



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:03 PM GMT

PDB ID : 1VQ6
Title : The structure of c-hpmn and CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.70 Å(reported)

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

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

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

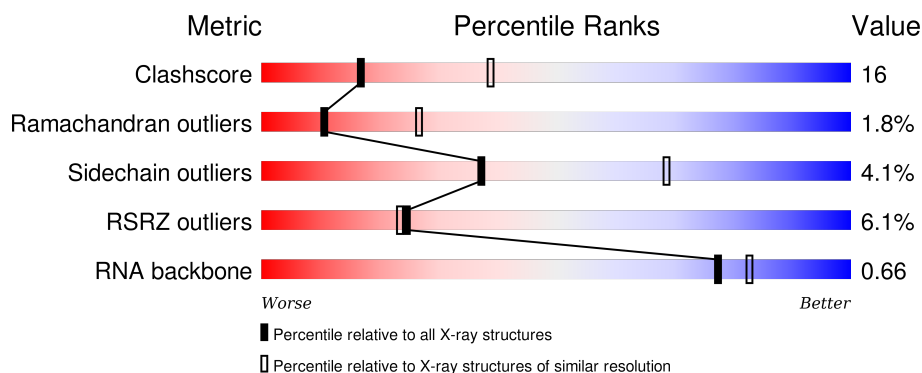
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	3	
4	5	6	
5	A	240	

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Mol	Chain	Length	Quality of chain
6	B	338	
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	

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Mol	Chain	Length	Quality of chain
31	2	50	
32	3	92	
33	I	162	

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	MG	0	8038	-	-	-	X
34	MG	0	8060	-	-	-	X
35	K	0	9001	-	-	-	X
36	NA	0	9110	-	-	-	X
36	NA	0	9114	-	-	-	X
36	NA	0	9120	-	-	-	X
36	NA	0	9121	-	-	-	X
36	NA	0	9125	-	-	-	X
36	NA	0	9129	-	-	-	X
36	NA	0	9140	-	-	-	X
36	NA	0	9150	-	-	-	X
36	NA	0	9156	-	-	-	X
36	NA	0	9161	-	-	-	X
36	NA	0	9162	-	-	-	X
36	NA	0	9164	-	-	-	X
36	NA	0	9165	-	-	-	X
36	NA	0	9168	-	-	-	X
36	NA	0	9169	-	-	-	X
36	NA	0	9171	-	-	-	X
36	NA	0	9172	-	-	-	X
36	NA	0	9173	-	-	-	X
36	NA	0	9174	-	-	-	X
36	NA	0	9176	-	-	-	X
36	NA	0	9177	-	-	-	X
36	NA	0	9178	-	-	-	X
36	NA	0	9182	-	-	-	X
36	NA	9	9183	-	-	-	X
36	NA	L	9180	-	-	-	X
36	NA	R	9186	-	-	-	X
37	CL	0	9315	-	-	-	X
37	CL	0	9316	-	-	-	X
37	CL	B	9319	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99029 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
			59021	26350	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 5'-R(*CP*(5AA)*(HFA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			52	30	9	12	1			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	0	0	0
			82	46	13	21	2			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	107	Total	Mg	0	0
			107	107		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	B	2	Total	Mg	0	0
			2	2		
34	A	2	Total	Mg	0	0
			2	2		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		
34	3	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	73	Total	Na	0	0
			73	73		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	H	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	A	1	Total 1	Na 1	0	0
36	R	3	Total 3	Na 3	0	0
36	9	2	Total 2	Na 2	0	0
36	L	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	8	Total 8	Cl 8	0	0
37	J	3	Total 3	Cl 3	0	0
37	K	1	Total 1	Cl 1	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	1	Total	Cl	0	0
			1	1		
37	3	1	Total	Cl	0	0
			1	1		
37	M	1	Total	Cl	0	0
			1	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5764	Total	O	0	0
			5764	5764		
39	9	135	Total	O	0	0
			135	135		
39	4	1	Total	O	0	0
			1	1		
39	5	1	Total	O	0	0
			1	1		
39	A	120	Total	O	0	0
			120	120		
39	B	156	Total	O	0	0
			156	156		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	49	Total	O	0	0
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	F	23	Total 23	O 23	0	0
39	G	16	Total 16	O 16	0	0
39	H	68	Total 68	O 68	0	0
39	J	50	Total 50	O 50	0	0
39	K	55	Total 55	O 55	0	0
39	L	89	Total 89	O 89	0	0
39	M	125	Total 125	O 125	0	0
39	N	64	Total 64	O 64	0	0
39	O	42	Total 42	O 42	0	0
39	P	63	Total 63	O 63	0	0
39	Q	50	Total 50	O 50	0	0
39	R	81	Total 81	O 81	0	0
39	S	35	Total 35	O 35	0	0
39	T	35	Total 35	O 35	0	0
39	U	29	Total 29	O 29	0	0
39	V	13	Total 13	O 13	0	0
39	W	70	Total 70	O 70	0	0
39	X	25	Total 25	O 25	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	30	Total 30	O 30	0	0
39	1	59	Total 59	O 59	0	0

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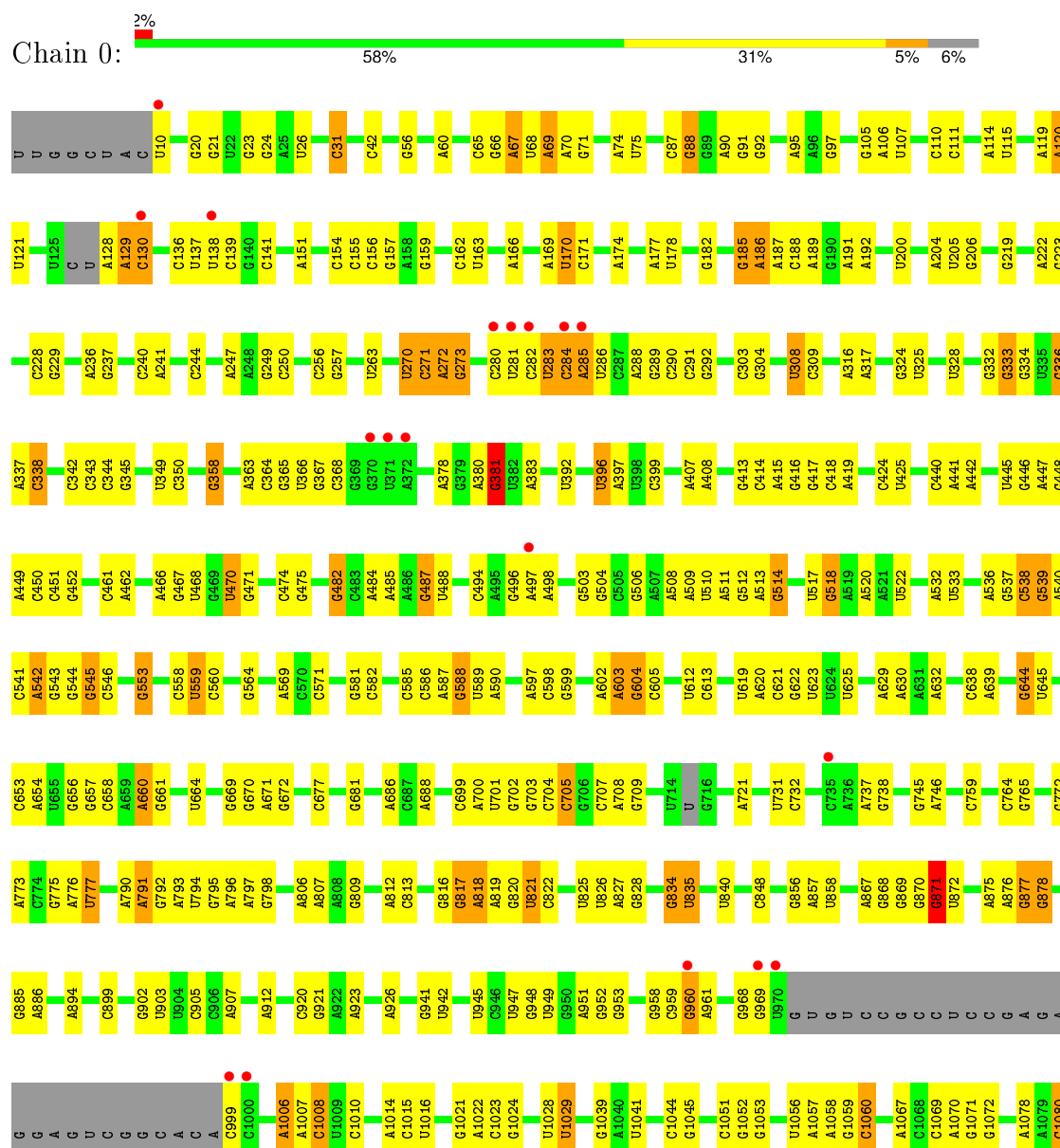
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	2	42	Total 42	O 42	0	0
39	3	71	Total 71	O 71	0	0
39	I	10	Total 10	O 10	0	0

