:O2'	1:0:2731:G:H5'	2.12	0.49
37:0:3479:HOH:O	22:S:82:THR:HA	2.12	0.49
6:C:27:ARG:NH1	6:C:27:ARG:HG2	2.27	0.49
13:J:34:VAL:CG2	13:J:47:ALA:HB2	2.41	0.49
37:J:7438:HOH:O	23:T:20:MET:HE1	2.10	0.49
14:K:112:GLY:O	14:K:132:LYS:NZ	2.44	0.49
15:L:35:PRO:HD2	15:L:38:VAL:HG21	1.93	0.49
16:M:22:GLN:HG2	16:M:26:LEU:HD22	1.93	0.49
16:M:37:ARG:CZ	37:M:8534:HOH:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:25:VAL:HG23	17:N:26:TRP:H	1.77	0.49
26:W:25:ARG:HG2	37:W:5356:HOH:O	2.11	0.49
1:O:1098:A:H2'	1:O:1099:G:O4'	2.12	0.49
1:O:1166:A:H61	1:O:1180:U:H3	1.59	0.49
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.11	0.49
13:J:58:THR:HG22	13:J:59:LYS:HG3	1.93	0.49
15:L:61:ILE:HA	37:L:8623:HOH:O	2.12	0.49
15:L:185:PRO:HG2	15:L:189:VAL:HG11	1.95	0.49
16:M:154:LEU:O	16:M:155:GLU:CB	2.61	0.49
20:Q:23:MET:HE3	20:Q:28:SER:OG	2.12	0.49
20:Q:132:ARG:NH1	37:Q:8580:HOH:O	2.46	0.49
22:S:37:GLN:OE1	22:S:118:SER:HA	2.12	0.49
1:O:316:A:H5'	22:S:54:ASP:OD2	2.12	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
1:O:2721:U:H4'	13:J:87:ARG:HG3	1.95	0.49
1:O:2780:C:H2'	1:O:2781:U:C6	2.48	0.49
37:O:6677:HOH:O	15:L:13:LYS:HE2	2.13	0.49
4:A:135:VAL:N	37:A:8596:HOH:O	2.44	0.49
4:A:179:MET:HG2	4:A:186:TRP:CB	2.43	0.49
5:B:7:ARG:HG2	5:B:7:ARG:NH1	2.22	0.49
26:W:76:ARG:HG3	26:W:76:ARG:NH1	2.25	0.49
1:O:1470:A:OP1	15:L:93:ARG:HD2	2.13	0.49
1:O:1940:C:H4'	37:O:6792:HOH:O	2.12	0.49
1:O:2481:G:C3'	1:O:2482:G:H5''	2.42	0.49
1:O:2524:G:H21	1:O:2526:C:N4	2.10	0.49
1:O:2791:U:H4'	1:O:2792:A:O5'	2.13	0.49
37:O:6904:HOH:O	6:C:188:ARG:HD2	2.13	0.49
5:B:305:ASP:O	5:B:306:LYS:HB2	2.12	0.49
7:D:95:THR:C	7:D:97:GLN:N	2.67	0.49
7:D:149:ARG:NH1	37:D:3066:HOH:O	2.32	0.49
13:J:29:LEU:HB3	13:J:55:VAL:CG1	2.31	0.49
13:J:55:VAL:HG12	13:J:56:SER:H	1.77	0.49
13:J:125:ALA:C	13:J:127:ALA:H	2.20	0.49
21:R:56:ASN:O	30:1:8:LYS:HE2	2.13	0.49
26:W:76:ARG:O	26:W:77:PHE:HB3	2.12	0.49
1:O:1878:G:O2'	1:O:1879:U:O5'	2.30	0.49
1:O:1947:G:N2	1:O:1966:U:C2	2.81	0.49
1:O:2387:U:H2'	1:O:2388:C:C6	2.48	0.49
2:9:3025:G:H2'	37:9:8460:HOH:O	2.12	0.49
2:9:3029:C:C2'	2:9:3030:C:H5'	2.43	0.49
7:D:19:GLU:O	7:D:133:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:14:TYR:N	11:H:91:HIS:HE1	2.10	0.49
12:I:75:PRO:HD3	12:I:136:SER:OG	2.13	0.49
16:M:182:GLY:O	16:M:183:ASP:O	2.30	0.49
22:S:41:ARG:NH1	22:S:42:VAL:O	2.46	0.49
1:0:766:A:O2'	1:0:767:A:H5''	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
2:9:3107:C:C5	37:9:8436:HOH:O	2.55	0.49
5:B:7:ARG:HD3	5:B:9:GLY:O	2.13	0.49
5:B:62:ARG:CB	5:B:65:MET:HE3	2.43	0.49
11:H:26:LYS:HD3	11:H:89:PRO:CG	2.43	0.49
22:S:38:ARG:NH1	22:S:38:ARG:HG3	2.26	0.49
22:S:38:ARG:HG3	22:S:38:ARG:HH11	1.78	0.49
25:V:139:GLY:O	25:V:141:HIS:CD2	2.64	0.49
26:W:15:ARG:HB3	26:W:15:ARG:NH1	2.27	0.49
28:Y:57:CYS:SG	28:Y:59:HIS:HB3	2.53	0.49
1:0:383:A:H4'	37:0:4793:HOH:O	2.13	0.49
1:0:1751:G:H2'	1:0:1752:G:C5'	2.33	0.49
1:0:2265:U:H2'	1:0:2266:A:H8	1.77	0.49
1:0:2756:U:N3	1:0:2896:A:H2	2.10	0.49
1:0:2834:G:OP1	26:W:39:LYS:HE2	2.12	0.49
4:A:96:LEU:HD22	4:A:128:LEU:HD13	1.93	0.49
6:C:237:GLU:N	37:C:8444:HOH:O	2.45	0.49
7:D:99:ASP:HB2	7:D:103:ASN:H	1.78	0.49
10:G:64:ASN:O	10:G:68:GLU:HG3	2.13	0.49
12:I:70:PHE:CD2	12:I:70:PHE:O	2.66	0.49
25:V:141:HIS:HB2	25:V:146:ILE:HG12	1.94	0.49
28:Y:59:HIS:HA	37:Y:8441:HOH:O	2.12	0.49
1:0:80:A:H3'	22:S:43:ASN:OD1	2.12	0.49
1:0:1176:C:H1'	37:0:3424:HOH:O	2.13	0.49
1:0:1180:U:H2'	1:0:1181:A:O4'	2.12	0.49
1:0:2363:G:O2'	19:P:11:ARG:HG3	2.13	0.49
5:B:241:PRO:HD2	37:B:8659:HOH:O	2.13	0.49
9:F:107:VAL:O	9:F:111:ILE:HG13	2.12	0.49
15:L:78:ASN:C	15:L:79:LYS:HG2	2.38	0.49
16:M:154:LEU:HG	16:M:155:GLU:N	2.27	0.49
22:S:52:ARG:HB2	22:S:95:ASN:HB3	1.95	0.49
22:S:65:VAL:HG22	22:S:72:ILE:HG22	1.95	0.49
25:V:22:GLU:HG2	25:V:27:HIS:CD2	2.48	0.49
25:V:90:TYR:CE2	25:V:99:ALA:HB2	2.48	0.49
26:W:15:ARG:HH11	26:W:15:ARG:CB	2.24	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2904:U:H4'	26:W:8:ARG:NH1	2.27	0.48
5:B:55:ASN:HB3	5:B:64:GLY:H	1.78	0.48
5:B:274:GLU:HA	5:B:292:GLY:O	2.13	0.48
14:K:17:SER:C	14:K:19:LYS:H	2.21	0.48
15:L:47:ASP:CG	15:L:48:ARG:N	2.71	0.48
20:Q:119:VAL:HG21	20:Q:142:ASP:CG	2.38	0.48
1:0:1015:C:H2'	1:0:1016:U:H6	1.77	0.48
1:0:1266:U:H4'	27:X:115:ARG:HH21	1.76	0.48
1:0:1333:U:H2'	1:0:1334:C:H6	1.78	0.48
1:0:1406:A:N1	37:0:5497:HOH:O	2.35	0.48
37:0:5655:HOH:O	30:1:44:ARG:HG2	2.12	0.48
2:9:3064:C:H2'	2:9:3065:A:H5'	1.95	0.48
5:B:145:HIS:CD2	5:B:146:THR:O	2.63	0.48
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.13	0.48
8:E:36:PRO:HD3	12:I:127:ILE:HD12	1.95	0.48
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.48
11:H:149:ALA:C	11:H:151:MET:H	2.20	0.48
11:H:165:GLY:C	11:H:166:ASN:HD22	2.21	0.48
12:I:26:VAL:HG13	12:I:36:VAL:HG11	1.94	0.48
15:L:35:PRO:HD2	15:L:38:VAL:CG2	2.43	0.48
16:M:23:ARG:NH1	37:M:8547:HOH:O	2.46	0.48
19:P:93:ARG:HH11	19:P:93:ARG:HG3	1.77	0.48
27:X:144:ARG:NH2	37:X:8601:HOH:O	2.46	0.48
1:0:776:A:OP1	29:Z:28:HIS:HE1	1.97	0.48
1:0:2717:C:H2'	1:0:2718:C:H5'	1.93	0.48
4:A:194:MET:CE	4:A:199:HIS:HB2	2.39	0.48
20:Q:119:VAL:O	20:Q:119:VAL:CG1	2.61	0.48
22:S:45:GLY:C	37:S:3851:HOH:O	2.56	0.48
28:Y:23:ARG:NH1	37:Y:8404:HOH:O	2.45	0.48
1:0:559:U:H2'	1:0:560:C:O4'	2.14	0.48
1:0:812:A:H1'	37:0:3451:HOH:O	2.12	0.48
1:0:1543:G:N1	1:0:1641:A:OP2	2.36	0.48
5:B:177:HIS:O	5:B:181:ILE:HG13	2.14	0.48
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.39	0.48
6:C:39:GLN:O	6:C:43:LYS:HD3	2.14	0.48
7:D:94:ALA:HB3	7:D:174:VAL:HA	1.96	0.48
11:H:47:GLU:HG2	11:H:133:ILE:HD12	1.94	0.48
12:I:131:THR:HG22	12:I:133:GLY:N	2.27	0.48
14:K:77:ALA:HB3	37:K:8532:HOH:O	2.12	0.48
16:M:38:LYS:HD2	16:M:114:LYS:HE3	1.94	0.48
21:R:29:ASP:OD1	21:R:31:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:858:U:H2'	1:0:859:C:C6	2.48	0.48
1:0:2408:A:H2	37:2:8514:HOH:O	1.96	0.48
37:0:4043:HOH:O	6:C:50:GLU:HG2	2.12	0.48
5:B:51:VAL:HG23	5:B:329:TYR:O	2.14	0.48
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.78	0.48
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.48
7:D:146:LYS:HE2	16:M:107:ASN:ND2	2.29	0.48
24:U:11:MET:HB3	24:U:15:GLU:HB2	1.95	0.48
25:V:21:LEU:HB3	25:V:26:ILE:CG1	2.43	0.48
28:Y:34:LYS:HE2	37:Y:8426:HOH:O	2.13	0.48
1:0:820:G:C6	4:A:171:LYS:HB2	2.49	0.48
1:0:825:U:H5''	1:0:826:U:OP1	2.13	0.48
1:0:1453:G:N2	1:0:1675:C:C2	2.81	0.48
1:0:1524:U:H4'	1:0:1525:G:C1'	2.41	0.48
1:0:1878:G:C1'	37:0:5583:HOH:O	2.55	0.48
5:B:205:VAL:O	5:B:307:ARG:NE	2.46	0.48
8:E:11:VAL:CG1	8:E:12:ASP:N	2.76	0.48
9:F:107:VAL:HG23	37:F:6617:HOH:O	2.13	0.48
14:K:148:GLU:HB2	37:K:8587:HOH:O	2.13	0.48
16:M:167:ASP:O	16:M:168:LEU:HD23	2.14	0.48
1:0:1787:C:OP1	18:O:68:LYS:HE2	2.13	0.48
2:9:3065:A:O2'	2:9:3066:G:OP2	2.32	0.48
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.42	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.81	0.48
11:H:137:ASN:O	11:H:139:ASP:N	2.46	0.48
15:L:115:LEU:HD13	15:L:116:ASN:HB2	1.95	0.48
25:V:38:THR:HB	37:V:5390:HOH:O	2.14	0.48
1:0:189:A:OP1	15:L:171:ARG:NH2	2.45	0.48
1:0:1087:G:H4'	1:0:1088:A:OP1	2.14	0.48
1:0:1214:G:O2'	1:0:1215:A:H8	1.96	0.48
1:0:2594:C:O2'	1:0:2595:U:H5'	2.13	0.48
9:F:78:GLU:HG3	37:F:5966:HOH:O	2.13	0.48
9:F:91:VAL:CG1	9:F:92:GLY:N	2.73	0.48
17:N:21:SER:OG	17:N:106:PRO:HB2	2.13	0.48
25:V:1:MET:HE3	25:V:101:LEU:HA	1.95	0.48
25:V:38:THR:HG22	25:V:39:ASP:H	1.79	0.48
1:0:775:G:OP1	29:Z:16:HIS:HE1	1.97	0.48
1:0:2359:G:H3'	37:0:5152:HOH:O	2.14	0.48
6:C:150:THR:HA	6:C:203:ALA:O	2.14	0.48
11:H:48:LEU:HD13	11:H:146:TRP:HB3	1.95	0.48
13:J:28:GLU:HB3	13:J:59:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:34:VAL:HB	37:J:7169:HOH:O	2.14	0.48
26:W:43:VAL:CG1	26:W:44:ASP:N	2.76	0.48
1:0:1058:A:H2'	1:0:1060:C:C5'	2.44	0.48
1:0:1205:U:O2'	1:0:1206:U:H5''	2.13	0.48
1:0:1218:U:H2'	1:0:1219:U:C6	2.49	0.48
1:0:2781:U:O2'	1:0:2782:G:H5'	2.14	0.48
37:0:9455:HOH:O	26:W:23:HIS:HD2	1.96	0.48
5:B:156:LYS:HE3	37:B:8633:HOH:O	2.13	0.48
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.44	0.48
7:D:67:ASP:O	7:D:69:ILE:HG13	2.14	0.48
10:G:12:ILE:CD1	37:G:692:HOH:O	2.58	0.48
1:0:396:U:HO2'	1:0:397:A:P	2.37	0.47
1:0:920:C:H5'	1:0:921:G:C4	2.49	0.47
1:0:1164:U:C4'	1:0:1165:G:OP1	2.53	0.47
2:9:3002:U:C4'	37:9:8477:HOH:O	2.61	0.47
2:9:3049:G:O2'	2:9:3050:G:H5'	2.14	0.47
5:B:144:THR:HG22	5:B:145:HIS:N	2.28	0.47
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.43	0.47
11:H:71:TYR:O	11:H:73:GLN:N	2.47	0.47
16:M:100:ALA:O	16:M:129:ILE:HG23	2.13	0.47
23:T:17:THR:HG22	23:T:18:GLY:N	2.29	0.47
27:X:187:VAL:HG23	27:X:192:ASP:HB3	1.92	0.47
28:Y:11:THR:HG21	28:Y:23:ARG:HB2	1.95	0.47
1:0:154:C:P	15:L:188:ARG:HH12	2.37	0.47
1:0:960:G:N3	1:0:960:G:C2'	2.76	0.47
1:0:1029:U:H5''	1:0:1031:G:N7	2.29	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.96	0.47
1:0:1862:C:H1'	37:0:6669:HOH:O	2.13	0.47
1:0:2241:C:O2'	1:0:2242:U:H5'	2.14	0.47
1:0:2720:C:O2	13:J:87:ARG:NH2	2.47	0.47
2:9:3020:G:O2'	2:9:3021:G:H5'	2.14	0.47
4:A:53:ALA:HB3	37:A:8605:HOH:O	2.15	0.47
4:A:105:VAL:CG1	4:A:106:CYS:N	2.77	0.47
5:B:54:VAL:O	5:B:55:ASN:C	2.55	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
11:H:35:ASN:ND2	11:H:79:ALA:O	2.47	0.47
11:H:86:ARG:NH1	11:H:130:HIS:CD2	2.82	0.47
15:L:165:SER:HB3	37:L:8532:HOH:O	2.14	0.47
16:M:163:PHE:HE1	16:M:171:HIS:HD1	1.62	0.47
18:O:18:LYS:O	18:O:21:VAL:HG22	2.14	0.47
21:R:57:THR:HG22	21:R:59:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:55:PHE:HB2	37:S:6384:HOH:O	2.13	0.47
1:0:764:C:C2'	1:0:765:G:H5'	2.43	0.47
1:0:949:U:O2'	19:P:40:HIS:HE1	1.98	0.47
1:0:1170:U:C2	1:0:1172:G:OP2	2.67	0.47
1:0:1500:U:OP2	18:O:41:ARG:NH2	2.47	0.47
1:0:1768:C:H2'	1:0:1769:C:O4'	2.14	0.47
1:0:1878:G:H2'	37:0:9758:HOH:O	2.13	0.47
1:0:2379:G:N7	1:0:2408:A:N1	2.61	0.47
4:A:109:GLU:HG2	4:A:116:GLY:N	2.29	0.47
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.38	0.47
5:B:221:GLN:HE22	13:J:42:ASN:ND2	2.04	0.47
14:K:125:PHE:CZ	14:K:140:VAL:HG13	2.49	0.47
22:S:43:ASN:C	22:S:45:GLY:H	2.22	0.47
26:W:30:MET:HE3	26:W:55:ASN:OD1	2.14	0.47
27:X:189:ASN:CA	27:X:217:ILE:HD11	2.42	0.47
1:0:484:A:N1	1:0:506:G:H4'	2.29	0.47
1:0:2276:U:H2'	1:0:2277:U:C6	2.49	0.47
5:B:243:ASN:HA	5:B:244:PRO:C	2.38	0.47
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.95	0.47
7:D:27:ILE:HD11	7:D:37:ALA:CB	2.44	0.47
7:D:81:GLU:O	7:D:85:GLN:HG3	2.15	0.47
8:E:157:LYS:NZ	37:E:2401:HOH:O	2.47	0.47
23:T:33:SER:O	23:T:37:GLU:HG3	2.14	0.47
1:0:236:A:H4'	1:0:237:G:C5'	2.35	0.47
1:0:289:G:O2'	1:0:290:C:H5'	2.14	0.47
1:0:844:A:C6	1:0:882:A:C5	3.02	0.47
1:0:1878:G:C4'	37:0:5583:HOH:O	2.62	0.47
1:0:1882:C:O2'	1:0:2012:U:OP2	2.30	0.47
1:0:2679:G:H2'	1:0:2681:A:OP2	2.13	0.47
2:9:3042:C:O2	7:D:76:ARG:NH1	2.48	0.47
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.77	0.47
4:A:179:MET:HA	4:A:179:MET:HE3	1.96	0.47
6:C:180:SER:N	37:C:8376:HOH:O	2.48	0.47
7:D:173:GLU:O	7:D:174:VAL:C	2.57	0.47
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.45	0.47
15:L:156:ARG:NH1	37:L:8557:HOH:O	2.47	0.47
16:M:62:HIS:HB3	16:M:65:ASP:OD1	2.14	0.47
17:N:96:VAL:HG13	17:N:100:GLN:HB2	1.96	0.47
20:Q:132:ARG:NH2	37:Q:8580:HOH:O	2.48	0.47
31:2:74:CYS:N	37:2:8549:HOH:O	2.47	0.47
1:0:2781:U:H2'	1:0:2782:G:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2832:C:H5	37:0:6663:HOH:O	1.97	0.47
5:B:72:THR:O	37:B:8604:HOH:O	2.20	0.47
6:C:33:LYS:HE2	37:C:8361:HOH:O	2.15	0.47
6:C:219:ASN:O	6:C:222:ASP:OD1	2.32	0.47
7:D:153:THR:HG22	37:D:5234:HOH:O	2.14	0.47
11:H:13:ALA:HA	11:H:91:HIS:HE1	1.78	0.47
11:H:139:ASP:N	11:H:140:PRO:CD	2.76	0.47
15:L:164:THR:HG23	15:L:165:SER:H	1.77	0.47
26:W:26:ALA:HB1	26:W:59:TRP:CE2	2.49	0.47
27:X:151:SER:HB3	27:X:154:ARG:HB3	1.95	0.47
1:0:130:C:H5'	37:0:4679:HOH:O	2.13	0.47
1:0:240:C:O2	1:0:240:C:H2'	2.15	0.47
1:0:702:G:O2'	1:0:703:G:H5'	2.15	0.47
1:0:941:G:O2'	1:0:942:U:H5'	2.15	0.47
1:0:1351:G:H1'	37:0:3543:HOH:O	2.14	0.47
1:0:1656:A:H2'	1:0:1657:A:O4'	2.15	0.47
1:0:1878:G:H4'	37:0:5583:HOH:O	2.14	0.47
1:0:1923:G:H4'	31:2:31:THR:O	2.15	0.47
1:0:2897:C:O2'	1:0:2898:G:H5'	2.15	0.47
37:0:4869:HOH:O	4:A:164:ARG:NE	2.47	0.47
37:0:5709:HOH:O	23:T:56:ARG:HD3	2.14	0.47
37:0:7149:HOH:O	6:C:94:THR:HG21	2.15	0.47
4:A:211:LYS:HD3	37:A:8610:HOH:O	2.13	0.47
5:B:84:LEU:HD13	5:B:84:LEU:O	2.14	0.47
9:F:1:PRO:HB2	37:F:5897:HOH:O	2.14	0.47
10:G:67:LEU:O	10:G:71:LEU:HG	2.15	0.47
14:K:90:ARG:NH1	14:K:119:THR:HG21	2.30	0.47
21:R:57:THR:CG2	21:R:58:MET:N	2.77	0.47
25:V:122:ARG:NH2	37:V:4276:HOH:O	2.39	0.47
1:0:128:A:O2'	1:0:129:A:H5'	2.15	0.47
1:0:240:C:H4'	15:L:146:GLN:NE2	2.30	0.47
1:0:820:G:C5	4:A:171:LYS:HB2	2.50	0.47
1:0:1791:U:O2'	1:0:1792:C:H5'	2.15	0.47
1:0:2349:G:OP1	7:D:20:LYS:NZ	2.38	0.47
10:G:12:ILE:HG13	37:G:6833:HOH:O	2.14	0.47
15:L:52:LEU:HD13	15:L:116:ASN:CG	2.38	0.47
1:0:128:A:H3'	1:0:128:A:H8	1.80	0.47
1:0:512:G:O3'	1:0:513:A:H8	1.97	0.47
1:0:631:A:C6	1:0:2074:A:H5'	2.50	0.47
1:0:1669:A:H2'	1:0:1670:G:H8	1.79	0.47
1:0:2094:G:H4'	5:B:245:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2563:U:H2'	1:0:2565:C:O5'	2.14	0.47
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.47
1:0:2657:G:OP1	5:B:17:LYS:HB2	2.15	0.47
1:0:2900:G:H2'	1:0:2901:C:O4'	2.15	0.47
5:B:23:THR:HG23	5:B:162:MET:HE3	1.97	0.47
5:B:275:GLY:O	5:B:291:ASP:HA	2.15	0.47
6:C:13:ASP:N	37:C:8437:HOH:O	2.48	0.47
16:M:67:ALA:HA	16:M:71:TRP:H	1.79	0.47
22:S:80:GLU:OE2	22:S:84:GLY:HA2	2.15	0.47
1:0:151:A:C2	1:0:442:A:C8	3.03	0.47
1:0:858:U:H2'	1:0:859:C:H6	1.80	0.47
1:0:1527:A:H1'	1:0:1528:A:C8	2.50	0.47
1:0:1804:A:H2'	1:0:1805:G:C8	2.49	0.47
1:0:2890:A:H1'	23:T:56:ARG:HH21	1.79	0.47
5:B:82:VAL:O	5:B:82:VAL:CG1	2.61	0.47
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.28	0.47
7:D:102:GLY:O	7:D:134:LEU:HD12	2.15	0.47
8:E:21:THR:HG23	8:E:30:THR:OG1	2.15	0.47
11:H:26:LYS:CD	11:H:28:ILE:HB	2.45	0.47
16:M:37:ARG:HA	16:M:37:ARG:HD3	1.82	0.47
19:P:25:PRO:HB2	37:P:4350:HOH:O	2.13	0.47
22:S:41:ARG:HG2	22:S:41:ARG:HH11	1.80	0.47
22:S:49:GLU:OE2	22:S:97:ARG:HD2	2.15	0.47
1:0:877:G:H3'	37:0:9614:HOH:O	2.15	0.46
1:0:1666:C:O2'	1:0:1667:A:C5'	2.58	0.46
1:0:1878:G:H5''	37:0:4633:HOH:O	2.13	0.46
1:0:2274:A:H1'	15:L:86:MET:SD	2.55	0.46
5:B:41:PHE:CE1	5:B:79:MET:HG3	2.49	0.46
7:D:146:LYS:CE	16:M:107:ASN:ND2	2.78	0.46
8:E:162:PHE:N	8:E:162:PHE:CD1	2.82	0.46
12:I:130:VAL:CG1	12:I:131:THR:N	2.77	0.46
13:J:82:ARG:HH21	13:J:115:ARG:HG2	1.76	0.46
15:L:49:ALA:C	15:L:54:TYR:HB3	2.40	0.46
1:0:926:A:O2'	14:K:41:HIS:CD2	2.69	0.46
1:0:1593:C:OP1	18:O:117:SER:CB	2.63	0.46
1:0:1857:A:N6	1:0:2247:C:H1'	2.30	0.46
1:0:2761:A:C4	1:0:2763:G:C8	3.03	0.46
4:A:48:ASP:HB3	37:A:8605:HOH:O	2.16	0.46
4:A:199:HIS:CD2	4:A:201:PHE:HB2	2.49	0.46
6:C:104:ASP:O	6:C:108:GLN:HG3	2.16	0.46
7:D:59:GLY:O	7:D:61:PHE:N	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.45	0.46
11:H:86:ARG:HD3	11:H:130:HIS:HD2	1.80	0.46
11:H:109:ASP:HB2	37:H:8345:HOH:O	2.15	0.46
15:L:77:PHE:HD2	37:L:8526:HOH:O	1.98	0.46
27:X:112:GLU:OE2	27:X:115:ARG:NH1	2.49	0.46
1:O:1139:U:H2'	1:O:1140:C:C6	2.50	0.46
1:O:1236:A:H2'	1:O:1237:U:O4'	2.16	0.46
1:O:1268:C:O2'	27:X:169:ARG:HB2	2.15	0.46
1:O:1450:C:H2'	1:O:1494:A:H5'	1.97	0.46
1:O:2004:U:H2'	1:O:2004:U:O2	2.14	0.46
3:3:1:G:C2'	3:3:2:C:H5'	2.45	0.46
5:B:60:SER:C	5:B:62:ARG:H	2.23	0.46
25:V:26:ILE:O	25:V:26:ILE:CG1	2.63	0.46
25:V:88:THR:CG2	25:V:110:GLN:NE2	2.72	0.46
1:O:2626:C:H2'	1:O:2627:G:C8	2.51	0.46
1:O:2717:C:OP1	5:B:207:LYS:HG3	2.15	0.46
37:O:9047:HOH:O	18:O:81:LYS:HG2	2.15	0.46
5:B:7:ARG:CG	5:B:7:ARG:NH1	2.75	0.46
7:D:23:VAL:HG23	7:D:41:LEU:HD22	1.97	0.46
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.45	0.46
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.45	0.46
11:H:46:VAL:O	11:H:146:TRP:CH2	2.66	0.46
15:L:45:ARG:CZ	15:L:48:ARG:HG3	2.46	0.46
16:M:67:ALA:C	16:M:69:TYR:N	2.74	0.46
20:Q:18:LEU:HG	20:Q:91:LEU:HD13	1.97	0.46
22:S:113:GLU:O	22:S:114:SER:C	2.58	0.46
24:U:5:VAL:CG1	24:U:9:ARG:NH1	2.79	0.46
28:Y:46:LYS:NZ	37:Y:8441:HOH:O	2.46	0.46
1:O:183:A:C5'	15:L:157:LEU:HD12	2.44	0.46
1:O:314:G:N2	1:O:316:A:H3'	2.30	0.46
1:O:795:G:O2'	1:O:817:G:N2	2.40	0.46
1:O:1535:G:H2'	1:O:1536:C:C6	2.51	0.46
1:O:1972:U:H2'	1:O:1973:A:C5'	2.46	0.46
6:C:127:ARG:HG2	6:C:127:ARG:NH1	2.31	0.46
7:D:65:GLU:HA	37:D:6752:HOH:O	2.14	0.46
9:F:34:ASN:HA	15:L:4:ALA:HB2	1.97	0.46
14:K:61:ALA:HA	37:K:8562:HOH:O	2.16	0.46
15:L:38:VAL:O	15:L:63:VAL:HG13	2.15	0.46
15:L:146:GLN:NE2	37:L:8643:HOH:O	2.48	0.46
15:L:169:ARG:HD2	37:L:8589:HOH:O	2.15	0.46
19:P:93:ARG:HG3	19:P:93:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:32:ALA:HA	21:R:36:GLU:OE1	2.15	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
2:9:3008:G:O6	16:M:11:ARG:NH1	2.47	0.46
5:B:79:MET:HE3	5:B:144:THR:HG21	1.98	0.46
7:D:63:ILE:C	37:D:5728:HOH:O	2.58	0.46
10:G:12:ILE:O	10:G:13:PRO:C	2.58	0.46
11:H:157:ILE:HG22	11:H:158:ASN:N	2.31	0.46
13:J:87:ARG:CZ	37:J:4854:HOH:O	2.63	0.46
20:Q:39:THR:CG2	20:Q:42:GLU:HG3	2.45	0.46
22:S:19:ARG:HD3	22:S:67:LEU:O	2.15	0.46
29:Z:1:THR:HB	37:Z:8455:HOH:O	2.15	0.46
29:Z:28:HIS:HD2	29:Z:31:LYS:H	1.63	0.46
1:0:45:A:H5''	1:0:47:G:O4'	2.16	0.46
1:0:169:A:O2'	31:2:48:ASN:ND2	2.49	0.46
1:0:686:A:O2'	1:0:747:G:H4'	2.16	0.46
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.46
4:A:164:ARG:HB2	28:Y:68:CYS:SG	2.55	0.46
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.45	0.46
15:L:57:LYS:HE2	15:L:140:ALA:O	2.16	0.46
16:M:47:LEU:CD1	16:M:97:VAL:HG11	2.45	0.46
22:S:48:VAL:HG23	22:S:98:VAL:HA	1.96	0.46
25:V:125:HIS:HE1	37:V:3071:HOH:O	1.97	0.46
30:1:18:ASN:ND2	30:1:40:ARG:H	2.14	0.46
1:0:1562:C:O2	1:0:1562:C:H2'	2.16	0.46
1:0:2729:C:H2'	1:0:2730:G:H8	1.81	0.46
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.74	0.46
6:C:21:VAL:C	6:C:23:GLU:H	2.24	0.46
7:D:169:THR:O	7:D:170:TYR:HB2	2.16	0.46
8:E:93:MET:HE2	8:E:107:PHE:CD1	2.51	0.46
9:F:26:THR:HB	9:F:102:GLY:C	2.40	0.46
9:F:113:ASP:O	9:F:117:GLU:HG3	2.16	0.46
24:U:16:ARG:NH2	24:U:63:GLU:HG3	2.31	0.46
29:Z:37:CYS:SG	29:Z:39:PHE:HB2	2.56	0.46
1:0:489:A:C8	22:S:82:THR:HG22	2.51	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.46
1:0:1185:U:H5'	37:0:6911:HOH:O	2.16	0.46
1:0:2656:G:O2'	1:0:2657:G:H5'	2.16	0.46
1:0:2719:A:C2	5:B:70:PRO:HG3	2.51	0.46
37:0:8858:HOH:O	21:R:63:LYS:NZ	2.48	0.46
2:9:3078:G:O2'	2:9:3079:U:OP2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.46	0.46
16:M:5:ARG:HG3	19:P:18:PRO:CB	2.46	0.46
26:W:27:ASP:OD2	26:W:27:ASP:N	2.49	0.46
1:O:212:A:O4'	1:O:214:U:C6	2.69	0.46
1:O:278:A:H2'	1:O:279:C:O4'	2.16	0.46
1:O:794:U:H3	1:O:819:A:H61	1.63	0.46
1:O:1166:A:H2'	1:O:1166:A:N3	2.31	0.46
1:O:1384:C:H5'	26:W:30:MET:HG2	1.98	0.46
1:O:2001:G:C2'	1:O:2002:C:H5'	2.46	0.46
1:O:2385:G:H2'	1:O:2386:U:C6	2.51	0.46
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.46
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.96	0.46
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.98	0.46
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.98	0.46
16:M:141:ARG:N	37:M:8569:HOH:O	2.48	0.46
25:V:13:MET:HE2	25:V:18:GLN:N	2.31	0.46
25:V:122:ARG:HG2	25:V:152:ALA:O	2.14	0.46
25:V:142:ASP:HB3	25:V:145:GLY:H	1.80	0.46
1:O:128:A:C8	1:O:128:A:C3'	2.98	0.45
1:O:1667:A:H2'	1:O:1668:U:H6	1.80	0.45
2:9:3013:A:O2'	2:9:3014:G:H5''	2.16	0.45
2:9:3065:A:C2'	2:9:3066:G:OP2	2.64	0.45
4:A:36:ASP:O	4:A:37:VAL:C	2.59	0.45
5:B:43:GLY:O	5:B:308:LEU:HD12	2.16	0.45
14:K:130:ARG:HA	37:K:8556:HOH:O	2.16	0.45
16:M:61:ALA:CB	16:M:88:ALA:HB2	2.46	0.45
21:R:6:LYS:HB2	21:R:27:ALA:O	2.15	0.45
21:R:8:PRO:HD2	24:U:32:ALA:HA	1.99	0.45
31:2:3:MET:O	31:2:90:PHE:HA	2.15	0.45
1:O:1056:U:H2'	1:O:1057:A:O4'	2.16	0.45
1:O:1119:G:H2'	12:I:52:GLN:NE2	2.31	0.45
1:O:1634:G:H2'	1:O:1635:U:C6	2.50	0.45
1:O:2837:U:H2'	37:O:6290:HOH:O	2.16	0.45
6:C:76:ARG:HG2	6:C:78:ARG:NH1	2.31	0.45
7:D:86:THR:CG2	37:D:7477:HOH:O	2.65	0.45
13:J:9:THR:O	13:J:10:GLN:C	2.57	0.45
14:K:148:GLU:HG2	37:K:8551:HOH:O	2.16	0.45
15:L:134:ILE:O	15:L:136:PRO:HD3	2.16	0.45
24:U:55:ARG:O	24:U:59:ILE:HG12	2.17	0.45
26:W:37:LEU:CD1	26:W:85:VAL:HG21	2.27	0.45
26:W:85:VAL:HG12	26:W:86:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:112:GLU:OE1	27:X:115:ARG:NH1	2.49	0.45
1:0:538:C:OP2	27:X:134:HIS:HE1	1.99	0.45
1:0:564:G:H1'	37:0:5770:HOH:O	2.16	0.45
1:0:1184:C:O2'	1:0:1185:U:H6	2.00	0.45
1:0:1759:A:N7	37:0:9067:HOH:O	2.36	0.45
1:0:1909:A:H2'	1:0:1910:A:C8	2.51	0.45
1:0:1942:A:O2'	1:0:1943:C:H5'	2.17	0.45
1:0:2019:A:H5'	37:0:4016:HOH:O	2.16	0.45
7:D:35:ALA:HB1	37:D:3279:HOH:O	2.15	0.45
11:H:39:GLY:O	11:H:41:THR:N	2.50	0.45
13:J:101:ASN:O	13:J:102:GLU:CB	2.65	0.45
14:K:146:GLY:C	14:K:148:GLU:H	2.24	0.45
15:L:87:MET:H	15:L:87:MET:HG3	1.28	0.45
1:0:177:A:H2'	1:0:178:U:O4'	2.16	0.45
1:0:962:C:H5''	37:0:4384:HOH:O	2.15	0.45
2:9:3041:C:C6	7:D:50:VAL:HG21	2.51	0.45
4:A:199:HIS:HD2	4:A:201:PHE:HB2	1.82	0.45
5:B:2:GLN:CD	37:B:8620:HOH:O	2.58	0.45
5:B:82:VAL:HG12	5:B:101:TRP:CE3	2.52	0.45
5:B:258:GLY:H	5:B:260:HIS:HE1	1.60	0.45
15:L:58:GLN:HG3	37:L:8606:HOH:O	2.15	0.45
16:M:161:GLY:O	16:M:162:ASP:C	2.58	0.45
23:T:49:LEU:CD1	37:T:3805:HOH:O	2.64	0.45
1:0:816:G:C6	1:0:817:G:N1	2.84	0.45
1:0:1299:G:N2	37:0:4158:HOH:O	2.48	0.45
1:0:1328:A:N7	1:0:1329:A:C5	2.85	0.45
1:0:1787:C:H4'	1:0:2883:A:O4'	2.16	0.45
2:9:3040:C:N4	7:D:51:ARG:HB2	2.31	0.45
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.51	0.45
6:C:109:LEU:HD12	6:C:109:LEU:O	2.16	0.45
7:D:58:VAL:CG1	7:D:59:GLY:N	2.78	0.45
7:D:92:GLU:O	7:D:93:LEU:O	2.34	0.45
8:E:152:THR:HG21	8:E:165:GLY:HA2	1.97	0.45
16:M:87:LEU:CD1	16:M:186:LEU:HD21	2.40	0.45
30:1:19:SER:O	30:1:36:ASN:ND2	2.50	0.45
1:0:299:U:C5'	37:0:6781:HOH:O	2.62	0.45
1:0:1245:C:O5'	1:0:1245:C:H6	2.00	0.45
1:0:1820:G:C6	1:0:2030:A:C2	3.05	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.17	0.45
2:9:3031:C:H2'	2:9:3032:G:O4'	2.15	0.45
10:G:63:ARG:O	10:G:67:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:72:ASN:O	14:K:76:LEU:HG	2.17	0.45
15:L:5:TYR:HE2	15:L:46:LEU:HD13	1.81	0.45
15:L:9:ARG:HG3	37:L:8543:HOH:O	2.16	0.45
15:L:59:GLY:C	15:L:141:ILE:HD11	2.41	0.45
16:M:80:SER:CB	37:M:8536:HOH:O	2.61	0.45
27:X:205:ILE:O	27:X:206:ALA:C	2.60	0.45
1:0:303:C:O2'	1:0:304:G:H5'	2.17	0.45
1:0:797:A:O4'	28:Y:10:ARG:N	2.49	0.45
1:0:1023:C:H2'	1:0:1024:G:O4'	2.17	0.45
1:0:1617:C:C4	1:0:1643:C:H4'	2.51	0.45
1:0:1845:A:OP2	4:A:190:ARG:NH1	2.50	0.45
1:0:2488:A:H1'	37:0:8611:HOH:O	2.17	0.45
1:0:2755:G:H1'	37:0:4157:HOH:O	2.16	0.45
37:0:5501:HOH:O	31:2:62:THR:HB	2.17	0.45
37:A:8612:HOH:O	28:Y:75:ALA:HB3	2.17	0.45
5:B:255:GLY:O	5:B:257:THR:HG23	2.17	0.45
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.75	0.45
7:D:64:ARG:O	7:D:67:ASP:OD2	2.34	0.45
9:F:58:GLU:HA	9:F:61:MET:HE2	1.98	0.45
12:I:93:ARG:HH11	12:I:93:ARG:CB	2.24	0.45
14:K:97:VAL:HG12	14:K:98:GLU:O	2.17	0.45
15:L:127:LYS:NZ	37:L:8564:HOH:O	2.50	0.45
15:L:138:HIS:C	15:L:139:PRO:O	2.52	0.45
17:N:59:VAL:HG23	17:N:111:VAL:HG23	1.97	0.45
19:P:25:PRO:HA	19:P:26:PRO:HD3	1.83	0.45
29:Z:1:THR:HA	37:Z:8410:HOH:O	2.16	0.45
1:0:134:U:C2	1:0:145:A:C2	3.05	0.45
1:0:911:G:H5'	1:0:932:U:OP1	2.17	0.45
1:0:963:C:H2'	1:0:964:G:C8	2.52	0.45
1:0:1422:U:H2'	1:0:1423:C:C6	2.52	0.45
1:0:2070:G:H5''	37:0:3279:HOH:O	2.17	0.45
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.98	0.45
4:A:132:ASP:OD1	4:A:133:ARG:N	2.49	0.45