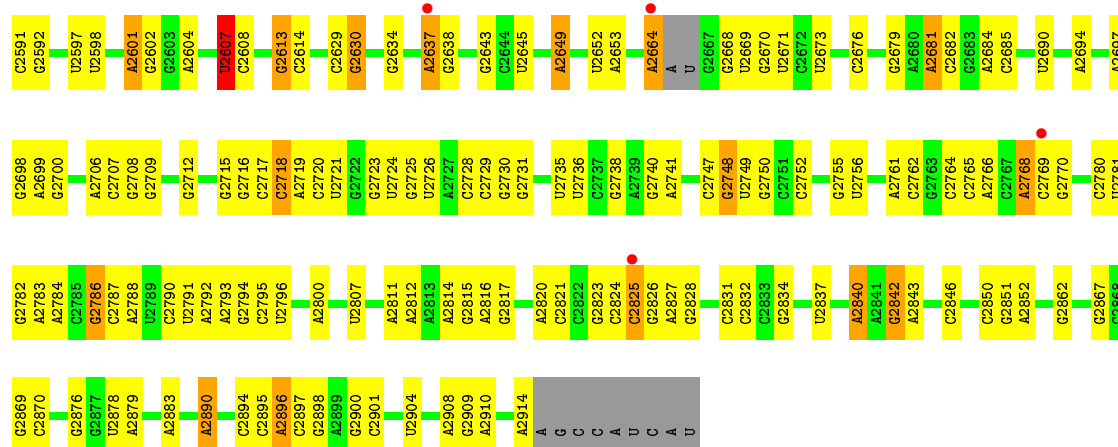
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

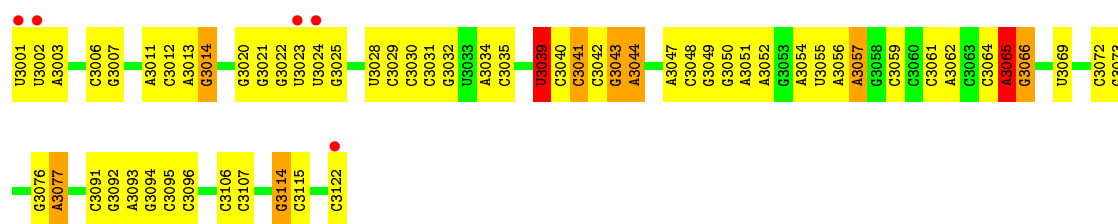
- Molecule 1: 23S ribosomal rna







• Molecule 2: 5S ribosomal RNA



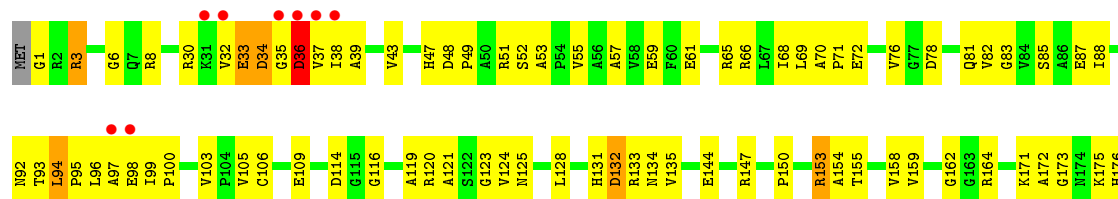
• Molecule 3: 5'-R(*CP*(5AA)*(HFA))-3'



• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

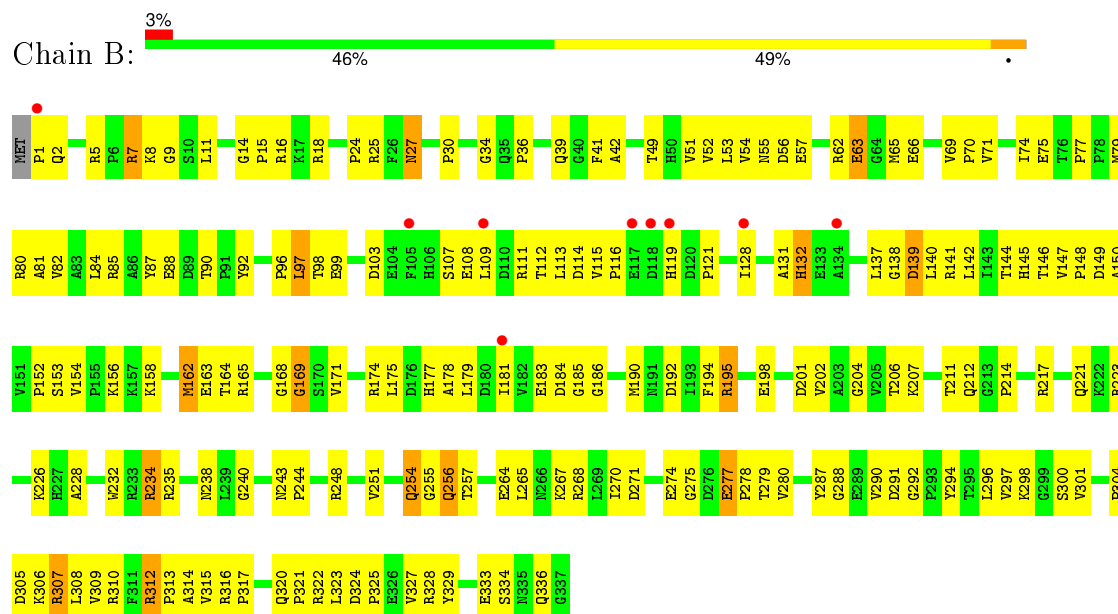


• Molecule 5: 50S ribosomal protein L2P

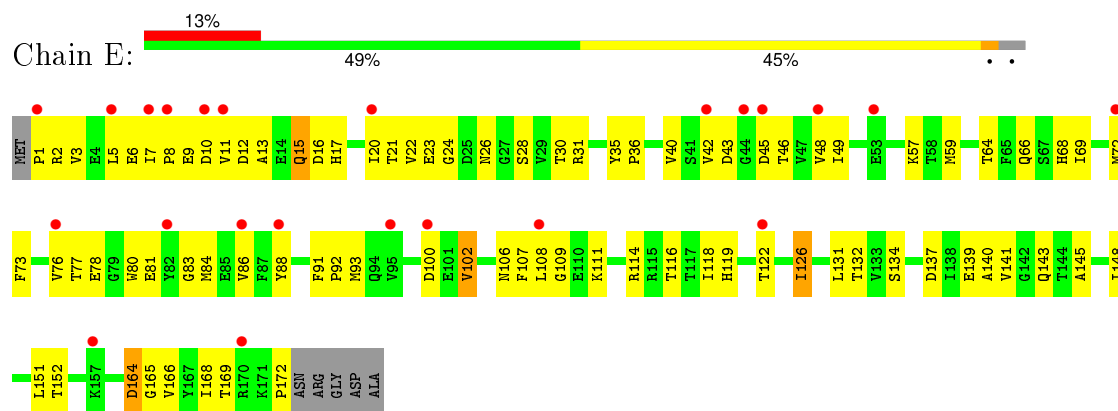




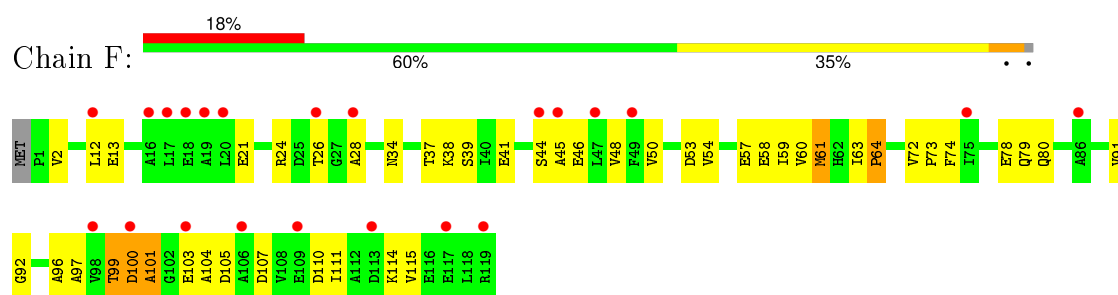
• Molecule 6: 50S ribosomal protein L3P



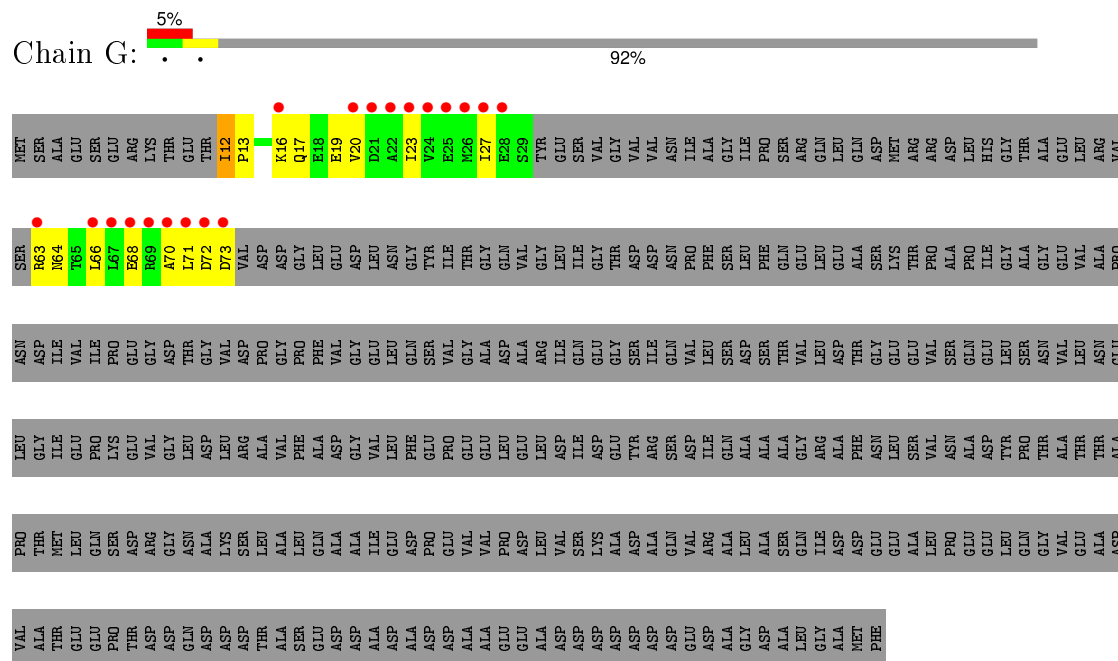
- Molecule 9: 50S ribosomal protein L6P



- Molecule 10: 50S ribosomal protein L7AE

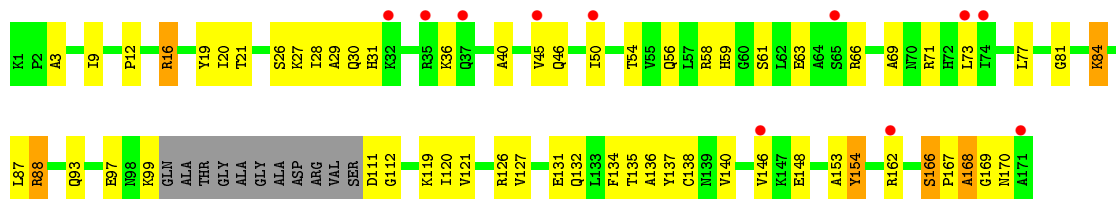


- Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



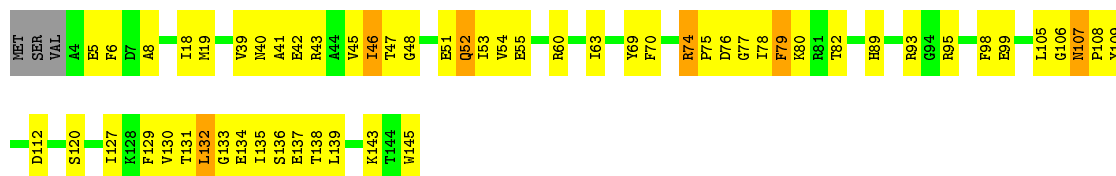
- Molecule 12: 50S RIBOSOMAL PROTEIN L10E