4:A:170:VAL:HG13	28:Y:22:ILE:CG2	2.46	0.45
5:B:1:PRO:O	5:B:2:GLN:HB2	2.17	0.45
5:B:185:GLY:HA2	37:B:8636:HOH:O	2.17	0.45
5:B:223:ARG:HG3	5:B:232:TRP:O	2.17	0.45
6:C:223:LEU:HD12	6:C:223:LEU:HA	1.87	0.45
14:K:21:ARG:N	37:K:8533:HOH:O	2.50	0.45
14:K:90:ARG:NH2	14:K:121:ILE:HD11	2.31	0.45
15:L:25:TRP:HE3	15:L:26:HIS:HD2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:139:TRP:HA	16:M:139:TRP:HE3	1.82	0.45
18:O:115:SER:C	18:O:117:SER:H	2.24	0.45
1:O:56:G:H5''	24:U:50:ARG:NH1	2.31	0.45
1:O:333:G:O2'	1:O:334:G:H5'	2.17	0.45
1:O:426:G:H2'	1:O:427:C:O4'	2.17	0.45
1:O:500:G:H21	20:Q:98:ASN:HD21	1.64	0.45
1:O:1134:G:C5'	11:H:151:MET:HE1	2.46	0.45
1:O:1221:G:C8	37:O:5452:HOH:O	2.68	0.45
1:O:1462:C:H2'	1:O:1463:A:C8	2.52	0.45
1:O:1589:G:N2	1:O:1605:G:O2'	2.42	0.45
2:9:3091:C:H2'	2:9:3092:G:O4'	2.17	0.45
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.16	0.45
11:H:26:LYS:HD2	11:H:28:ILE:HB	1.98	0.45
12:I:52:GLN:HG3	12:I:53:ILE:H	1.81	0.45
12:I:88:PRO:O	12:I:94:GLY:HA3	2.17	0.45
15:L:81:ARG:O	15:L:86:MET:HE2	2.17	0.45
22:S:9:LYS:HD2	37:S:7242:HOH:O	2.16	0.45
22:S:48:VAL:CG2	22:S:98:VAL:HA	2.46	0.45
25:V:54:PHE:CZ	25:V:140:LYS:HB2	2.51	0.45
26:W:12:ILE:HD12	26:W:36:HIS:ND1	2.32	0.45
27:X:122:ARG:NH2	37:X:8533:HOH:O	2.50	0.45
28:Y:11:THR:HG23	28:Y:23:ARG:HD2	1.99	0.45
1:O:397:A:P	37:O:3830:HOH:O	2.75	0.45
1:O:678:G:OP2	6:C:107:ARG:NH2	2.49	0.45
1:O:790:A:H2'	1:O:791:A:O4'	2.17	0.45
1:O:1450:C:C2'	1:O:1494:A:H5'	2.47	0.45
1:O:2769:C:H2'	1:O:2770:G:C5'	2.46	0.45
2:9:3051:A:H5'	16:M:160:SER:CB	2.44	0.45
4:A:51:ARG:NH1	4:A:120:ARG:O	2.50	0.45
6:C:1:MET:HG2	6:C:2:GLN:NE2	2.32	0.45
6:C:13:ASP:OD1	6:C:13:ASP:O	2.35	0.45
7:D:35:ALA:C	7:D:37:ALA:N	2.75	0.45
11:H:1:LYS:N	37:H:8351:HOH:O	2.49	0.45
11:H:157:ILE:CG2	11:H:158:ASN:N	2.80	0.45
13:J:30:LYS:O	13:J:55:VAL:HG13	2.17	0.45
13:J:118:ALA:C	13:J:120:ARG:H	2.25	0.45
16:M:38:LYS:HB2	16:M:38:LYS:HE3	1.65	0.45
17:N:77:ALA:HA	17:N:96:VAL:O	2.17	0.45
18:O:16:VAL:CG1	18:O:17:GLY:N	2.80	0.45
25:V:88:THR:HG23	25:V:110:GLN:HB3	1.98	0.45
1:O:559:U:H5'	1:O:559:U:C6	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1183:C:N3	37:0:5509:HOH:O	2.48	0.44
1:0:2392:C:H4'	37:P:2875:HOH:O	2.17	0.44
1:0:2502:C:H4'	11:H:151:MET:SD	2.57	0.44
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.45	0.44
11:H:150:LYS:HA	11:H:153:VAL:HG22	1.99	0.44
16:M:71:TRP:CE3	16:M:175:LEU:CD2	2.99	0.44
28:Y:46:LYS:O	28:Y:57:CYS:HA	2.17	0.44
1:0:40:C:O5'	1:0:40:C:H6	2.01	0.44
1:0:69:A:C8	1:0:69:A:H5'	2.51	0.44
1:0:920:C:H4'	1:0:921:G:N2	2.31	0.44
1:0:929:A:O5'	1:0:929:A:H8	2.01	0.44
1:0:1524:U:O2'	1:0:1525:G:OP2	2.33	0.44
37:0:8835:HOH:O	28:Y:16:PRO:HG3	2.16	0.44
4:A:192:VAL:CG1	4:A:192:VAL:O	2.65	0.44
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.48	0.44
5:B:321:PRO:HG3	37:B:8598:HOH:O	2.18	0.44
11:H:114:PRO:O	11:H:115:PHE:C	2.59	0.44
12:I:77:GLY:O	12:I:78:ILE:C	2.60	0.44
15:L:108:LYS:HE3	37:L:8614:HOH:O	2.16	0.44
27:X:112:GLU:CD	27:X:115:ARG:HH12	2.25	0.44
30:1:40:ARG:HG3	30:1:45:ASN:CB	2.47	0.44
31:2:42:ARG:HG3	31:2:42:ARG:HH11	1.82	0.44
31:2:91:GLN:O	31:2:92:GLU:HB2	2.17	0.44
1:0:154:C:H2'	1:0:155:C:C6	2.52	0.44
1:0:338:C:H4'	6:C:174:ILE:HD11	1.99	0.44
1:0:1079:A:N1	1:0:2068:G:O2'	2.41	0.44
1:0:1119:G:C8	12:I:52:GLN:NE2	2.86	0.44
1:0:1269:G:H2'	1:0:1270:U:C6	2.53	0.44
1:0:2780:C:H2'	1:0:2781:U:H6	1.82	0.44
37:0:9276:HOH:O	14:K:41:HIS:HE1	2.00	0.44
2:9:3017:G:N2	2:9:3064:C:C2	2.86	0.44
5:B:60:SER:C	5:B:62:ARG:N	2.74	0.44
9:F:32:GLY:N	37:F:3111:HOH:O	2.49	0.44
12:I:39:VAL:CG1	12:I:107:ASN:HB2	2.48	0.44
18:O:115:SER:O	18:O:117:SER:N	2.50	0.44
23:T:20:MET:CG	23:T:28:THR:HG23	2.48	0.44
23:T:31:PHE:CG	23:T:37:GLU:HG2	2.53	0.44
25:V:122:ARG:HH11	25:V:122:ARG:CG	2.23	0.44
28:Y:13:ARG:NH1	37:Y:8421:HOH:O	2.48	0.44
1:0:10:U:HO2'	1:0:11:A:P	2.41	0.44
1:0:684:G:H2'	1:0:685:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1211:G:O2'	1:0:1212:C:H5'	2.16	0.44
1:0:1268:C:H2'	1:0:1269:G:H8	1.83	0.44
5:B:215:VAL:HA	5:B:220:VAL:HG22	1.99	0.44
7:D:21:VAL:HG13	7:D:131:THR:O	2.18	0.44
9:F:22:VAL:CG2	9:F:104:ALA:HB2	2.48	0.44
9:F:26:THR:HG21	9:F:103:ALA:CB	2.47	0.44
15:L:122:GLU:HB2	15:L:126:HIS:O	2.18	0.44
16:M:138:ASP:O	16:M:140:GLN:N	2.44	0.44
18:O:131:PHE:CD1	18:O:137:LEU:HD13	2.52	0.44
22:S:24:ARG:HH21	22:S:39:ASN:ND2	2.14	0.44
28:Y:17:ARG:O	28:Y:18:TYR:HB2	2.17	0.44
1:0:464:G:O2'	1:0:465:U:OP2	2.35	0.44
1:0:1194:A:C6	1:0:1206:U:C4	3.06	0.44
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.17	0.44
5:B:333:GLU:HB2	23:T:14:GLU:OE2	2.17	0.44
7:D:59:GLY:C	7:D:61:PHE:N	2.74	0.44
11:H:95:GLU:HB3	11:H:119:VAL:HG11	2.00	0.44
14:K:3:LYS:O	14:K:4:LYS:C	2.59	0.44
14:K:30:ARG:NH2	37:K:8522:HOH:O	2.36	0.44
15:L:182:LYS:HD2	15:L:193:LYS:HB2	1.99	0.44
16:M:43:VAL:O	16:M:43:VAL:HG12	2.17	0.44
18:O:106:ARG:HG3	37:O:7156:HOH:O	2.18	0.44
24:U:39:ALA:C	24:U:41:GLU:N	2.75	0.44
1:0:1205:U:H2'	1:0:1206:U:C5'	2.47	0.44
1:0:1741:U:O2'	1:0:2723:G:H4'	2.18	0.44
1:0:2434:A:O3'	31:2:28:GLY:HA3	2.18	0.44
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.44
1:0:2779:G:H21	8:E:143:GLN:HE22	1.66	0.44
1:0:2812:A:C2	1:0:2814:A:N6	2.74	0.44
4:A:93:THR:C	4:A:94:LEU:HD23	2.42	0.44
4:A:186:TRP:CG	4:A:187:PRO:HA	2.52	0.44
5:B:168:GLY:H	5:B:174:ARG:HD3	1.81	0.44
7:D:94:ALA:HB3	7:D:174:VAL:CA	2.48	0.44
9:F:21:GLU:O	9:F:24:ARG:HG3	2.16	0.44
9:F:117:GLU:C	9:F:119:ARG:N	2.76	0.44
10:G:64:ASN:N	10:G:64:ASN:ND2	2.61	0.44
13:J:81:ARG:HD3	13:J:87:ARG:HH12	1.82	0.44
14:K:62:ALA:HB2	14:K:103:ALA:CB	2.47	0.44
28:Y:11:THR:OG1	28:Y:23:ARG:HB2	2.18	0.44
28:Y:56:MET:HA	28:Y:62:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:2:GLY:O	29:Z:6:PRO:HG2	2.18	0.44
1:0:1003:U:O2'	11:H:90:PHE:HE1	2.01	0.44
1:0:1594:C:O2'	1:0:1607:A:H4'	2.17	0.44
2:9:3065:A:O2'	2:9:3066:G:P	2.75	0.44
5:B:88:GLU:O	5:B:88:GLU:HG3	2.17	0.44
7:D:60:GLU:C	7:D:62:ASP:N	2.73	0.44
7:D:128:LEU:N	37:D:6007:HOH:O	2.50	0.44
12:I:6:PHE:O	12:I:8:ALA:N	2.50	0.44
16:M:73:ALA:HB1	16:M:74:PRO:CD	2.47	0.44
20:Q:39:THR:O	20:Q:40:ALA:C	2.60	0.44
31:2:7:PHE:HE2	31:2:22:VAL:HG21	1.82	0.44
1:0:65:C:O2'	1:0:66:G:H5'	2.17	0.44
1:0:222:A:H2'	1:0:223:G:O4'	2.17	0.44
1:0:244:C:H6	1:0:244:C:O5'	2.00	0.44
1:0:396:U:O2'	1:0:397:A:P	2.75	0.44
1:0:1235:G:C1'	12:I:63:ILE:HG23	2.47	0.44
1:0:2247:C:H5''	37:0:6790:HOH:O	2.17	0.44
1:0:2779:G:O2'	1:0:2780:C:H5'	2.18	0.44
2:9:3076:G:C8	2:9:3077:A:H2'	2.53	0.44
4:A:130:THR:HG22	4:A:131:HIS:O	2.18	0.44
5:B:54:VAL:HB	37:B:8611:HOH:O	2.18	0.44
5:B:85:ARG:NH1	37:B:8637:HOH:O	2.51	0.44
5:B:313:PRO:O	5:B:314:ALA:C	2.61	0.44
6:C:173:LYS:NZ	37:C:8412:HOH:O	2.51	0.44
7:D:48:MET:HA	7:D:49:PRO:HD3	1.85	0.44
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.48	0.44
9:F:27:GLY:HA3	37:F:5413:HOH:O	2.18	0.44
14:K:24:ALA:HB2	14:K:30:ARG:HD2	1.99	0.44
15:L:137:ASP:HA	15:L:142:LYS:HE3	1.99	0.44
16:M:175:LEU:O	16:M:176:ARG:C	2.61	0.44
1:0:111:C:H2'	1:0:112:G:O4'	2.18	0.44
1:0:1168:C:H5	37:0:6942:HOH:O	2.00	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.44
1:0:2072:G:C6	1:0:2533:C:H1'	2.53	0.44
1:0:2598:U:O2	1:0:2600:A:C8	2.71	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.58	0.44
5:B:275:GLY:C	37:B:8654:HOH:O	2.60	0.44
6:C:27:ARG:CD	6:C:29:ASP:OD1	2.66	0.44
6:C:115:LEU:HD12	6:C:115:LEU:HA	1.85	0.44
8:E:11:VAL:HG11	8:E:22:VAL:HG13	1.99	0.44
15:L:42:ARG:HA	15:L:43:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:14:ALA:HB3	20:Q:147:LEU:HB2	2.00	0.44
25:V:6:GLN:HA	25:V:52:VAL:HG23	1.99	0.44
25:V:146:ILE:HG22	25:V:147:ASP:N	2.32	0.44
1:O:432:G:O2'	1:O:433:C:H5'	2.18	0.43
1:O:716:G:H2'	1:O:717:C:O5'	2.18	0.43
1:O:1184:C:O2'	1:O:1185:U:OP2	2.35	0.43
1:O:1919:A:H4'	37:O:4319:HOH:O	2.18	0.43
1:O:1970:G:H4'	1:O:1971:G:O5'	2.17	0.43
1:O:2563:U:O2'	1:O:2564:G:H3'	2.18	0.43
1:O:2712:G:O2'	1:O:2713:G:H5'	2.18	0.43
1:O:2724:U:H2'	1:O:2725:G:O4'	2.18	0.43
2:9:3064:C:C2'	2:9:3065:A:H5'	2.48	0.43
4:A:8:ARG:NH1	37:A:8550:HOH:O	2.46	0.43
4:A:36:ASP:HB2	4:A:84:VAL:N	2.33	0.43
5:B:320:GLN:HG3	5:B:321:PRO:CD	2.47	0.43
10:G:71:LEU:C	10:G:73:ASP:N	2.76	0.43
18:O:13:VAL:HG11	18:O:40:VAL:CG1	2.48	0.43
21:R:53:ASN:ND2	37:R:8321:HOH:O	2.51	0.43
27:X:117:LEU:HD12	27:X:174:VAL:HG11	1.99	0.43
1:O:1159:G:P	37:O:3782:HOH:O	2.75	0.43
1:O:1815:A:H4'	1:O:2751:C:O4'	2.18	0.43
1:O:2316:G:H5'	1:O:2317:C:O4'	2.18	0.43
1:O:2346:C:O3'	7:D:52:THR:HG23	2.17	0.43
2:9:3001:U:O3'	2:9:3003:A:H5''	2.19	0.43
2:9:3008:G:C6	2:9:3009:C:C4	3.06	0.43
2:9:3056:A:H1'	7:D:14:ARG:HG2	2.01	0.43
5:B:51:VAL:HG21	5:B:327:VAL:HG13	2.00	0.43
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.47	0.43
8:E:12:ASP:HA	37:E:1750:HOH:O	2.18	0.43
10:G:73:ASP:C	37:G:2994:HOH:O	2.61	0.43
11:H:113:ALA:N	11:H:114:PRO:HD3	2.33	0.43
15:L:107:ARG:NH1	37:L:8575:HOH:O	2.47	0.43
16:M:139:TRP:HH2	16:M:176:ARG:HH11	1.65	0.43
20:Q:39:THR:CB	20:Q:42:GLU:HG3	2.48	0.43
22:S:75:GLU:O	22:S:76:ASP:HB2	2.17	0.43
23:T:9:CYS:HA	23:T:52:THR:CG2	2.45	0.43
26:W:71:ARG:HD3	37:W:2171:HOH:O	2.18	0.43
1:O:816:G:H5'	1:O:1598:A:H4'	1.98	0.43
1:O:1164:U:C4	1:O:1192:A:H2	2.36	0.43
5:B:138:GLY:O	5:B:139:ASP:C	2.60	0.43
18:O:120:ARG:NH2	18:O:123:TYR:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:29:ASP:CG	21:R:31:ARG:NH1	2.76	0.43
23:T:36:CYS:O	23:T:37:GLU:C	2.60	0.43
24:U:57:LYS:HA	24:U:60:GLN:HE21	1.84	0.43
28:Y:48:LYS:NZ	37:Y:8438:HOH:O	2.50	0.43
1:0:51:G:O2'	1:0:52:A:H5'	2.19	0.43
1:0:328:U:O4'	6:C:202:THR:HG22	2.17	0.43
1:0:1684:A:O2'	1:0:1685:A:H5''	2.18	0.43
1:0:2667:G:H1'	1:0:2914:A:N3	2.32	0.43
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.43
1:0:2906:A:H5'	1:0:2907:C:O4'	2.18	0.43
1:0:2909:G:H2'	1:0:2910:A:H8	1.84	0.43
37:0:8601:HOH:O	15:L:174:ARG:HG3	2.18	0.43
2:9:3026:C:P	37:9:8440:HOH:O	2.77	0.43
4:A:192:VAL:O	4:A:207:GLN:HG2	2.18	0.43
5:B:63:GLU:O	5:B:63:GLU:HG3	2.18	0.43
5:B:162:MET:HE2	5:B:310:ARG:CG	2.48	0.43
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.00	0.43
7:D:101:THR:HG22	7:D:101:THR:O	2.18	0.43
8:E:95:VAL:O	8:E:126:ILE:HD13	2.18	0.43
12:I:47:THR:HG22	12:I:48:GLY:N	2.33	0.43
16:M:110:THR:HB	16:M:113:SER:OG	2.18	0.43
22:S:26:THR:HA	22:S:39:ASN:HB3	1.99	0.43
24:U:42:ASN:O	24:U:44:GLY:N	2.51	0.43
28:Y:56:MET:HE2	28:Y:63:LYS:CD	2.48	0.43
1:0:40:C:H4'	37:0:6454:HOH:O	2.17	0.43
1:0:283:U:H5''	1:0:284:C:P	2.58	0.43
1:0:539:G:H2'	1:0:540:A:C8	2.53	0.43
1:0:1072:G:OP2	27:X:154:ARG:NH2	2.50	0.43
1:0:1495:C:H1'	1:0:1573:A:H1'	2.01	0.43
1:0:1592:G:H2'	1:0:1593:C:C6	2.54	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.53	0.43
1:0:2656:G:C2'	1:0:2657:G:H5'	2.48	0.43
2:9:3092:G:C6	2:9:3093:A:C6	3.07	0.43
4:A:179:MET:HG2	4:A:186:TRP:CG	2.53	0.43
8:E:84:MET:HB2	8:E:131:LEU:HB2	2.00	0.43
14:K:143:THR:HG21	37:K:8539:HOH:O	2.18	0.43
16:M:143:ARG:NH1	16:M:173:ASP:CG	2.77	0.43
17:N:23:GLY:C	37:N:3062:HOH:O	2.61	0.43
25:V:122:ARG:NE	37:V:5817:HOH:O	2.52	0.43
27:X:184:GLU:OE1	27:X:204:ARG:NH1	2.51	0.43
1:0:628:A:O2'	1:0:630:A:OP2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1154:A:H2'	1:0:1155:G:C8	2.54	0.43
1:0:1367:A:C2'	1:0:1368:U:H5'	2.49	0.43
1:0:2575:C:H2'	1:0:2576:A:O4'	2.19	0.43
8:E:20:ILE:O	8:E:30:THR:HA	2.18	0.43
13:J:22:ASP:C	13:J:22:ASP:OD1	2.62	0.43
13:J:87:ARG:NE	37:J:4854:HOH:O	2.51	0.43
16:M:15:GLU:HB2	16:M:17:ARG:HG3	2.00	0.43
16:M:108:SER:HA	16:M:109:PRO:HD3	1.81	0.43
25:V:41:TYR:HA	25:V:44:MET:HE3	2.01	0.43
31:2:30:GLN:NE2	37:2:8543:HOH:O	2.48	0.43
1:0:101:C:H2'	1:0:102:A:H8	1.83	0.43
1:0:553:G:OP2	27:X:204:ARG:NH2	2.50	0.43
1:0:1778:A:O2'	1:0:1822:A:OP1	2.30	0.43
1:0:1810:C:OP1	23:T:44:ARG:NE	2.31	0.43
1:0:2079:G:H2'	1:0:2080:G:O4'	2.19	0.43
1:0:2241:C:H2'	1:0:2242:U:C6	2.53	0.43
1:0:2860:G:H1'	37:0:6253:HOH:O	2.18	0.43
5:B:162:MET:HG3	5:B:310:ARG:CZ	2.49	0.43
10:G:27:ILE:HD12	10:G:70:ALA:HB1	1.99	0.43
11:H:112:ARG:O	11:H:113:ALA:C	2.62	0.43
12:I:6:PHE:HB3	12:I:109:TYR:OH	2.19	0.43
14:K:89:PHE:N	37:K:8569:HOH:O	2.52	0.43
14:K:130:ARG:O	14:K:131:GLU:C	2.62	0.43
21:R:23:LYS:HD3	21:R:65:VAL:HG12	2.00	0.43
22:S:3:GLN:HA	22:S:4:PRO:HD3	1.88	0.43
22:S:49:GLU:HB3	22:S:59:GLU:CG	2.48	0.43
25:V:21:LEU:CD2	25:V:48:VAL:HG11	2.47	0.43
27:X:106:THR:HG22	27:X:107:PRO:O	2.19	0.43
27:X:112:GLU:OE1	27:X:112:GLU:HA	2.19	0.43
1:0:716:G:C2'	1:0:717:C:O5'	2.67	0.43
1:0:885:G:H5''	1:0:886:A:H5'	2.01	0.43
1:0:1119:G:H2'	12:I:52:GLN:HE22	1.84	0.43
1:0:1367:A:H2'	1:0:1368:U:H5'	2.01	0.43
1:0:1450:C:C4'	1:0:1451:C:OP2	2.64	0.43
2:9:3104:A:O2'	2:9:3105:A:H5'	2.19	0.43
4:A:1:GLY:N	37:A:8607:HOH:O	2.40	0.43
4:A:131:HIS:O	4:A:132:ASP:CB	2.62	0.43
4:A:211:LYS:HB2	37:A:8619:HOH:O	2.17	0.43
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.49	0.43
7:D:81:GLU:C	7:D:83:PHE:N	2.75	0.43
8:E:7:ILE:HG22	8:E:45:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:84:MET:HE2	8:E:133:VAL:HG23	1.99	0.43
11:H:117:LYS:HB2	37:H:8338:HOH:O	2.18	0.43
14:K:17:SER:C	14:K:19:LYS:N	2.75	0.43
22:S:111:ARG:HB3	22:S:119:ALA:HB2	2.01	0.43
29:Z:28:HIS:O	29:Z:32:LYS:N	2.44	0.43
1:0:45:A:N6	1:0:147:G:C4	2.87	0.43
1:0:354:A:H2'	1:0:355:C:C6	2.54	0.43
1:0:401:C:P	37:0:5254:HOH:O	2.76	0.43
1:0:1684:A:O2'	30:1:43:ARG:NH2	2.52	0.43
1:0:2547:C:H2'	1:0:2548:C:H6	1.83	0.43
37:0:8905:HOH:O	28:Y:34:LYS:HD3	2.19	0.43
2:9:3114:G:H2'	2:9:3115:C:C6	2.54	0.43
6:C:20:ASP:O	6:C:23:GLU:HB2	2.19	0.43
11:H:56:ILE:HG21	11:H:61:LEU:HD13	2.01	0.43
25:V:4:LEU:HD23	25:V:4:LEU:HA	1.85	0.43
1:0:584:U:H3'	37:0:5557:HOH:O	2.17	0.43
1:0:794:U:H5	37:0:3677:HOH:O	2.01	0.43
1:0:902:G:N7	14:K:18:HIS:CD2	2.85	0.43
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.43
1:0:1669:A:H2	37:0:3203:HOH:O	2.02	0.43
1:0:2866:U:H4'	1:0:2867:G:H5'	2.00	0.43
1:0:2912:C:H2'	1:0:2913:A:O4'	2.19	0.43
2:9:3003:A:H2'	37:9:8420:HOH:O	2.19	0.43
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.87	0.43
6:C:98:ARG:NH1	37:C:8356:HOH:O	2.48	0.43
6:C:133:ARG:NH2	37:C:8425:HOH:O	2.52	0.43
6:C:214:THR:HB	37:C:8326:HOH:O	2.18	0.43
7:D:167:GLU:C	7:D:169:THR:H	2.27	0.43
11:H:130:HIS:CG	11:H:133:ILE:HD11	2.53	0.43
13:J:98:VAL:HG22	13:J:102:GLU:C	2.44	0.43
15:L:191:GLY:O	15:L:192:ALA:HB3	2.18	0.43
16:M:163:PHE:O	16:M:164:ASP:O	2.36	0.43
17:N:35:LYS:HD3	37:N:3360:HOH:O	2.19	0.43
19:P:31:GLU:CD	19:P:93:ARG:HH12	2.27	0.43
20:Q:96:VAL:HG13	20:Q:106:GLY:HA3	2.01	0.43
24:U:5:VAL:HG11	24:U:9:ARG:NH1	2.33	0.43
27:X:99:ALA:HB2	27:X:233:TYR:CE2	2.53	0.43
1:0:331:A:C6	1:0:332:G:C4	3.06	0.42
1:0:470:U:H2'	1:0:471:G:O4'	2.19	0.42
1:0:474:C:O3'	6:C:73:LEU:CD2	2.66	0.42
1:0:585:C:H6	37:0:5557:HOH:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1200:A:H4'	37:0:6786:HOH:O	2.17	0.42
1:0:1625:U:H5''	37:0:5484:HOH:O	2.18	0.42
1:0:2505:G:H8	37:0:5100:HOH:O	2.02	0.42
2:9:3020:G:H3'	37:9:8434:HOH:O	2.19	0.42
2:9:3047:A:C2	2:9:3048:C:C2	3.06	0.42
4:A:93:THR:HG23	4:A:154:ALA:O	2.19	0.42
5:B:36:PRO:HA	5:B:168:GLY:HA2	1.97	0.42
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.00	0.42
15:L:65:VAL:HG21	15:L:105:ALA:HB2	2.01	0.42
16:M:64:SER:C	16:M:66:LEU:N	2.77	0.42
16:M:67:ALA:C	16:M:69:TYR:H	2.27	0.42
16:M:139:TRP:CH2	16:M:176:ARG:NH1	2.87	0.42
21:R:80:ARG:NH1	37:R:8345:HOH:O	2.52	0.42
22:S:28:SER:O	22:S:32:ARG:HG3	2.19	0.42
23:T:13:ILE:HG12	23:T:32:CYS:CB	2.49	0.42
29:Z:28:HIS:CD2	29:Z:31:LYS:H	2.37	0.42
1:0:101:C:H2'	1:0:102:A:C8	2.54	0.42
1:0:1114:A:H2'	1:0:1115:U:H6	1.83	0.42
1:0:2044:G:OP1	26:W:23:HIS:CE1	2.69	0.42
1:0:2346:C:H4'	7:D:52:THR:CG2	2.48	0.42
37:0:4549:HOH:O	5:B:216:LYS:HA	2.19	0.42
2:9:3092:G:H22	11:H:52:LYS:NZ	2.17	0.42
4:A:150:PRO:HG3	37:A:8596:HOH:O	2.19	0.42
5:B:141:ARG:HG2	5:B:165:ARG:HA	2.01	0.42
6:C:168:ARG:NH2	6:C:190:ALA:O	2.52	0.42
16:M:79:PRO:HG3	16:M:142:THR:O	2.19	0.42
16:M:129:ILE:HA	16:M:130:PRO:HD3	1.93	0.42
19:P:30:VAL:O	19:P:30:VAL:HG12	2.19	0.42
20:Q:32:ALA:O	20:Q:33:ARG:C	2.62	0.42
20:Q:40:ALA:O	20:Q:44:VAL:HG23	2.19	0.42
25:V:122:ARG:CG	25:V:152:ALA:O	2.67	0.42
1:0:57:C:H5''	37:0:6211:HOH:O	2.18	0.42
1:0:447:A:O2'	1:0:448:G:H5'	2.19	0.42
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.55	0.42
1:0:1241:G:N3	12:I:86:MET:HE2	2.33	0.42
1:0:1308:A:O4'	6:C:226:GLY:HA3	2.20	0.42
1:0:1477:C:O2'	1:0:1478:U:H5'	2.18	0.42
1:0:1887:U:OP1	28:Y:21:LYS:HE3	2.20	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:2791:U:C1'	1:0:2792:A:H5''	2.48	0.42
5:B:24:PRO:O	5:B:25:ARG:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.53	0.42
5:B:152:PRO:HD2	37:B:8634:HOH:O	2.19	0.42
6:C:14:GLY:N	37:C:8437:HOH:O	2.49	0.42
6:C:196:THR:HG23	37:C:8400:HOH:O	2.19	0.42
9:F:39:SER:CB	9:F:45:ALA:HB2	2.50	0.42
11:H:56:ILE:HG22	11:H:61:LEU:CD2	2.47	0.42
18:O:2:ASP:OD1	18:O:2:ASP:C	2.62	0.42
18:O:10:ALA:CA	18:O:13:VAL:HG12	2.46	0.42
29:Z:44:LYS:NZ	37:Z:8456:HOH:O	2.53	0.42
1:0:291:C:H2'	1:0:292:G:O4'	2.20	0.42
1:0:593:A:N7	37:0:3883:HOH:O	2.51	0.42
1:0:1114:A:H2'	1:0:1115:U:C6	2.55	0.42
1:0:1224:G:H2'	1:0:1225:C:C6	2.54	0.42
1:0:1527:A:HO2'	1:0:1528:A:H8	1.63	0.42
1:0:1593:C:H5'	18:O:116:SER:O	2.20	0.42
1:0:1943:C:O4'	4:A:212:PRO:HA	2.18	0.42
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.42
1:0:2445:U:H2'	1:0:2446:G:H8	1.82	0.42
37:0:6904:HOH:O	6:C:188:ARG:HD3	2.18	0.42
2:9:3036:C:C5	2:9:3037:C:C5	3.08	0.42
7:D:25:MET:HE1	7:D:37:ALA:HB1	2.01	0.42
9:F:2:VAL:HG11	15:L:23:LEU:HD23	2.00	0.42
12:I:142:ASN:O	12:I:144:THR:N	2.52	0.42
14:K:128:GLY:O	14:K:132:LYS:HG3	2.18	0.42
15:L:39:ARG:HA	15:L:63:VAL:HG22	2.02	0.42
17:N:98:LEU:HD12	17:N:98:LEU:HA	1.88	0.42
18:O:115:SER:C	18:O:117:SER:N	2.77	0.42
20:Q:35:ILE:O	20:Q:38:LYS:HB2	2.19	0.42
26:W:9:VAL:HG13	26:W:88:GLU:OE2	2.20	0.42
31:2:36:ILE:HD12	31:2:36:ILE:HA	1.93	0.42
31:2:69:TYR:HB2	31:2:78:HIS:CE1	2.54	0.42
1:0:814:G:H4'	37:0:9635:HOH:O	2.19	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.19	0.42
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.85	0.42
1:0:2456:A:H2'	1:0:2457:U:C6	2.55	0.42
4:A:199:HIS:HD2	4:A:201:PHE:N	2.06	0.42
5:B:132:HIS:HB2	5:B:137:LEU:HD22	2.01	0.42
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.19	0.42
7:D:93:LEU:CB	7:D:97:GLN:OE1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:103:ASN:ND2	7:D:134:LEU:H	2.16	0.42
8:E:23:GLU:HG2	8:E:28:SER:HB2	2.02	0.42
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.80	0.42
9:F:111:ILE:O	9:F:115:VAL:HG23	2.19	0.42
13:J:78:LYS:HA	13:J:79:PRO:HD3	1.86	0.42
13:J:99:ASP:C	13:J:99:ASP:OD1	2.61	0.42
27:X:133:HIS:CD2	37:X:8573:HOH:O	2.54	0.42
27:X:216:ARG:CD	37:X:8561:HOH:O	2.59	0.42
1:O:120:A:H2'	1:O:120:A:N3	2.34	0.42
1:O:450:C:H4'	6:C:46:TYR:CE1	2.55	0.42
1:O:731:U:H2'	1:O:732:C:C6	2.55	0.42
1:O:821:U:O2'	1:O:822:C:H5'	2.19	0.42
1:O:1385:G:O3'	26:W:49:ARG:NH1	2.52	0.42
37:O:4344:HOH:O	15:L:174:ARG:HG2	2.19	0.42
2:9:3059:C:H2'	2:9:3060:C:C6	2.54	0.42
9:F:100:ASP:O	9:F:101:ALA:O	2.38	0.42
14:K:65:ASP:CG	14:K:111:ALA:HB3	2.45	0.42
22:S:71:VAL:HG11	22:S:90:PRO:CB	2.26	0.42
24:U:12:THR:HG23	24:U:14:ALA:H	1.84	0.42
25:V:38:THR:O	25:V:42:ARG:HB2	2.19	0.42
1:O:2353:A:H4'	1:O:2354:A:O5'	2.20	0.42
2:9:3054:A:O2'	2:9:3055:U:H5'	2.19	0.42
4:A:81:GLN:CB	4:A:92:ASN:ND2	2.82	0.42
4:A:123:GLY:HA3	4:A:162:GLY:HA2	2.02	0.42
6:C:16:VAL:CG1	6:C:17:ASP:N	2.81	0.42
7:D:84:LEU:HA	7:D:87:ALA:HB3	2.02	0.42
9:F:101:ALA:HA	37:F:5413:HOH:O	2.20	0.42
10:G:16:LYS:O	10:G:20:VAL:HG23	2.20	0.42
11:H:72:VAL:HG11	11:H:81:TYR:CZ	2.55	0.42
11:H:111:MET:O	11:H:114:PRO:HD3	2.19	0.42
14:K:134:GLU:HA	14:K:138:GLY:O	2.19	0.42
16:M:143:ARG:NH1	16:M:173:ASP:OD1	2.53	0.42
23:T:14:GLU:OE1	23:T:15:PRO:CD	2.63	0.42
25:V:3:ALA:O	25:V:54:PHE:HA	2.20	0.42
28:Y:39:CYS:HA	28:Y:47:LEU:HD11	2.00	0.42
1:O:92:G:H4'	24:U:44:GLY:HA3	2.01	0.42
1:O:513:A:H3'	37:O:3350:HOH:O	2.20	0.42
1:O:1242:A:OP2	12:I:60:ARG:NH2	2.50	0.42
1:O:1574:C:O5'	1:O:1574:C:H6	2.03	0.42
1:O:1743:G:H1'	37:O:4360:HOH:O	2.20	0.42
1:O:2289:G:H21	1:O:2291:A:H2	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2405:C:H5'	37:0:6051:HOH:O	2.18	0.42
1:0:2735:U:H2'	1:0:2736:U:C6	2.55	0.42
1:0:2821:C:H4'	5:B:116:PRO:CB	2.46	0.42
37:0:5737:HOH:O	17:N:7:LEU:HD22	2.18	0.42
2:9:3001:U:O3'	2:9:3003:A:C5'	2.68	0.42
2:9:3004:G:OP1	2:9:3059:C:O2'	2.38	0.42
4:A:192:VAL:O	4:A:192:VAL:HG12	2.20	0.42
4:A:217:ARG:HG2	4:A:229:ALA:HB2	2.01	0.42
6:C:129:HIS:CE1	6:C:232:LEU:H	2.38	0.42
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.49	0.42
7:D:64:ARG:HG2	7:D:66:GLY:O	2.20	0.42
11:H:1:LYS:HA	11:H:2:PRO:HD3	1.76	0.42
16:M:71:TRP:N	37:M:8538:HOH:O	2.52	0.42
19:P:40:HIS:CE1	19:P:94:GLN:HA	2.55	0.42
22:S:101:LEU:HD13	22:S:112:LEU:HD11	2.02	0.42
1:0:289:G:N1	1:0:363:A:C2	2.86	0.42
1:0:1377:C:H2'	1:0:1723:G:O6	2.20	0.42
1:0:1594:C:C2	1:0:1601:G:C2	3.08	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
5:B:74:ILE:HG13	37:B:8604:HOH:O	2.19	0.42
7:D:166:ILE:O	7:D:169:THR:N	2.53	0.42
8:E:91:PHE:HA	8:E:92:PRO:HD3	1.88	0.42
8:E:98:GLU:N	37:E:4191:HOH:O	2.52	0.42
8:E:139:GLU:CD	37:E:5919:HOH:O	2.61	0.42
12:I:39:VAL:HG12	12:I:40:ASN:ND2	2.35	0.42
16:M:73:ALA:HB1	16:M:74:PRO:HD2	2.01	0.42
20:Q:25:PHE:CE2	20:Q:29:LYS:CE	3.02	0.42
20:Q:82:GLU:O	20:Q:86:LYS:HG3	2.19	0.42
24:U:20:LEU:HD22	24:U:60:GLN:HE22	1.84	0.42
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.42
1:0:303:C:H2'	1:0:304:G:O4'	2.20	0.42
1:0:306:A:P	22:S:38:ARG:HH21	2.43	0.42
1:0:694:A:C2'	1:0:695:C:H5'	2.50	0.42
1:0:941:G:C5	1:0:942:U:C4	3.08	0.42
1:0:1603:A:H5'	1:0:1605:G:C4'	2.50	0.42
1:0:2346:C:H4'	7:D:52:THR:HG22	2.02	0.42
1:0:2507:G:H2'	1:0:2510:C:H42	1.85	0.42
37:0:3893:HOH:O	4:A:11:ARG:CZ	2.68	0.42
4:A:51:ARG:NH2	37:A:8605:HOH:O	2.52	0.42
4:A:99:ILE:O	4:A:131:HIS:CE1	2.72	0.42
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.88	0.42
5:B:127:GLN:HG3	37:B:8645:HOH:O	2.19	0.42
11:H:45:GLN:CB	11:H:163:PRO:HD2	2.25	0.42
12:I:107:ASN:ND2	12:I:107:ASN:C	2.72	0.42
14:K:98:GLU:O	14:K:99:GLU:CB	2.68	0.42
17:N:26:TRP:HB2	37:N:3062:HOH:O	2.19	0.42
20:Q:129:ALA:O	20:Q:130:MET:CB	2.67	0.42
1:O:2668:G:H2'	1:O:2669:U:C6	2.55	0.41
5:B:268:ARG:NE	37:B:8606:HOH:O	2.53	0.41
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.35	0.41
11:H:57:ARG:HG3	11:H:57:ARG:HH11	1.85	0.41
20:Q:82:GLU:HG3	20:Q:83:LYS:H	1.85	0.41
22:S:88:PRO:HB3	37:S:6320:HOH:O	2.19	0.41
23:T:52:THR:HG21	23:T:54:THR:HB	2.01	0.41
25:V:122:ARG:CG	25:V:122:ARG:NH1	2.82	0.41
1:O:282:C:H2'	1:O:283:U:O4'	2.19	0.41
1:O:392:U:C5'	15:L:193:LYS:HB3	2.50	0.41
1:O:567:U:O2'	1:O:568:G:H5'	2.19	0.41
1:O:736:A:H2'	1:O:737:A:O4'	2.19	0.41
1:O:945:U:H2'	1:O:946:C:C6	2.56	0.41
1:O:1947:G:H2'	1:O:1948:G:C8	2.54	0.41
4:A:184:THR:HG22	4:A:185:LYS:N	2.35	0.41
5:B:41:PHE:HB3	5:B:190:MET:CE	2.49	0.41
5:B:84:LEU:HD13	5:B:84:LEU:C	2.46	0.41
6:C:120:ASP:OD1	6:C:120:ASP:C	2.63	0.41
8:E:11:VAL:HG13	8:E:23:GLU:O	2.19	0.41
12:I:126:ASN:O	12:I:129:PHE:HE2	2.03	0.41
17:N:26:TRP:CE3	17:N:26:TRP:HA	2.55	0.41
18:O:16:VAL:CG1	18:O:20:ARG:HB2	2.51	0.41
24:U:38:GLY:C	24:U:40:PRO:HD2	2.45	0.41
25:V:5:VAL:O	25:V:52:VAL:CG2	2.69	0.41
25:V:65:VAL:HG12	25:V:116:LEU:HD13	2.01	0.41
25:V:146:ILE:HD13	25:V:146:ILE:HA	1.85	0.41
26:W:12:ILE:HG23	26:W:36:HIS:CG	2.55	0.41
27:X:177:LYS:HD3	27:X:181:GLY:O	2.20	0.41
1:O:68:U:O2'	1:O:69:A:H5''	2.20	0.41
1:O:553:G:P	27:X:204:ARG:NH2	2.91	0.41
1:O:656:G:H5'	17:N:3:THR:CG2	2.50	0.41
1:O:1200:A:C4'	37:O:6786:HOH:O	2.67	0.41
1:O:1252:A:H2'	1:O:1253:C:O4'	2.20	0.41