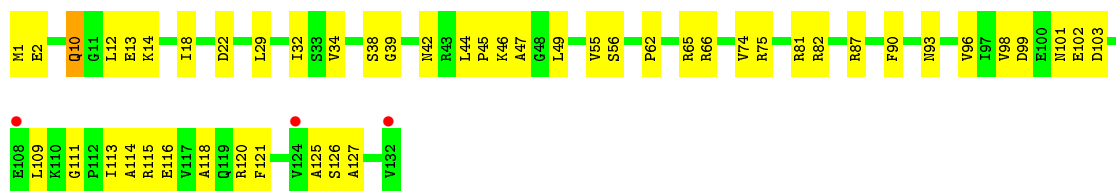
- Molecule 13: 50S ribosomal protein L13P

Chain J: 59% 35%



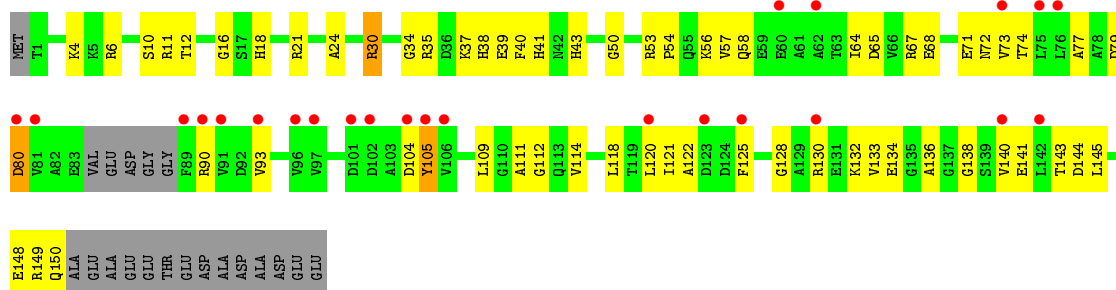
- Molecule 14: 50S ribosomal protein L14P

Chain K: 2% 63% 36%



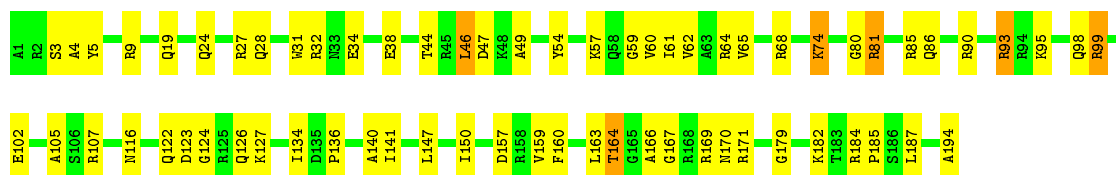
- Molecule 15: 50S ribosomal protein L15P

Chain L: 15% 50% 36% 12%

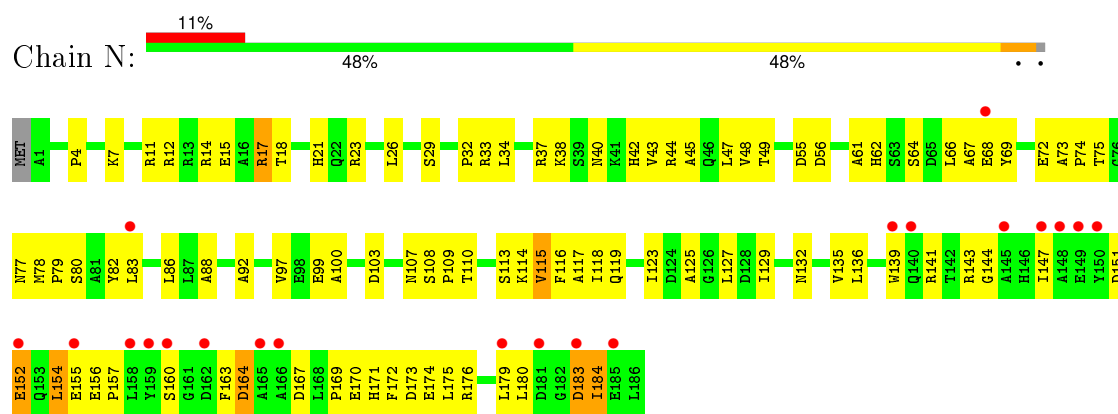


- Molecule 16: 50S Ribosomal Protein L15E

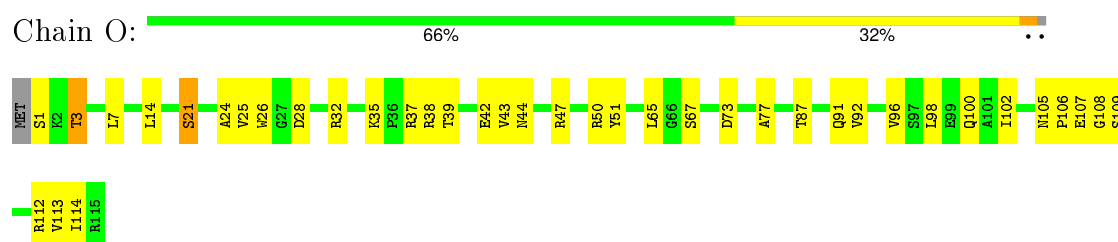
Chain M: 66% 31%



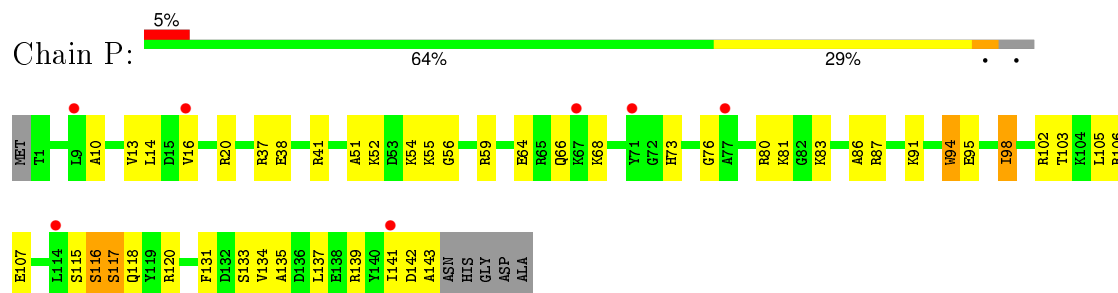
- Molecule 17: 50S ribosomal protein L18P



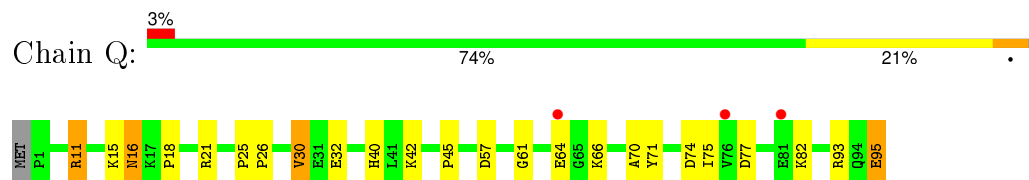
- Molecule 18: 50S ribosomal protein L18e