1:O:1462:C:O2'	1:O:1463:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1947:G:N2	1:0:1966:U:O2	2.53	0.41
1:0:2481:G:H3'	1:0:2482:G:H5''	2.02	0.41
1:0:2691:A:H8	1:0:2691:A:OP1	2.03	0.41
4:A:109:GLU:HG2	4:A:116:GLY:H	1.85	0.41
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.85	0.41
8:E:31:ARG:CZ	37:E:5919:HOH:O	2.68	0.41
11:H:132:PHE:O	11:H:133:ILE:HD13	2.20	0.41
11:H:150:LYS:CG	37:H:8380:HOH:O	2.67	0.41
13:J:90:PHE:N	13:J:90:PHE:CD1	2.89	0.41
19:P:16:ASN:HD22	19:P:16:ASN:HA	1.68	0.41
27:X:154:ARG:O	27:X:154:ARG:HG2	2.18	0.41
27:X:213:LYS:HE3	27:X:213:LYS:HB2	1.85	0.41
1:0:541:C:O2'	1:0:542:A:H5''	2.21	0.41
1:0:590:A:H2'	1:0:591:A:H5'	2.03	0.41
1:0:622:G:O2'	1:0:623:U:H5'	2.20	0.41
1:0:1299:G:H5'	37:0:3564:HOH:O	2.20	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.21	0.41
1:0:1714:C:O2'	1:0:1715:C:H5'	2.20	0.41
1:0:2443:C:H3'	37:0:9977:HOH:O	2.19	0.41
6:C:115:LEU:HD13	6:C:223:LEU:CD2	2.33	0.41
8:E:9:GLU:HG3	8:E:10:ASP:N	2.35	0.41
9:F:60:VAL:O	9:F:60:VAL:HG12	2.20	0.41
15:L:20:ILE:O	15:L:24:MET:HG2	2.20	0.41
17:N:26:TRP:N	37:N:3062:HOH:O	2.53	0.41
19:P:41:LEU:HB3	19:P:52:PHE:CZ	2.55	0.41
1:0:952:G:OP1	19:P:42:LYS:HE2	2.20	0.41
1:0:1299:G:N7	14:K:6:ARG:NH1	2.68	0.41
1:0:1717:A:H5''	18:O:54:LYS:HB2	2.03	0.41
1:0:2644:C:H2'	37:0:4072:HOH:O	2.20	0.41
2:9:3056:A:C3'	2:9:3057:A:H5''	2.50	0.41
6:C:187:ARG:O	6:C:187:ARG:HG3	2.19	0.41
7:D:23:VAL:HG12	7:D:130:VAL:HG22	2.03	0.41
15:L:35:PRO:CD	15:L:38:VAL:HG23	2.50	0.41
15:L:134:ILE:HG23	15:L:141:ILE:HD13	2.02	0.41
18:O:83:LYS:O	18:O:86:ALA:HB3	2.21	0.41
22:S:77:VAL:HG11	22:S:91:LEU:HD11	2.02	0.41
25:V:151:GLU:O	25:V:154:ARG:HB3	2.20	0.41
25:V:154:ARG:HB3	25:V:154:ARG:HE	1.66	0.41
30:1:40:ARG:HA	30:1:45:ASN:ND2	2.35	0.41
1:0:23:G:H1'	1:0:520:A:N6	2.36	0.41
1:0:183:A:O2'	1:0:184:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:255:A:H2'	1:0:256:C:C6	2.55	0.41
1:0:558:C:C2	1:0:600:G:N2	2.88	0.41
1:0:1183:C:C2	37:0:5509:HOH:O	2.54	0.41
4:A:69:LEU:CD2	4:A:120:ARG:HB3	2.45	0.41
5:B:33:ASP:O	5:B:34:GLY:O	2.37	0.41
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.55	0.41
6:C:178:GLN:C	6:C:180:SER:N	2.75	0.41
8:E:132:THR:HG23	8:E:132:THR:O	2.21	0.41
9:F:12:LEU:HD23	9:F:12:LEU:O	2.21	0.41
14:K:73:VAL:HG11	14:K:118:LEU:HD21	2.01	0.41
16:M:149:GLU:O	16:M:152:GLU:HB2	2.21	0.41
22:S:49:GLU:HB3	22:S:59:GLU:HG3	2.03	0.41
28:Y:38:LYS:HG3	37:Y:8431:HOH:O	2.20	0.41
1:0:883:U:O2	1:0:883:U:C2'	2.67	0.41
1:0:1137:G:O2'	37:0:3373:HOH:O	2.21	0.41
1:0:2282:U:H4'	1:0:2309:C:C5	2.56	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
1:0:2911:C:H2'	1:0:2912:C:C6	2.56	0.41
4:A:29:HIS:CE1	4:A:107:ASN:ND2	2.89	0.41
4:A:57:ALA:HA	4:A:67:LEU:HD23	2.02	0.41
4:A:101:GLU:HG2	4:A:131:HIS:ND1	2.35	0.41
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.20	0.41
4:A:192:VAL:HG12	4:A:207:GLN:HB3	2.03	0.41
7:D:93:LEU:HG	37:D:3862:HOH:O	2.21	0.41
12:I:131:THR:CG2	12:I:133:GLY:H	2.34	0.41
13:J:28:GLU:OE2	13:J:58:THR:HG21	2.20	0.41
15:L:108:LYS:N	15:L:108:LYS:HD3	2.36	0.41
15:L:183:VAL:HG12	15:L:184:ARG:N	2.36	0.41
18:O:31:ILE:HG12	18:O:43:LEU:HD13	2.03	0.41
22:S:12:ARG:NH1	37:S:3035:HOH:O	2.53	0.41
24:U:42:ASN:N	24:U:43:PRO:HD3	2.35	0.41
28:Y:59:HIS:CE1	37:Y:8422:HOH:O	2.73	0.41
1:0:10:U:H5'	37:0:5500:HOH:O	2.20	0.41
1:0:100:C:H4'	22:S:16:LEU:HB2	2.03	0.41
1:0:175:G:O2'	1:0:176:U:P	2.79	0.41
1:0:394:G:H1	15:L:181:GLU:CD	2.29	0.41
1:0:488:U:H2'	37:0:3498:HOH:O	2.20	0.41
1:0:1634:G:H2'	1:0:1635:U:H6	1.86	0.41
1:0:2135:A:C2	1:0:2241:C:C2	3.09	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
4:A:34:ASP:OD1	4:A:35:GLY:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:55:VAL:HG22	4:A:68:ILE:O	2.21	0.41
5:B:310:ARG:HD2	37:B:8652:HOH:O	2.20	0.41
6:C:8:LEU:N	6:C:8:LEU:HD23	2.35	0.41
7:D:35:ALA:C	7:D:37:ALA:H	2.28	0.41
16:M:119:GLN:O	16:M:123:ILE:HG13	2.21	0.41
23:T:6:CYS:O	23:T:8:TYR:N	2.54	0.41
30:1:36:ASN:HB3	30:1:39:ARG:NE	2.36	0.41
1:0:60:A:C2	1:0:61:G:C8	3.09	0.41
1:0:213:G:O2'	1:0:214:U:OP2	2.39	0.41
1:0:282:C:O2'	1:0:283:U:C5'	2.66	0.41
1:0:407:A:H2'	1:0:408:A:C8	2.56	0.41
1:0:812:A:H2'	1:0:813:C:O4'	2.20	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.36	0.41
1:0:1185:U:C5'	37:0:6911:HOH:O	2.68	0.41
1:0:1218:U:H2'	1:0:1219:U:H6	1.86	0.41
1:0:1335:C:OP2	27:X:207:SER:CB	2.69	0.41
1:0:1504:A:O2'	1:0:1506:U:OP2	2.33	0.41
1:0:1586:G:O2'	1:0:1587:U:H5'	2.20	0.41
1:0:2016:U:H2'	1:0:2017:U:C6	2.56	0.41
1:0:2768:A:H3'	37:0:3907:HOH:O	2.21	0.41
1:0:2820:A:H2'	1:0:2821:C:O4'	2.21	0.41
1:0:2896:A:H2'	1:0:2896:A:N3	2.36	0.41
37:0:4450:HOH:O	15:L:125:ARG:CZ	2.69	0.41
37:0:5501:HOH:O	31:2:84:ARG:HD3	2.21	0.41
2:9:3048:C:H4'	16:M:141:ARG:NH2	2.29	0.41
2:9:3078:G:O2'	2:9:3079:U:P	2.78	0.41
7:D:160:ALA:C	7:D:162:ALA:N	2.78	0.41
8:E:54:ASP:OD1	8:E:54:ASP:N	2.54	0.41
9:F:99:THR:O	9:F:100:ASP:HB2	2.21	0.41
12:I:103:VAL:CG1	37:I:5907:HOH:O	2.61	0.41
14:K:101:ASP:C	14:K:103:ALA:N	2.79	0.41
15:L:43:PRO:HG3	15:L:62:VAL:HG21	2.03	0.41
15:L:55:LYS:O	15:L:60:ILE:HD12	2.21	0.41
15:L:62:VAL:C	15:L:63:VAL:HG23	2.46	0.41
15:L:94:LYS:CE	37:L:8580:HOH:O	2.46	0.41
15:L:114:VAL:HG21	15:L:159:THR:HG21	2.03	0.41
16:M:154:LEU:CG	16:M:155:GLU:H	2.28	0.41
16:M:184:ILE:HG22	16:M:185:GLU:N	2.34	0.41
22:S:96:VAL:HG13	22:S:97:ARG:N	2.36	0.41
24:U:45:ARG:C	24:U:47:LYS:N	2.77	0.41
25:V:64:THR:O	25:V:68:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:106:THR:CG2	27:X:107:PRO:HD2	2.51	0.41
1:0:39:G:N2	1:0:444:C:C2	2.89	0.41
1:0:396:U:OP2	31:2:38:ARG:HD2	2.21	0.41
1:0:637:C:OP1	27:X:136:LYS:NZ	2.48	0.41
1:0:1842:A:C4	1:0:1979:G:C6	3.09	0.41
1:0:2111:G:H1'	37:0:8563:HOH:O	2.20	0.41
1:0:2506:A:H2'	1:0:2507:G:C5'	2.51	0.41
1:0:2601:A:N1	13:J:38:SER:HB2	2.36	0.41
1:0:2783:A:O2'	1:0:2784:A:H5'	2.21	0.41
16:M:67:ALA:HA	16:M:71:TRP:HB3	2.03	0.41
25:V:131:PRO:HD2	25:V:134:GLU:HB2	2.02	0.41
1:0:10:U:O2'	1:0:11:A:O5'	2.38	0.40
1:0:66:G:H4'	1:0:69:A:O4'	2.21	0.40
1:0:290:C:O2'	1:0:291:C:H5'	2.20	0.40
1:0:1102:C:H2'	1:0:1103:C:C6	2.56	0.40
1:0:2684:A:H2'	1:0:2685:C:C6	2.56	0.40
1:0:2897:C:H2'	1:0:2898:G:C8	2.55	0.40
4:A:51:ARG:HB2	37:A:8605:HOH:O	2.20	0.40
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.39	0.40
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.50	0.40
8:E:9:GLU:HA	37:E:5240:HOH:O	2.20	0.40
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.88	0.40
11:H:26:LYS:HE3	11:H:28:ILE:HB	2.03	0.40
12:I:49:ARG:O	12:I:50:GLU:C	2.62	0.40
16:M:32:PRO:HD2	16:M:99:GLU:O	2.21	0.40
16:M:93:GLN:HG2	37:M:8556:HOH:O	2.21	0.40
21:R:73:ASP:OD1	21:R:75:GLN:HB2	2.21	0.40
24:U:1:THR:C	24:U:3:LEU:N	2.79	0.40
1:0:226:A:H1'	1:0:393:G:C5	2.56	0.40
1:0:407:A:H3'	37:0:3940:HOH:O	2.21	0.40
1:0:876:A:N3	1:0:876:A:C2'	2.84	0.40
1:0:1025:C:H5'	25:V:23:MET:O	2.21	0.40
1:0:1129:C:H5''	1:0:1130:U:OP2	2.21	0.40
1:0:1154:A:H2'	1:0:1155:G:H8	1.86	0.40
1:0:1314:U:H2'	37:0:5336:HOH:O	2.21	0.40
1:0:1413:A:H2'	1:0:1414:A:O4'	2.21	0.40
1:0:1845:A:H2'	1:0:1846:U:O4'	2.21	0.40
1:0:2269:C:C2'	1:0:2270:G:H5'	2.50	0.40
1:0:2692:G:O2'	1:0:2693:U:OP2	2.40	0.40
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.40
37:0:4811:HOH:O	22:S:3:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:23:THR:HA	5:B:24:PRO:HD3	1.92	0.40
6:C:7:ASP:OD1	6:C:11:ASN:O	2.39	0.40
7:D:27:ILE:O	7:D:69:ILE:HG22	2.21	0.40
7:D:35:ALA:O	7:D:37:ALA:N	2.54	0.40
7:D:48:MET:HE2	7:D:48:MET:HB3	1.98	0.40
7:D:57:THR:C	7:D:58:VAL:HG23	2.46	0.40
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.51	0.40
18:O:7:LYS:CD	18:O:21:VAL:CG2	3.00	0.40
25:V:11:VAL:O	25:V:12:ASN:HB2	2.20	0.40
27:X:187:VAL:HG12	27:X:205:ILE:HA	2.03	0.40
28:Y:25:ARG:O	28:Y:29:VAL:HG23	2.22	0.40
1:O:74:A:H2'	1:O:75:U:C6	2.56	0.40
1:O:424:C:H2'	1:O:425:U:C6	2.55	0.40
1:O:766:A:HO2'	1:O:767:A:H5''	1.85	0.40
1:O:1076:G:C2	1:O:1084:C:C2	3.08	0.40
1:O:1756:G:H1'	37:O:5725:HOH:O	2.20	0.40
5:B:27:ASN:HD22	5:B:27:ASN:H	1.69	0.40
5:B:72:THR:HB	37:B:8604:HOH:O	2.21	0.40
5:B:307:ARG:HD3	37:B:8523:HOH:O	2.20	0.40
7:D:52:THR:N	7:D:70:GLY:O	2.54	0.40
14:K:98:GLU:O	14:K:99:GLU:HB2	2.21	0.40
15:L:12:TRP:O	15:L:15:PRO:HD3	2.21	0.40
15:L:52:LEU:HD13	15:L:116:ASN:CB	2.51	0.40
16:M:90:LEU:CB	16:M:186:LEU:HD22	2.51	0.40
16:M:164:ASP:OD1	16:M:164:ASP:C	2.64	0.40
17:N:47:ARG:NH1	17:N:47:ARG:CG	2.77	0.40
18:O:14:LEU:HD13	18:O:51:ALA:HB2	2.02	0.40
22:S:32:ARG:NH1	22:S:38:ARG:NH1	2.68	0.40
1:O:305:A:C5	1:O:329:A:C2	3.09	0.40
1:O:765:G:O3'	6:C:69:HIS:HB3	2.22	0.40
1:O:2255:A:C6	1:O:2256:G:C5	3.09	0.40
1:O:2388:C:O2'	1:O:2389:U:H5'	2.22	0.40
2:9:3059:C:H6	2:9:3059:C:O5'	2.05	0.40
4:A:81:GLN:HB2	4:A:92:ASN:HD22	1.86	0.40
4:A:212:PRO:HB2	37:A:8559:HOH:O	2.21	0.40
5:B:102:THR:HG21	5:B:182:VAL:O	2.21	0.40
5:B:139:ASP:CB	5:B:165:ARG:HE	2.34	0.40
5:B:207:LYS:HG2	5:B:304:PRO:HB3	2.03	0.40
5:B:316:ARG:N	5:B:317:PRO:HD3	2.37	0.40
7:D:11:HIS:O	7:D:12:GLU:CB	2.68	0.40
8:E:139:GLU:CG	37:E:5919:HOH:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:43:PRO:HD2	11:H:137:ASN:HA	2.03	0.40
20:Q:15:LYS:HE3	37:Q:8575:HOH:O	2.20	0.40
20:Q:84:ALA:O	20:Q:88:PHE:HD1	2.05	0.40
21:R:69:SER:C	21:R:71:ASP:N	2.80	0.40
22:S:71:VAL:CG1	22:S:72:ILE:N	2.84	0.40
23:T:14:GLU:HA	23:T:15:PRO:HD2	1.96	0.40
26:W:61:ARG:HH12	26:W:67:PRO:HD3	1.87	0.40
1:O:290:C:H2'	1:O:291:C:O4'	2.21	0.40
1:O:380:A:OP2	15:L:9:ARG:HD2	2.21	0.40
1:O:412:C:H2'	1:O:413:G:O4'	2.20	0.40
1:O:746:A:C6	17:N:65:LEU:HD13	2.57	0.40
1:O:951:A:C2'	1:O:952:G:H5'	2.51	0.40
1:O:1162:G:H2'	1:O:1162:G:N3	2.36	0.40
1:O:1783:A:O2'	1:O:1784:U:H5'	2.21	0.40
1:O:1878:G:H4'	37:O:3608:HOH:O	2.22	0.40
5:B:76:THR:N	5:B:77:PRO:HD3	2.36	0.40
8:E:81:GLU:HA	8:E:133:VAL:O	2.21	0.40
11:H:26:LYS:NZ	11:H:31:PHE:CZ	2.89	0.40
11:H:42:TYR:HA	11:H:43:PRO:HD3	1.93	0.40
13:J:99:ASP:OD1	13:J:101:ASN:N	2.53	0.40
15:L:32:ARG:NH2	37:L:8596:HOH:O	2.55	0.40
15:L:66:ALA:O	15:L:67:ILE:HD13	2.22	0.40
15:L:139:PRO:HA	15:L:142:LYS:HB2	2.02	0.40
18:O:134:VAL:O	18:O:137:LEU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	235/239 (98%)	210 (89%)	22 (9%)	3 (1%)	9 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	335/337 (99%)	306 (91%)	22 (7%)	7 (2%)	5	25
6	C	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	30	61
7	D	134/176 (76%)	96 (72%)	25 (19%)	13 (10%)	0	3
8	E	170/177 (96%)	162 (95%)	7 (4%)	1 (1%)	21	52
9	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	30
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	152/167 (91%)	134 (88%)	12 (8%)	6 (4%)	2	14
12	I	140/145 (97%)	128 (91%)	9 (6%)	3 (2%)	5	25
13	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	47
14	K	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	9	34
15	L	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	12	41
16	M	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	3	17
17	N	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	O	141/148 (95%)	136 (96%)	4 (3%)	1 (1%)	18	49
19	P	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
20	Q	148/154 (96%)	141 (95%)	6 (4%)	1 (1%)	18	49
21	R	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
22	S	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	6	25
24	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	18
25	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	49
26	W	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	4	21
27	X	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
28	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	34
29	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	1	42/48 (88%)	42 (100%)	0	0	100	100
31	2	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3633/4235 (86%)	3327 (92%)	250 (7%)	56 (2%)	8	32

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP

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Mol	Chain	Res	Type
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	162	SER
11	H	164	ALA
14	K	80	ASP
16	M	154	LEU
16	M	164	ASP
16	M	183	ASP
24	U	43	PRO
4	A	34	ASP
4	A	37	VAL
4	A	132	ASP
5	B	34	GLY
5	B	169	GLY
7	D	11	HIS
7	D	20	LYS
7	D	171	ASP
16	M	162	ASP
16	M	181	ASP
25	V	77	ALA
5	B	107	SER
5	B	184	ASP
6	C	8	LEU
7	D	16	PRO
7	D	36	ASN
7	D	61	PHE
12	I	5	GLU
12	I	7	ASP
12	I	143	LYS
13	J	119	GLN
14	K	21	ARG
15	L	140	ALA
18	O	116	SER
23	T	7	ASP
26	W	77	PHE
28	Y	81	LYS
5	B	185	GLY
11	H	40	PRO
7	D	170	TYR

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Mol	Chain	Res	Type
9	F	64	PRO
11	H	72	VAL
11	H	138	PRO
15	L	165	SER
16	M	167	ASP
24	U	40	PRO
5	B	2	GLN
7	D	96	SER
7	D	147	ALA
11	H	139	ASP
8	E	44	GLY
20	Q	81	PRO
26	W	70	ILE