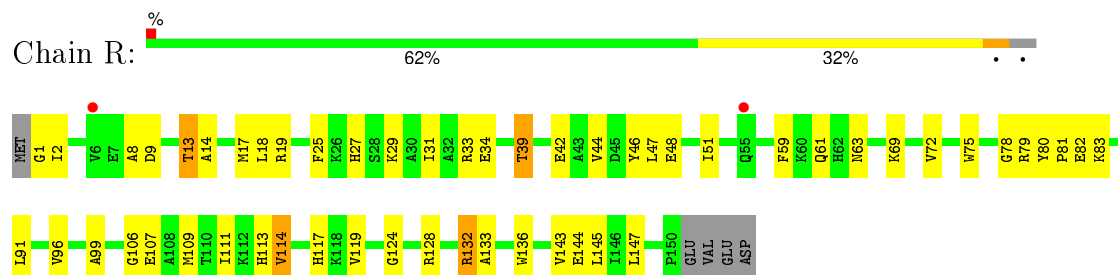
- Molecule 19: 50S ribosomal protein L19E



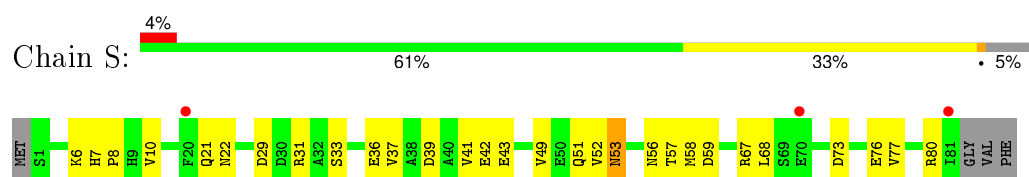
- Molecule 20: 50S ribosomal protein L21e



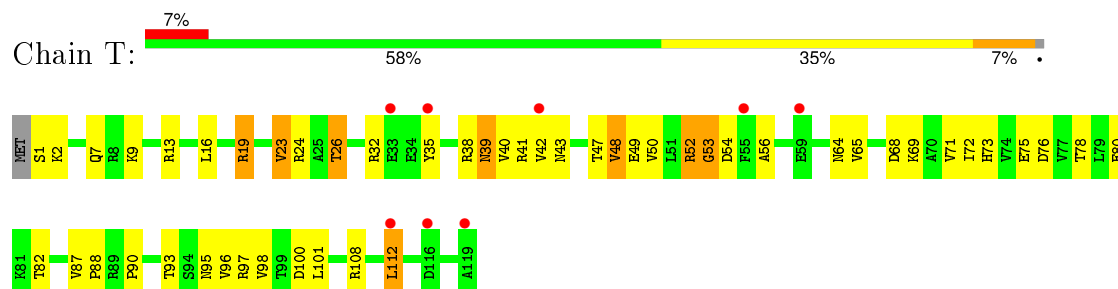
- Molecule 21: 50S ribosomal protein L22P



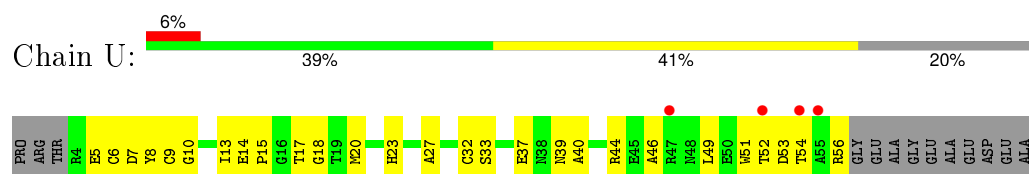
- Molecule 22: 50S ribosomal protein L23P



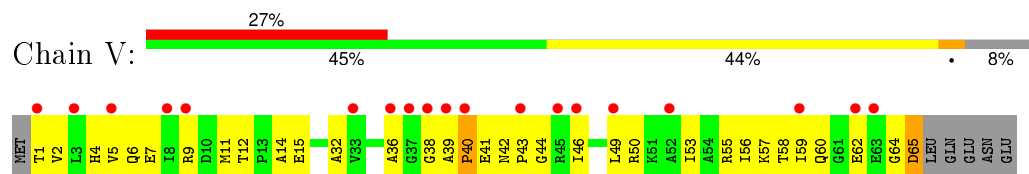
- Molecule 23: 50S ribosomal protein L24P



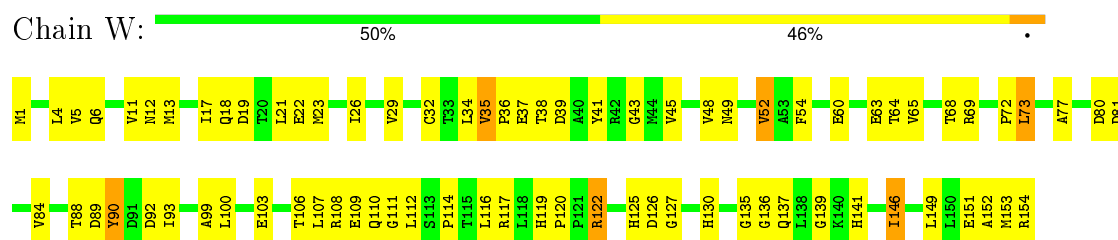
- Molecule 24: 50S ribosomal protein L24E



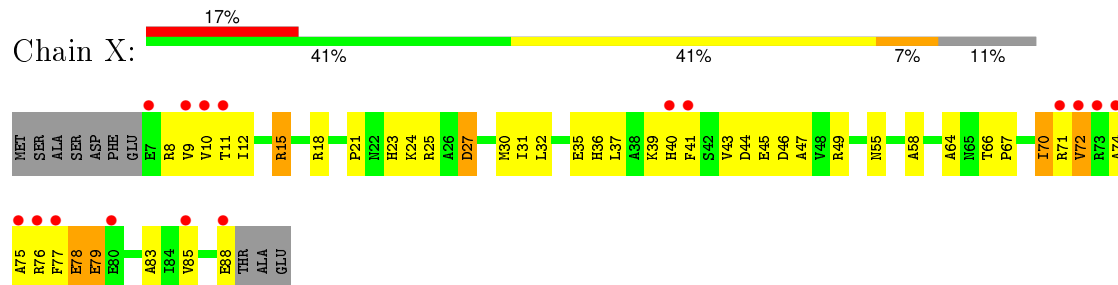
- Molecule 25: 50S ribosomal protein L29P



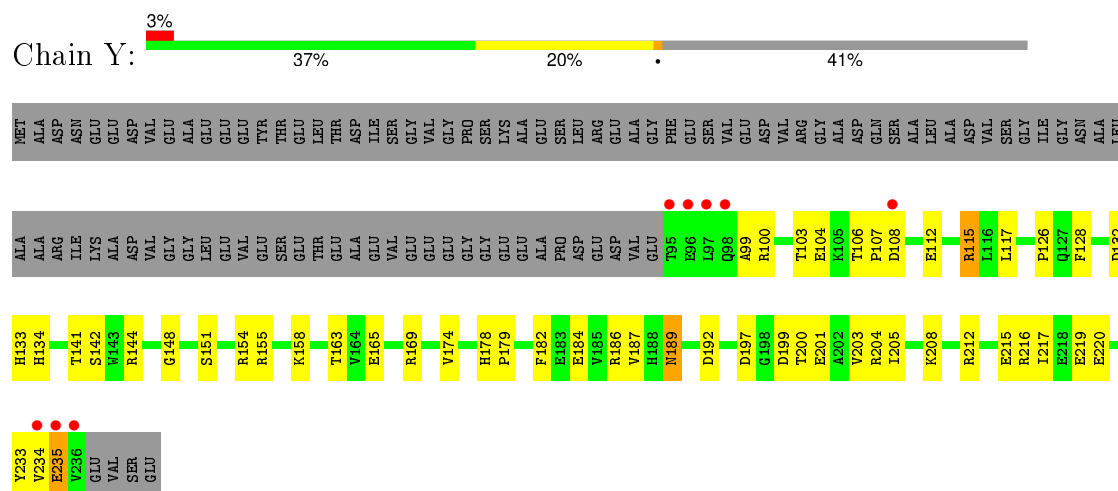
- Molecule 26: 50S ribosomal protein L30P