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	
4	A	179/181 (99%)	166 (93%)	13 (7%)	13	40
5	B	282/282 (100%)	263 (93%)	19 (7%)	15	43
6	C	193/193 (100%)	179 (93%)	14 (7%)	13	40
7	D	117/147 (80%)	108 (92%)	9 (8%)	12	38
8	E	152/155 (98%)	147 (97%)	5 (3%)	33	63
9	F	92/92 (100%)	89 (97%)	3 (3%)	33	63
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	108 (88%)	14 (12%)	5	23
12	I	118/121 (98%)	110 (93%)	8 (7%)	14	42
13	J	106/106 (100%)	103 (97%)	3 (3%)	38	66
14	K	112/126 (89%)	109 (97%)	3 (3%)	39	67
15	L	166/166 (100%)	158 (95%)	8 (5%)	23	54
16	M	149/149 (100%)	141 (95%)	8 (5%)	20	50
17	N	93/93 (100%)	89 (96%)	4 (4%)	26	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	113/116 (97%)	110 (97%)	3 (3%)	39	67
19	P	79/79 (100%)	74 (94%)	5 (6%)	16	45
20	Q	117/121 (97%)	114 (97%)	3 (3%)	40	68
21	R	71/73 (97%)	70 (99%)	1 (1%)	59	76
22	S	105/105 (100%)	100 (95%)	5 (5%)	23	54
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	50 (98%)	1 (2%)	48	72
25	V	130/130 (100%)	121 (93%)	9 (7%)	14	41
26	W	66/73 (90%)	61 (92%)	5 (8%)	12	39
27	X	120/195 (62%)	111 (92%)	9 (8%)	12	39
28	Y	56/56 (100%)	54 (96%)	2 (4%)	31	62
29	Z	46/46 (100%)	46 (100%)	0	100	100
30	1	42/44 (96%)	41 (98%)	1 (2%)	43	69
31	2	79/79 (100%)	76 (96%)	3 (4%)	29	60
All	All	3027/3441 (88%)	2869 (95%)	158 (5%)	21	51

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	55	VAL
4	A	68	ILE
4	A	69	LEU
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	175	LYS
4	A	179	MET
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	33	ASP
5	B	53	LEU

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Mol	Chain	Res	Type
5	B	63	GLU
5	B	84	LEU
5	B	97	LEU
5	B	98	THR
5	B	103	ASP
5	B	162	MET
5	B	195	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	304	PRO
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	67	GLN
6	C	78	ARG
6	C	94	THR
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS
7	D	50	VAL
7	D	92	GLU
7	D	95	THR
7	D	99	ASP
7	D	131	THR
7	D	136	ARG
7	D	137	PRO
7	D	149	ARG
8	E	7	ILE
8	E	36	PRO
8	E	54	ASP
8	E	86	VAL
8	E	102	VAL

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Mol	Chain	Res	Type
9	F	1	PRO
9	F	12	LEU
9	F	46	GLU
11	H	18	GLU
11	H	30	GLN
11	H	59	ASN
11	H	61	LEU
11	H	72	VAL
11	H	73	GLN
11	H	82	LYS
11	H	85	ILE
11	H	86	ARG
11	H	93	ILE
11	H	118	PRO
11	H	142	VAL
11	H	150	LYS
11	H	166	ASN
12	I	46	ILE
12	I	52	GLN
12	I	74	ARG
12	I	93	ARG
12	I	120	SER
12	I	125	SER
12	I	127	ILE
12	I	131	THR
13	J	7	ASP
13	J	10	GLN
13	J	98	VAL
14	K	35	ARG
14	K	117	GLU
14	K	140	VAL
15	L	38	VAL
15	L	46	LEU
15	L	81	ARG
15	L	87	MET
15	L	93	ARG
15	L	99	ARG
15	L	159	THR
15	L	164	THR
16	M	12	ARG
16	M	26	LEU
16	M	43	VAL

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Mol	Chain	Res	Type
16	M	47	LEU
16	M	127	LEU
16	M	128	ASP
16	M	152	GLU
16	M	163	PHE
17	N	3	THR
17	N	28	ASP
17	N	98	LEU
17	N	111	VAL
18	O	52	LYS
18	O	91	LYS
18	O	98	ILE
19	P	11	ARG
19	P	16	ASN
19	P	54	PRO
19	P	57	ASP
19	P	95	GLU
20	Q	13	THR
20	Q	39	THR
20	Q	82	GLU
21	R	10	VAL
22	S	26	THR
22	S	39	ASN
22	S	47	THR
22	S	48	VAL
22	S	96	VAL
24	U	43	PRO
25	V	4	LEU
25	V	35	VAL
25	V	45	VAL
25	V	52	VAL
25	V	73	LEU
25	V	122	ARG
25	V	142	ASP
25	V	146	ILE
25	V	154	ARG
26	W	15	ARG
26	W	27	ASP
26	W	52	PRO
26	W	66	THR
26	W	72	VAL
27	X	103	THR

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Mol	Chain	Res	Type
27	X	141	THR
27	X	154	ARG
27	X	163	THR
27	X	172	THR
27	X	189	ASN
27	X	200	THR
27	X	203	VAL
27	X	235	GLU
28	Y	11	THR
28	Y	64	ILE
30	1	18	ASN
31	2	14	CYS
31	2	42	ARG
31	2	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	47	HIS
4	A	92	ASN
4	A	127	GLN
4	A	199	HIS
4	A	218	ASN
5	B	27	ASN
5	B	55	ASN
5	B	94	GLN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	260	HIS
5	B	318	ASN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	67	GLN
6	C	129	HIS
6	C	163	HIS
7	D	103	ASN
8	E	96	ASN
8	E	106	ASN
8	E	119	HIS

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Mol	Chain	Res	Type
8	E	143	GLN
10	G	17	GLN
10	G	64	ASN
11	H	8	ASN
11	H	30	GLN
11	H	35	ASN
11	H	45	GLN
11	H	55	GLN
11	H	58	HIS
11	H	59	ASN
11	H	74	ASN
11	H	91	HIS
11	H	129	ASN
11	H	130	HIS
11	H	137	ASN
11	H	158	ASN
11	H	166	ASN
12	I	52	GLN
12	I	107	ASN
12	I	126	ASN
13	J	10	GLN
14	K	18	HIS
14	K	41	HIS
14	K	42	ASN
14	K	58	GLN
14	K	116	HIS
15	L	26	HIS
15	L	58	GLN
15	L	89	ASN
15	L	176	GLN
16	M	107	ASN
16	M	140	GLN
16	M	153	GLN
17	N	53	GLN
18	O	50	GLN
18	O	66	GLN
18	O	73	HIS
18	O	118	GLN
19	P	16	ASN
19	P	40	HIS
19	P	94	GLN
20	Q	22	GLN

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Mol	Chain	Res	Type
20	Q	61	GLN
20	Q	94	ASN
20	Q	98	ASN
20	Q	113	HIS
20	Q	117	HIS
20	Q	122	GLN
20	Q	140	GLN
21	R	51	GLN
21	R	53	ASN
21	R	55	GLN
22	S	39	ASN
22	S	73	HIS
22	S	95	ASN
23	T	39	ASN
24	U	4	HIS
24	U	60	GLN
25	V	6	GLN
25	V	14	HIS
25	V	27	HIS
25	V	110	GLN
25	V	119	HIS
25	V	125	HIS
25	V	141	HIS
26	W	23	HIS
27	X	133	HIS
27	X	134	HIS
27	X	149	GLN
27	X	153	GLN
27	X	189	ASN
28	Y	33	HIS
29	Z	8	GLN
29	Z	16	HIS
29	Z	28	HIS
30	1	16	ASN
30	1	18	ASN
30	1	37	HIS
30	1	41	HIS
30	1	45	ASN
31	2	30	GLN
31	2	39	GLN
31	2	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2748/2922 (94%)	300 (10%)	96 (3%)
2	9	121/122 (99%)	24 (19%)	7 (5%)
3	3	10/28 (35%)	3 (30%)	0
All	All	2879/3072 (93%)	327 (11%)	103 (3%)

All (327) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	59	A
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	175	G
1	0	176	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U

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Mol	Chain	Res	Type
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	338	C
1	0	339	A
1	0	345	G
1	0	358	G
1	0	368	C
1	0	381	G
1	0	396	U
1	0	397	A
1	0	417	G
1	0	418	C
1	0	428	G
1	0	461	C
1	0	464	G
1	0	465	U
1	0	486	A
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	518	G
1	0	519	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G

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Mol	Chain	Res	Type
1	0	660	A
1	0	688	A
1	0	701	U
1	0	705	C
1	0	717	C
1	0	747	G
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	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	885	G
1	0	894	A
1	0	898	G
1	0	899	C
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	952	G
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G

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Mol	Chain	Res	Type
1	0	1073	A
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1124	A
1	0	1130	U
1	0	1137	G
1	0	1138	G
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	1184	C
1	0	1185	U
1	0	1192	A
1	0	1206	U
1	0	1215	A
1	0	1216	G
1	0	1232	A
1	0	1233	A
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1245	C
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1370	G
1	0	1377	C
1	0	1380	U
1	0	1381	A
1	0	1407	A
1	0	1448	A

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Mol	Chain	Res	Type
1	0	1451	C
1	0	1473	U
1	0	1474	C
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1702	U
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1753	C
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1857	A
1	0	1875	A
1	0	1878	G

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Mol	Chain	Res	Type
1	0	1879	U
1	0	1904	A
1	0	1919	A
1	0	1941	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1972	U
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	1995	G
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	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	2103	A
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	2316	G
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2346	C

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2370	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2503	A
1	0	2504	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2681	A
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

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Mol	Chain	Res	Type
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2836	G
1	0	2837	U
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2897	C
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3003	A
2	9	3004	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3026	C
2	9	3033	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3055	U
2	9	3056	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3103	A
2	9	3104	A
2	9	3113	C
2	9	3114	G
2	9	3122	C
3	3	4	G
3	3	75	C
3	3	76	A

All (103) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	59	A
1	0	87	C
1	0	114	A
1	0	129	A
1	0	166	A
1	0	169	A
1	0	175	G
1	0	236	A
1	0	270	U
1	0	284	C
1	0	337	A
1	0	338	C
1	0	396	U
1	0	417	G
1	0	428	G
1	0	464	G
1	0	518	G
1	0	603	A
1	0	604	G
1	0	628	A
1	0	699	C
1	0	716	G
1	0	776	A
1	0	834	G
1	0	857	A
1	0	868	G
1	0	871	G
1	0	877	G
1	0	893	C
1	0	898	G
1	0	952	G
1	0	1072	G
1	0	1080	C
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1184	C
1	0	1215	A
1	0	1232	A
1	0	1237	U
1	0	1352	A

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Mol	Chain	Res	Type
1	0	1370	G
1	0	1380	U
1	0	1406	A
1	0	1431	C
1	0	1450	C
1	0	1488	U
1	0	1524	U
1	0	1527	A
1	0	1563	G
1	0	1603	A
1	0	1653	A
1	0	1684	A
1	0	1730	G
1	0	1752	G
1	0	1842	A
1	0	1856	C
1	0	1874	U
1	0	1878	G
1	0	1941	A
1	0	1942	A
1	0	1970	G
1	0	1971	G
1	0	1977	U
1	0	1979	G
1	0	1980	U
1	0	1995	G
1	0	2011	A
1	0	2072	G
1	0	2101	A
1	0	2102	G
1	0	2237	G
1	0	2283	G
1	0	2292	C
1	0	2309	C
1	0	2313	C
1	0	2316	G
1	0	2320	U
1	0	2369	A
1	0	2379	G
1	0	2421	G
1	0	2467	A
1	0	2469	A