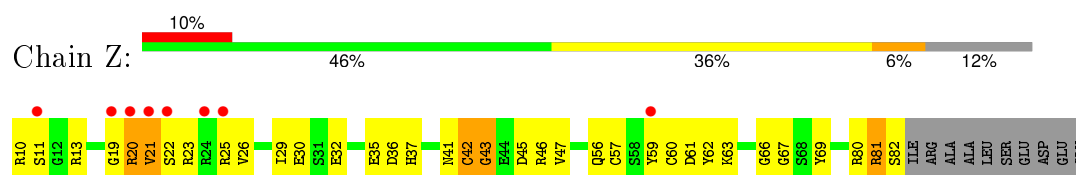
- Molecule 27: 50S ribosomal protein L31e



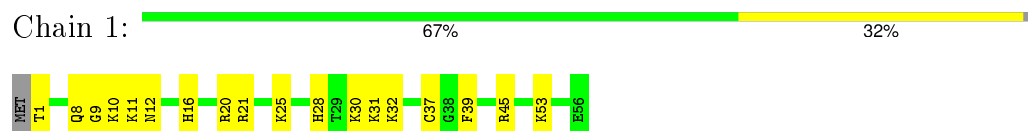
• Molecule 28: 50S ribosomal protein L32E



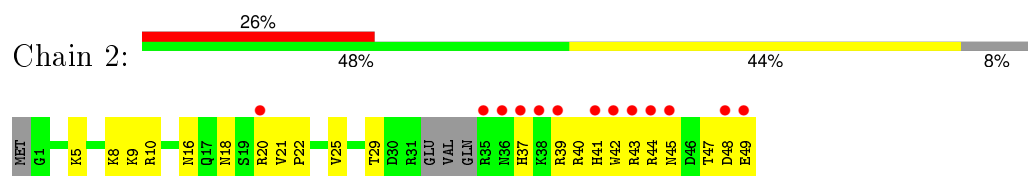
• Molecule 29: 50S ribosomal protein L37Ae



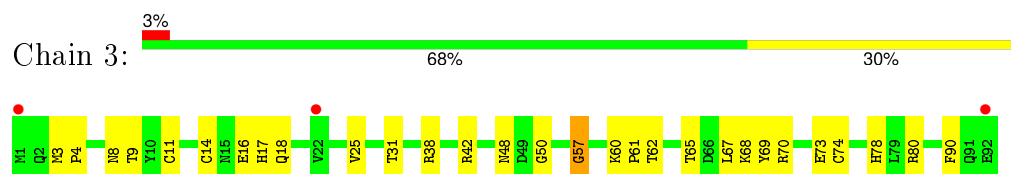
• Molecule 30: 50S ribosomal protein L37e



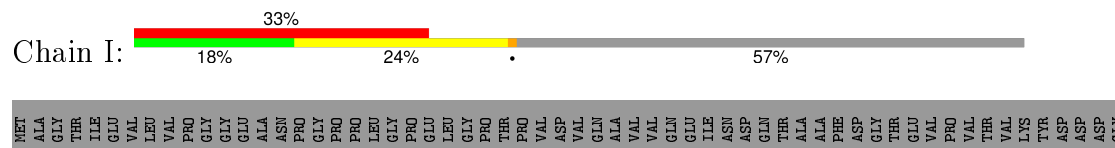
• Molecule 31: 50S ribosomal protein L39e

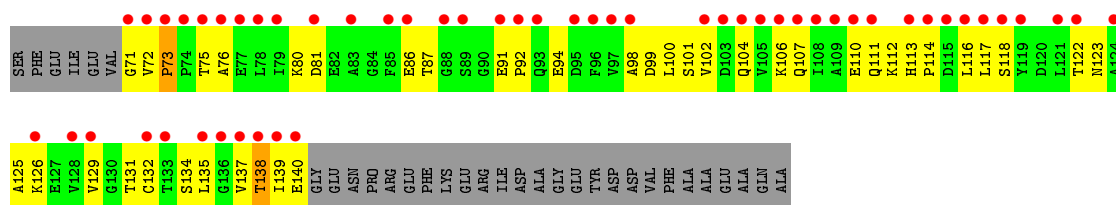


• Molecule 32: 50S ribosomal protein L44E



• Molecule 33: 50S RIBOSOMAL PROTEIN L11P





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.05Å 300.19Å 573.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.70) 93.2 (48.36-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.233 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 492017 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99029	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, ACA, CD, HFA, OMU, UR3, 5AA, 1MA, BTN, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.38	0/65959	0.69	19/102870 (0.0%)
2	9	0.35	0/2905	0.70	1/4528 (0.0%)
3	4	0.30	0/18	0.52	0/26
4	5	0.53	0/76	0.91	1/112 (0.9%)
5	A	0.32	0/1786	0.64	0/2408
6	B	0.33	0/2690	0.64	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.30	0/1111	0.53	0/1498
9	E	0.32	0/1382	0.57	0/1880
10	F	0.31	0/901	0.56	0/1224
11	G	0.29	0/241	0.46	0/324
12	H	0.33	0/1287	0.64	1/1725 (0.1%)
13	J	0.36	0/1136	0.61	0/1530
14	K	0.35	0/1001	0.69	0/1347
15	L	0.33	0/1130	0.66	0/1509
16	M	0.35	0/1584	0.61	0/2119
17	N	0.29	0/1474	0.62	0/1999
18	O	0.33	0/874	0.60	0/1181
19	P	0.34	0/1147	0.55	0/1528
20	Q	0.36	0/749	0.70	0/1005
21	R	0.35	0/1172	0.64	0/1578
22	S	0.33	0/648	0.60	0/875
23	T	0.33	0/958	0.63	1/1289 (0.1%)
24	U	0.34	0/417	0.60	0/562
25	V	0.29	0/502	0.53	0/675
26	W	0.34	0/1219	0.64	0/1655
27	X	0.34	0/664	0.58	0/895
28	Y	0.36	0/1146	0.65	0/1536
29	Z	0.36	0/589	0.64	0/787
30	1	0.42	0/438	0.64	0/578
31	2	0.33	0/401	0.53	0/529
32	3	0.40	0/771	0.60	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.30	0/526	0.56	0/716
All	All	0.37	0/98786	0.67	23/147715 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	49
2	9	0	2
26	W	0	1
All	All	1	52

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.66	130.76	109.50
1	0	871	G	C5'-C4'-O4'	-7.33	100.30	109.10
1	0	1942	A	C5'-C4'-C3'	7.21	127.54	116.00
2	9	3039	U	N1-C1'-C2'	6.70	122.70	114.00
1	0	2467	A	C1'-O4'-C4'	-6.33	104.84	109.90
1	0	1504	A	C1'-O4'-C4'	-6.29	104.87	109.90
1	0	1819	G	C5'-C4'-C3'	5.64	125.03	116.00
1	0	2291	A	N9-C1'-C2'	5.64	121.33	114.00
1	0	2313	C	C5'-C4'-O4'	5.61	115.83	109.10
1	0	1979	G	C2'-C3'-O3'	5.51	122.51	113.70
1	0	2316	G	C5'-C4'-C3'	-5.44	107.30	116.00
12	H	112	GLY	N-CA-C	-5.41	99.56	113.10
1	0	206	G	C5'-C4'-C3'	-5.36	107.43	116.00
1	0	1120	U	C5'-C4'-C3'	-5.34	107.46	116.00
1	0	381	G	N9-C1'-C2'	5.34	120.94	114.00
1	0	1592	G	N9-C1'-C2'	5.31	120.91	114.00
1	0	1504	A	N9-C1'-C2'	5.28	120.86	114.00
1	0	1165	G	C1'-O4'-C4'	-5.16	105.77	109.90
4	5	76	A	C4'-C3'-O3'	-5.13	98.63	109.40
23	T	52	ARG	N-CA-C	5.08	124.72	111.00
1	0	1971	G	N9-C1'-C2'	5.03	120.53	114.00
1	0	1979	G	N9-C1'-C2'	5.02	120.53	114.00
1	0	2607	U	N1-C1'-C2'	5.01	120.51	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain
1	0	1376	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1993	C	Sidechain
1	0	2101	A	Sidechain
1	0	2301	A	Sidechain
1	0	2315	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2543	G	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	270	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	791	A	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	867	A	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
26	W	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	59021	0	29810	904	0
2	9	2600	0	1326	60	0
3	4	52	0	36	2	0
4	5	82	0	55	3	0
5	A	1753	0	1766	128	0
6	B	2625	0	2533	202	0
7	C	1859	0	1816	113	0
8	D	1094	0	1085	84	0
9	E	1357	0	1266	86	0
10	F	890	0	843	45	0
11	G	240	0	231	15	0
12	H	1266	0	1268	66	0
13	J	1120	0	1098	69	0
14	K	992	0	1031	63	0
15	L	1118	0	1076	59	0
16	M	1560	0	1568	64	0
17	N	1445	0	1401	104	0
18	O	865	0	873	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	1136	0	1123	50	0
20	Q	735	0	729	20	0
21	R	1149	0	1122	56	0
22	S	641	0	605	22	0
23	T	950	0	923	54	0
24	U	410	0	364	31	0
25	V	499	0	511	34	0
26	W	1196	0	1137	100	0
27	X	654	0	653	51	0
28	Y	1130	0	1133	63	0
29	Z	578	0	539	27	0
30	1	431	0	426	24	0
31	2	396	0	413	31	0
32	3	755	0	728	27	0
33	I	519	0	500	46	0
34	0	107	0	0	0	0
34	3	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	73	0	0	0	0
36	9	2	0	0	0	0
36	A	1	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	3	0	0	0	0
36	S	1	0	0	0	0
37	0	8	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	0	0
37	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	2	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5764	0	0	115	0
39	1	59	0	0	2	0
39	2	42	0	0	1	0
39	3	71	0	0	5	0
39	4	1	0	0	0	0
39	5	1	0	0	0	0
39	9	135	0	0	2	0
39	A	120	0	0	11	0
39	B	156	0	0	21	0
39	C	168	0	0	18	0
39	D	45	0	0	8	0
39	E	49	0	0	8	0
39	F	23	0	0	3	0
39	G	16	0	0	1	0
39	H	68	0	0	6	0
39	I	10	0	0	2	0
39	J	50	0	0	2	0
39	K	55	0	0	8	0
39	L	89	0	0	15	0
39	M	125	0	0	3	0
39	N	64	0	0	8	0
39	O	42	0	0	7	0
39	P	63	0	0	3	0
39	Q	50	0	0	6	0
39	R	81	0	0	4	0
39	S	35	0	0	2	0
39	T	35	0	0	3	0
39	U	29	0	0	1	0
39	V	13	0	0	1	0
39	W	70	0	0	4	0
39	X	25	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Y	95	0	0	8	0
39	Z	30	0	0	1	0
All	All	99029	0	59988	2476	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2476) 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)
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.27	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.18	1.10
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.30	1.08
1:0:1242:A:H5'	13:J:82:THR:HG23	1.37	1.07
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.40	1.04
1:0:156:C:H5''	16:M:171:ARG:HD3	1.39	1.02
7:C:236:THR:HG22	7:C:239:ALA:H	1.15	1.02
21:R:39:THR:HG22	21:R:42:GLU:H	1.26	1.01
1:0:871:G:C8	1:0:871:G:H5'	1.95	1.00
31:2:41:HIS:H	31:2:45:ASN:HD22	1.11	0.99
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.22	0.99
8:D:25:MET:HE2	8:D:41:LEU:HG	1.45	0.98
1:0:871:G:H8	1:0:871:G:H5'	1.24	0.98
2:9:3076:G:H3'	2:9:3077:A:H5''	1.42	0.97
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.79	0.97
1:0:2717:C:H2'	1:0:2718:C:H5''	1.44	0.96
1:0:2364:A:H5''	20:Q:15:LYS:HD3	1.48	0.96
28:Y:187:VAL:HG23	28:Y:192:ASP:HB2	1.47	0.94
1:0:541:C:H2'	1:0:542:A:H5''	1.48	0.94
7:C:1:MET:HG2	7:C:2:GLN:H	1.31	0.94
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.49	0.94
16:M:99:ARG:HD2	16:M:167:GLY:HA2	1.49	0.93
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.49	0.93
1:0:1474:C:H6	1:0:1474:C:H5'	1.34	0.93
14:K:10:GLN:H	14:K:10:GLN:HE21	0.96	0.93
6:B:307:ARG:HB2	6:B:307:ARG:HH11	1.34	0.93
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.82	0.93
1:0:21:G:H5'	21:R:2:ILE:HA	1.50	0.93
5:A:211:LYS:HB3	5:A:212:PRO:HD2	1.50	0.92
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.92
22:S:57:THR:HG22	22:S:59:ASP:H	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
1:0:1751:G:H2'	1:0:1752:G:H5''	1.49	0.91
5:A:35:GLY:O	5:A:36:ASP:HB3	1.68	0.91
19:P:115:SER:H	19:P:118:GLN:NE2	1.69	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.51	0.90
1:0:1667:A:H8	1:0:1667:A:H5'	1.37	0.90
1:0:289:G:H22	1:0:363:A:H2	1.18	0.90
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.90
1:0:1160:G:C5'	1:0:1161:A:H5'	2.00	0.90
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.84	0.90
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.54	0.90
1:0:870:G:H2'	1:0:871:G:H5''	1.53	0.90
8:D:154:LYS:HD2	8:D:154:LYS:H	1.36	0.89
1:0:1119:G:H2'	13:J:52:GLN:HE22	1.35	0.89
16:M:164:THR:HG22	16:M:167:GLY:H	1.36	0.89