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Mol	Chain	Res	Type
1	0	2483	A
1	0	2503	A
1	0	2526	C
1	0	2536	C
1	0	2601	A
1	0	2749	U
1	0	2791	U
1	0	2811	A
1	0	2836	G
1	0	2837	U
1	0	2896	A
1	0	2902	A
2	9	3002	U
2	9	3023	U
2	9	3024	U
2	9	3055	U
2	9	3065	A
2	9	3103	A
2	9	3113	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 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	19 (0%) 84 68	28, 55, 104, 159	0
2	9	122/122 (100%)	-0.02	4 (3%) 49 29	37, 71, 106, 162	0
3	3	12/28 (42%)	0.74	0 100 100	80, 132, 141, 145	0
4	A	237/239 (99%)	-0.03	2 (0%) 82 65	36, 64, 100, 123	0
5	B	337/337 (100%)	-0.02	1 (0%) 90 80	32, 65, 90, 100	0
6	C	246/246 (100%)	-0.15	0 100 100	27, 58, 84, 91	0
7	D	140/176 (79%)	0.80	13 (9%) 14 8	66, 110, 129, 134	0
8	E	172/177 (97%)	0.19	4 (2%) 61 39	49, 75, 99, 106	0
9	F	119/119 (100%)	0.33	1 (0%) 82 65	62, 87, 111, 120	0
10	G	29/348 (8%)	0.93	3 (10%) 12 6	79, 97, 104, 106	0
11	H	156/167 (93%)	0.15	6 (3%) 44 25	36, 62, 87, 94	0
12	I	142/145 (97%)	-0.15	0 100 100	42, 55, 80, 99	0
13	J	132/132 (100%)	0.06	1 (0%) 82 65	42, 64, 89, 97	0
14	K	145/164 (88%)	0.22	7 (4%) 35 19	33, 82, 117, 125	0
15	L	194/194 (100%)	0.04	4 (2%) 63 42	40, 58, 78, 90	0
16	M	186/186 (100%)	0.52	9 (4%) 35 19	48, 80, 122, 133	0
17	N	115/115 (100%)	0.09	0 100 100	54, 69, 86, 89	0
18	O	143/148 (96%)	0.09	1 (0%) 84 68	45, 68, 85, 94	0
19	P	95/95 (100%)	-0.15	0 100 100	38, 55, 72, 90	0
20	Q	150/154 (97%)	-0.28	0 100 100	36, 51, 74, 84	0
21	R	81/84 (96%)	-0.00	0 100 100	56, 77, 96, 100	0
22	S	119/119 (100%)	0.08	2 (1%) 69 48	50, 70, 97, 116	0
23	T	53/66 (80%)	0.02	0 100 100	53, 67, 82, 91	0
24	U	65/70 (92%)	0.34	3 (4%) 37 20	64, 90, 123, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	154/154 (100%)	-0.29	0 100 100	38, 53, 74, 84	0
26	W	82/91 (90%)	0.14	1 (1%) 76 58	51, 66, 87, 107	0
27	X	142/240 (59%)	-0.19	1 (0%) 84 68	31, 54, 75, 96	0
28	Y	73/73 (100%)	0.48	1 (1%) 73 53	57, 73, 87, 95	0
29	Z	56/56 (100%)	-0.51	0 100 100	34, 44, 51, 53	0
30	1	46/48 (95%)	0.40	0 100 100	48, 80, 110, 119	0
31	2	92/92 (100%)	0.15	0 100 100	47, 68, 82, 97	0
All	All	6589/7307 (90%)	-0.12	83 (1%) 75 56	27, 62, 106, 162	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	1	PRO	5.2
24	U	1	THR	4.9
16	M	162	ASP	4.3
14	K	83	GLU	4.2
2	9	3025	G	4.1
7	D	10	PHE	3.9
1	0	10	U	3.6
1	0	1192	A	3.4
2	9	3001	U	3.4
28	Y	22	ILE	3.4
11	H	40	PRO	3.3
14	K	82	ALA	3.3
1	0	1176	C	3.3
2	9	3024	U	3.2
1	0	1172	G	3.1
1	0	138	U	3.1
1	0	1173	A	3.1
2	9	3002	U	3.0
22	S	1	SER	3.0
1	0	1175	G	3.0
1	0	2748	G	3.0
15	L	63	VAL	3.0
11	H	39	GLY	2.9
8	E	10	ASP	2.9
4	A	36	ASP	2.9
15	L	89	ASN	2.9
18	O	116	SER	2.8
10	G	26	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	2344	G	2.7
10	G	27	ILE	2.7
15	L	87	MET	2.6
11	H	38	ALA	2.6
1	0	1193	A	2.6
7	D	174	VAL	2.6
24	U	2	VAL	2.6
1	0	2345	A	2.6
16	M	158	LEU	2.5
1	0	960	G	2.5
14	K	102	ASP	2.5
16	M	168	LEU	2.5
4	A	31	LYS	2.5
1	0	1160	G	2.5
7	D	63	ILE	2.5
10	G	63	ARG	2.5
16	M	159	TYR	2.5
22	S	119	ALA	2.4
1	0	1161	A	2.4
7	D	55	LYS	2.4
7	D	62	ASP	2.4
16	M	38	LYS	2.4
27	X	235	GLU	2.4
16	M	186	LEU	2.4
11	H	167	ALA	2.3
26	W	65	ASN	2.3
14	K	104	ASP	2.3
14	K	89	PHE	2.3
9	F	90	GLU	2.3
7	D	107	GLY	2.3
16	M	167	ASP	2.3
1	0	1171	A	2.3
7	D	22	VAL	2.3
14	K	56	LYS	2.3
8	E	100	ASP	2.3
1	0	1964	U	2.2
7	D	35	ALA	2.2
8	E	45	ASP	2.2
7	D	131	THR	2.2
7	D	43	GLU	2.2
1	0	1524	U	2.2
8	E	126	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
11	H	41	THR	2.1
11	H	164	ALA	2.1
15	L	194	ALA	2.1
14	K	81	VAL	2.1
7	D	72	LYS	2.1
16	M	1	ALA	2.1
16	M	160	SER	2.1
7	D	138	GLY	2.1
13	J	119	GLN	2.1
24	U	39	ALA	2.0
7	D	21	VAL	2.0
1	0	1167	G	2.0
1	0	1181	A	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8119	1/1	0.32	0.20	112,112,112,112	0
34	NA	9	8351	1/1	0.58	0.21	91,91,91,91	0
34	NA	0	8385	1/1	0.60	0.41	72,72,72,72	0
34	NA	0	8329	1/1	0.64	0.46	108,108,108,108	0
34	NA	R	8312	1/1	0.64	0.32	167,167,167,167	0
34	NA	0	8363	1/1	0.69	0.23	68,68,68,68	0
32	MG	2	8118	1/1	0.74	0.12	70,70,70,70	0
34	NA	0	8371	1/1	0.75	0.29	51,51,51,51	0
34	NA	0	8341	1/1	0.75	0.13	52,52,52,52	0
34	NA	Q	8386	1/1	0.76	0.50	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8384	1/1	0.79	0.27	122,122,122,122	0
34	NA	0	8328	1/1	0.80	0.27	51,51,51,51	0
34	NA	0	8360	1/1	0.81	0.36	47,47,47,47	0
34	NA	0	8369	1/1	0.81	0.31	84,84,84,84	0
35	CL	0	8515	1/1	0.81	0.27	107,107,107,107	0
32	MG	0	8023	1/1	0.82	0.11	35,35,35,35	0
34	NA	0	8381	1/1	0.82	0.09	76,76,76,76	0
34	NA	H	8322	1/1	0.83	0.29	59,59,59,59	0
32	MG	0	8050	1/1	0.83	0.11	71,71,71,71	0
34	NA	0	8367	1/1	0.84	0.18	60,60,60,60	0
34	NA	0	8373	1/1	0.84	0.18	58,58,58,58	0
35	CL	N	8508	1/1	0.84	0.14	92,92,92,92	0
32	MG	0	8044	1/1	0.85	0.10	74,74,74,74	0
32	MG	A	8065	1/1	0.85	0.12	38,38,38,38	0
32	MG	0	8092	1/1	0.85	0.18	89,89,89,89	0
34	NA	0	8310	1/1	0.86	0.15	35,35,35,35	0
35	CL	0	8522	1/1	0.86	0.33	89,89,89,89	0
34	NA	0	8324	1/1	0.86	0.29	55,55,55,55	0
34	NA	0	8366	1/1	0.87	0.09	66,66,66,66	0
34	NA	0	8333	1/1	0.87	0.16	52,52,52,52	0
35	CL	A	8509	1/1	0.87	0.18	78,78,78,78	0
32	MG	0	8103	1/1	0.87	0.13	67,67,67,67	0
32	MG	0	8114	1/1	0.88	0.17	93,93,93,93	0
32	MG	0	8082	1/1	0.88	0.13	58,58,58,58	0
34	NA	0	8365	1/1	0.88	0.34	62,62,62,62	0
34	NA	0	8340	1/1	0.88	0.17	47,47,47,47	0
34	NA	0	8301	1/1	0.88	0.06	44,44,44,44	0
34	NA	0	8357	1/1	0.88	0.14	66,66,66,66	0
34	NA	9	8383	1/1	0.88	0.21	71,71,71,71	0
34	NA	0	8354	1/1	0.89	0.12	51,51,51,51	0
34	NA	Q	8337	1/1	0.89	0.10	57,57,57,57	0
34	NA	0	8326	1/1	0.89	0.29	98,98,98,98	0
34	NA	0	8321	1/1	0.89	0.24	42,42,42,42	0
34	NA	0	8379	1/1	0.90	0.16	53,53,53,53	0
34	NA	0	8327	1/1	0.90	0.08	44,44,44,44	0
34	NA	0	8352	1/1	0.90	0.20	54,54,54,54	0
32	MG	0	8087	1/1	0.90	0.08	60,60,60,60	0
32	MG	0	8085	1/1	0.90	0.10	91,91,91,91	0
34	NA	0	8302	1/1	0.90	0.09	52,52,52,52	0
34	NA	0	8303	1/1	0.90	0.15	58,58,58,58	0
34	NA	0	8362	1/1	0.91	0.18	59,59,59,59	0
34	NA	0	8308	1/1	0.91	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8375	1/1	0.91	0.37	85,85,85,85	0
34	NA	K	8380	1/1	0.91	0.17	63,63,63,63	0
34	NA	0	8377	1/1	0.91	0.28	77,77,77,77	0
34	NA	0	8378	1/1	0.91	0.29	38,38,38,38	0
32	MG	0	8011	1/1	0.91	0.31	1,1,1,1	0
34	NA	0	8355	1/1	0.91	0.18	50,50,50,50	0
34	NA	0	8382	1/1	0.91	0.30	99,99,99,99	0
34	NA	0	8332	1/1	0.91	0.09	47,47,47,47	0
35	CL	B	8519	1/1	0.91	0.18	65,65,65,65	0
34	NA	0	8343	1/1	0.91	0.12	40,40,40,40	0
32	MG	0	8049	1/1	0.92	0.08	59,59,59,59	0
34	NA	C	8304	1/1	0.92	0.07	41,41,41,41	0
34	NA	0	8374	1/1	0.92	0.30	62,62,62,62	0
34	NA	0	8315	1/1	0.92	0.13	65,65,65,65	0
34	NA	0	8361	1/1	0.92	0.12	44,44,44,44	0
34	NA	0	8334	1/1	0.92	0.10	39,39,39,39	0
32	MG	0	8100	1/1	0.92	0.17	99,99,99,99	0
35	CL	0	8505	1/1	0.92	0.11	69,69,69,69	0
32	MG	0	8101	1/1	0.92	0.09	48,48,48,48	0
32	MG	0	8046	1/1	0.92	0.08	80,80,80,80	0
32	MG	0	8053	1/1	0.92	0.09	59,59,59,59	0
34	NA	0	8306	1/1	0.92	0.25	57,57,57,57	0
35	CL	L	8518	1/1	0.92	0.10	55,55,55,55	0
32	MG	0	8090	1/1	0.92	0.09	46,46,46,46	0
35	CL	X	8520	1/1	0.92	0.11	47,47,47,47	0
32	MG	0	8081	1/1	0.93	0.08	79,79,79,79	0
32	MG	0	8024	1/1	0.93	0.69	187,187,187,187	0
35	CL	0	8503	1/1	0.93	0.17	61,61,61,61	0
32	MG	0	8116	1/1	0.93	0.06	58,58,58,58	0
35	CL	0	8513	1/1	0.93	0.12	68,68,68,68	0
35	CL	0	8514	1/1	0.93	0.09	54,54,54,54	0
32	MG	0	8045	1/1	0.93	0.10	70,70,70,70	0
35	CL	0	8517	1/1	0.93	0.07	56,56,56,56	0
32	MG	0	8070	1/1	0.93	0.09	63,63,63,63	0
32	MG	0	8102	1/1	0.93	0.11	48,48,48,48	0
34	NA	0	8311	1/1	0.93	0.10	48,48,48,48	0
35	CL	K	8510	1/1	0.93	0.06	75,75,75,75	0
34	NA	0	8314	1/1	0.93	0.08	32,32,32,32	0
34	NA	L	8347	1/1	0.93	0.07	31,31,31,31	0
34	NA	0	8368	1/1	0.93	0.17	58,58,58,58	0
33	K	0	8202	1/1	0.94	0.16	76,76,76,76	0
32	MG	0	8076	1/1	0.94	0.07	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8089	1/1	0.94	0.10	84,84,84,84	0
32	MG	0	8084	1/1	0.94	0.06	30,30,30,30	0
32	MG	9	8095	1/1	0.94	0.13	80,80,80,80	0
35	CL	I	8502	1/1	0.94	0.14	74,74,74,74	0
34	NA	0	8307	1/1	0.94	0.08	55,55,55,55	0
32	MG	0	8054	1/1	0.94	0.07	25,25,25,25	0
35	CL	M	8507	1/1	0.94	0.12	66,66,66,66	0
32	MG	0	8112	1/1	0.94	0.10	59,59,59,59	0
34	NA	0	8353	1/1	0.94	0.07	49,49,49,49	0
35	CL	0	8511	1/1	0.95	0.15	87,87,87,87	0
32	MG	0	8094	1/1	0.95	0.12	63,63,63,63	0
34	NA	0	8305	1/1	0.95	0.08	44,44,44,44	0
32	MG	Y	8105	1/1	0.95	0.07	28,28,28,28	0
34	NA	0	8356	1/1	0.95	0.18	62,62,62,62	0
34	NA	0	8372	1/1	0.95	0.19	66,66,66,66	0
34	NA	0	8323	1/1	0.95	0.13	50,50,50,50	0
32	MG	0	8009	1/1	0.95	0.05	18,18,18,18	0
32	MG	0	8064	1/1	0.95	0.20	37,37,37,37	0
32	MG	0	8015	1/1	0.95	0.07	23,23,23,23	0
34	NA	0	8344	1/1	0.95	0.03	31,31,31,31	0
34	NA	0	8364	1/1	0.95	0.10	51,51,51,51	0
34	NA	0	8349	1/1	0.95	0.06	59,59,59,59	0
32	MG	0	8043	1/1	0.95	0.07	48,48,48,48	0
36	CD	N	8405	1/1	0.95	0.07	118,118,118,118	0
32	MG	0	8104	1/1	0.96	0.04	52,52,52,52	0
34	NA	0	8370	1/1	0.96	0.20	53,53,53,53	0
34	NA	0	8358	1/1	0.96	0.25	91,91,91,91	0
34	NA	0	8359	1/1	0.96	0.27	72,72,72,72	0
32	MG	0	8067	1/1	0.96	0.05	57,57,57,57	0
32	MG	0	8088	1/1	0.96	0.10	36,36,36,36	0
32	MG	0	8059	1/1	0.96	0.06	76,76,76,76	0
35	CL	I	8501	1/1	0.96	0.07	80,80,80,80	0
34	NA	0	8330	1/1	0.96	0.05	38,38,38,38	0
35	CL	I	8521	1/1	0.96	0.08	66,66,66,66	0
34	NA	Q	8338	1/1	0.96	0.06	68,68,68,68	0
34	NA	0	8331	1/1	0.96	0.16	66,66,66,66	0
32	MG	0	8075	1/1	0.96	0.06	56,56,56,56	0
32	MG	0	8051	1/1	0.96	0.06	89,89,89,89	0
34	NA	0	8325	1/1	0.96	0.08	56,56,56,56	0
34	NA	0	8335	1/1	0.96	0.13	58,58,58,58	0
34	NA	0	8342	1/1	0.97	0.10	46,46,46,46	0
32	MG	0	8115	1/1	0.97	0.04	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	0	8516	1/1	0.97	0.13	51,51,51,51	0
32	MG	0	8047	1/1	0.97	0.06	74,74,74,74	0
34	NA	I	8346	1/1	0.97	0.07	43,43,43,43	0
32	MG	0	8041	1/1	0.97	0.04	62,62,62,62	0
34	NA	0	8376	1/1	0.97	0.10	53,53,53,53	0
34	NA	0	8319	1/1	0.97	0.07	40,40,40,40	0
32	MG	0	8057	1/1	0.97	0.11	38,38,38,38	0
32	MG	0	8042	1/1	0.97	0.07	52,52,52,52	0
32	MG	A	8066	1/1	0.97	0.05	60,60,60,60	0
32	MG	J	8069	1/1	0.97	0.05	72,72,72,72	0
34	NA	0	8339	1/1	0.97	0.04	25,25,25,25	0
32	MG	0	8096	1/1	0.97	0.04	49,49,49,49	0
35	CL	0	8512	1/1	0.97	0.08	50,50,50,50	0
35	CL	2	8504	1/1	0.97	0.07	67,67,67,67	0
32	MG	0	8040	1/1	0.97	0.06	67,67,67,67	0
32	MG	0	8072	1/1	0.98	0.07	114,114,114,114	0
32	MG	0	8093	1/1	0.98	0.04	38,38,38,38	0
32	MG	0	8037	1/1	0.98	0.04	72,72,72,72	0
34	NA	P	8348	1/1	0.98	0.04	34,34,34,34	0
32	MG	S	8073	1/1	0.98	0.04	59,59,59,59	0
32	MG	0	8001	1/1	0.98	0.04	43,43,43,43	0
32	MG	0	8097	1/1	0.98	0.10	36,36,36,36	0
32	MG	0	8098	1/1	0.98	0.13	50,50,50,50	0
32	MG	0	8099	1/1	0.98	0.06	57,57,57,57	0
32	MG	0	8079	1/1	0.98	0.04	38,38,38,38	0
32	MG	0	8012	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8013	1/1	0.98	0.04	57,57,57,57	0
34	NA	0	8336	1/1	0.98	0.03	48,48,48,48	0
32	MG	0	8083	1/1	0.98	0.08	58,58,58,58	0
32	MG	0	8063	1/1	0.98	0.06	107,107,107,107	0
32	MG	0	8111	1/1	0.98	0.05	45,45,45,45	0
32	MG	0	8025	1/1	0.98	0.03	32,32,32,32	0
32	MG	0	8113	1/1	0.98	0.07	53,53,53,53	0
34	NA	0	8313	1/1	0.98	0.05	57,57,57,57	0
32	MG	0	8028	1/1	0.98	0.06	52,52,52,52	0
34	NA	0	8350	1/1	0.98	0.14	36,36,36,36	0
32	MG	0	8068	1/1	0.98	0.03	70,70,70,70	0
34	NA	0	8316	1/1	0.98	0.13	47,47,47,47	0
34	NA	0	8317	1/1	0.98	0.04	51,51,51,51	0
32	MG	0	8052	1/1	0.98	0.05	36,36,36,36	0
34	NA	0	8320	1/1	0.98	0.04	25,25,25,25	0
32	MG	0	8117	1/1	0.98	0.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	Q	8506	1/1	0.98	0.09	68,68,68,68	0
34	NA	A	8345	1/1	0.98	0.06	53,53,53,53	0
32	MG	0	8071	1/1	0.98	0.04	100,100,100,100	0
32	MG	0	8091	1/1	0.98	0.04	47,47,47,47	0
32	MG	0	8027	1/1	0.99	0.05	43,43,43,43	0
32	MG	0	8004	1/1	0.99	0.04	60,60,60,60	0
32	MG	0	8030	1/1	0.99	0.04	44,44,44,44	0
32	MG	0	8035	1/1	0.99	0.07	55,55,55,55	0
32	MG	0	8016	1/1	0.99	0.03	55,55,55,55	0
32	MG	0	8039	1/1	0.99	0.02	53,53,53,53	0
32	MG	0	8021	1/1	0.99	0.05	28,28,28,28	0
34	NA	0	8318	1/1	0.99	0.05	38,38,38,38	0
32	MG	0	8074	1/1	0.99	0.04	27,27,27,27	0
32	MG	0	8022	1/1	0.99	0.04	41,41,41,41	0
32	MG	0	8006	1/1	0.99	0.02	57,57,57,57	0
32	MG	B	8055	1/1	0.99	0.05	37,37,37,37	0
32	MG	0	8056	1/1	0.99	0.02	67,67,67,67	0
32	MG	0	8080	1/1	0.99	0.03	44,44,44,44	0
32	MG	0	8007	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8008	1/1	0.99	0.03	45,45,45,45	0
33	K	0	8201	1/1	0.99	0.11	89,89,89,89	0
32	MG	0	8060	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8061	1/1	0.99	0.05	36,36,36,36	0
34	NA	H	8309	1/1	0.99	0.05	24,24,24,24	0
32	MG	0	8062	1/1	0.99	0.05	63,63,63,63	0
32	MG	0	8106	1/1	0.99	0.04	45,45,45,45	0
32	MG	0	8107	1/1	0.99	0.04	61,61,61,61	0
32	MG	0	8108	1/1	0.99	0.07	83,83,83,83	0
32	MG	0	8110	1/1	0.99	0.10	30,30,30,30	0
32	MG	0	8086	1/1	0.99	0.06	67,67,67,67	0
36	CD	T	8401	1/1	0.99	0.02	82,82,82,82	0
36	CD	Y	8403	1/1	0.99	0.02	79,79,79,79	0
36	CD	2	8404	1/1	0.99	0.03	74,74,74,74	0
32	MG	0	8026	1/1	1.00	0.02	35,35,35,35	0
32	MG	0	8017	1/1	1.00	0.03	34,34,34,34	0
32	MG	0	8018	1/1	1.00	0.05	48,48,48,48	0
32	MG	0	8029	1/1	1.00	0.02	73,73,73,73	0
32	MG	0	8019	1/1	1.00	0.04	41,41,41,41	0
32	MG	0	8048	1/1	1.00	0.02	33,33,33,33	0
32	MG	0	8031	1/1	1.00	0.04	43,43,43,43	0
32	MG	0	8032	1/1	1.00	0.05	42,42,42,42	0
32	MG	0	8033	1/1	1.00	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8034	1/1	1.00	0.02	42,42,42,42	0
32	MG	0	8077	1/1	1.00	0.02	34,34,34,34	0
32	MG	0	8020	1/1	1.00	0.03	29,29,29,29	0
32	MG	0	8036	1/1	1.00	0.04	45,45,45,45	0
32	MG	0	8005	1/1	1.00	0.02	66,66,66,66	0
32	MG	X	8109	1/1	1.00	0.06	34,34,34,34	0
32	MG	0	8038	1/1	1.00	0.01	47,47,47,47	0
32	MG	2	8078	1/1	1.00	0.02	46,46,46,46	0
32	MG	0	8058	1/1	1.00	0.03	41,41,41,41	0
32	MG	0	8003	1/1	1.00	0.05	26,26,26,26	0
32	MG	0	8014	1/1	1.00	0.08	24,24,24,24	0
32	MG	0	8010	1/1	1.00	0.02	34,34,34,34	0
36	CD	Z	8402	1/1	1.00	0.03	68,68,68,68	0
32	MG	0	8002	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.