19:P:115:SER:N	19:P:118:GLN:HE21	1.70	0.88
1:0:1116:U:HO2'	1:0:1118:A:H2	0.90	0.88
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.87	0.88
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.56	0.88
1:0:796:A:HO2'	29:Z:10:ARG:N	1.72	0.88
23:T:9:LYS:HE3	23:T:13:ARG:HH11	1.39	0.88
26:W:21:LEU:HD22	26:W:26:ILE:HD11	1.54	0.88
6:B:238:ASN:HD22	6:B:240:GLY:H	1.16	0.87
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.58	0.86
1:0:1160:G:H5'	1:0:1161:A:C5'	2.04	0.86
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.57	0.86
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.19	0.86
7:C:236:THR:HG22	7:C:239:ALA:N	1.90	0.86
39:0:6381:HOH:O	5:A:223:ARG:HG3	1.75	0.86
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.41	0.86
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.55	0.86
1:0:2812:A:H2	1:0:2814:A:H62	1.23	0.85
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.85
14:K:74:VAL:HG12	14:K:75:ARG:HG3	1.57	0.85
19:P:115:SER:H	19:P:118:GLN:HE21	0.86	0.84
14:K:39:GLY:HA2	39:K:4183:HOH:O	1.78	0.84
1:0:542:A:H5'	1:0:542:A:H8	1.42	0.84
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.78	0.84
14:K:10:GLN:N	14:K:10:GLN:HE21	1.74	0.84
17:N:144:GLY:O	17:N:147:ILE:HG22	1.76	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.24	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.83
1:0:1603:A:H5'	1:0:1605:G:O4'	1.78	0.83
6:B:7:ARG:NH1	6:B:11:LEU:HD21	1.93	0.83
26:W:13:MET:HE2	26:W:18:GLN:HA	1.59	0.83
28:Y:117:LEU:HD12	28:Y:174:VAL:HG13	1.61	0.83
33:I:138:THR:HG22	33:I:139:ILE:H	1.43	0.83
6:B:168:GLY:H	6:B:174:ARG:HD3	1.41	0.83
17:N:113:SER:HB2	39:N:9356:HOH:O	1.78	0.82
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.61	0.82
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.62	0.82
6:B:98:THR:HG22	6:B:99:GLU:H	1.44	0.82
6:B:27:ASN:H	6:B:27:ASN:HD22	1.24	0.82
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.60	0.82
1:0:282:C:H1'	1:0:368:C:N4	1.94	0.81
1:0:1187:U:HO2'	1:0:1189:A:H2	1.26	0.81
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.61	0.81
39:0:3528:HOH:O	33:I:92:PRO:HD2	1.80	0.80
23:T:101:LEU:HD13	23:T:112:LEU:HD11	1.62	0.80
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.78	0.80
12:H:166:SER:HB2	12:H:167:PRO:HD3	1.64	0.80
1:0:2716:G:H5''	6:B:206:THR:HG21	1.63	0.80
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.46	0.80
27:X:30:MET:HE1	27:X:55:ASN:HA	1.61	0.80
30:1:25:LYS:HG3	31:2:49:GLU:H	1.47	0.80
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.63	0.79
1:0:871:G:H8	1:0:871:G:C5'	1.95	0.79
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.81	0.79
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.62	0.79
2:9:3014:G:H8	2:9:3014:G:H5'	1.45	0.79
1:0:541:C:C2'	1:0:542:A:H5''	2.12	0.79
5:A:135:VAL:HG21	5:A:147:ARG:HG2	1.63	0.79
1:0:545:G:H8	1:0:545:G:H5'	1.48	0.79
28:Y:235:GLU:H	28:Y:235:GLU:CD	1.84	0.79
1:0:2291:A:C8	1:0:2309:C:H5'	2.16	0.79
18:O:14:LEU:HD23	18:O:102:ILE:HD11	1.63	0.79
1:0:21:G:C5'	21:R:2:ILE:HA	2.13	0.79
8:D:57:THR:HG23	8:D:63:ILE:HA	1.65	0.79
22:S:33:SER:O	22:S:37:VAL:HG23	1.83	0.79
1:0:2533:C:H5'	1:0:2533:C:H6	1.47	0.79
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.78
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.66	0.78
1:0:1641:A:H2'	1:0:1642:A:H5'	1.65	0.78
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.12	0.78
1:0:1559:A:H1'	39:0:6094:HOH:O	1.83	0.78
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.66	0.78
1:0:2908:A:H2'	1:0:2909:G:O4'	1.83	0.78
17:N:7:LYS:HE3	20:Q:21:ARG:O	1.84	0.78
6:B:320:GLN:NE2	6:B:321:PRO:HD2	1.98	0.78
26:W:72:PRO:HG2	26:W:77:ALA:HB3	1.65	0.77
26:W:88:THR:HB	39:W:6679:HOH:O	1.83	0.77
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.47	0.77
12:H:166:SER:HB2	12:H:167:PRO:CD	2.15	0.77
6:B:179:LEU:O	6:B:183:GLU:HG2	1.83	0.77
1:0:2506:A:O2'	1:0:2507:G:H8	1.66	0.77
25:V:1:THR:HG23	25:V:2:VAL:H	1.50	0.77
1:0:1162:G:H1'	33:I:117:LEU:HD11	1.67	0.77
26:W:122:ARG:NH2	26:W:154:ARG:HB3	2.00	0.77
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.65	0.77
16:M:27:ARG:NH2	16:M:44:THR:HG23	2.00	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.65	0.77
17:N:151:ASP:O	17:N:154:LEU:HB2	1.85	0.77
1:0:877:G:H5'	1:0:878:G:OP1	1.84	0.77
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.50	0.77
1:0:1450:C:H4'	1:0:1451:C:OP2	1.84	0.77
26:W:4:LEU:HD23	26:W:54:PHE:HB3	1.65	0.77
28:Y:117:LEU:HD12	28:Y:174:VAL:CG1	2.15	0.77
18:O:105:ASN:HD21	18:O:109:SER:H	1.31	0.77
8:D:135:VAL:HG22	8:D:136:ARG:H	1.50	0.77
1:0:2073:G:H5''	39:0:4116:HOH:O	1.85	0.76
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.66	0.76
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.66	0.76
1:0:1328:A:OP1	28:Y:169:ARG:HD2	1.85	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.50	0.76
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.33	0.76
1:0:793:A:H5''	19:P:83:LYS:HG2	1.68	0.75
1:0:381:G:H5''	39:0:4600:HOH:O	1.86	0.75
9:E:7:ILE:HG22	9:E:45:ASP:O	1.86	0.75
19:P:115:SER:OG	19:P:118:GLN:HG3	1.87	0.75
26:W:80:ASP:O	26:W:84:VAL:HG23	1.86	0.75
12:H:58:ARG:HG3	12:H:58:ARG:HH11	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:5:ILE:HD11	7:C:16:VAL:HG23	1.67	0.75
1:0:1474:C:C6	1:0:1474:C:H5'	2.22	0.75
1:0:281:U:H2'	1:0:282:C:O4'	1.86	0.75
1:0:2756:U:H3	1:0:2896:A:H2	1.35	0.75
1:0:1184:C:H1'	39:0:7637:HOH:O	1.87	0.75
1:0:657:G:OP1	7:C:27:ARG:NH2	2.20	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.52	0.74
6:B:36:PRO:CA	6:B:168:GLY:HA3	2.16	0.74
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.69	0.74
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.17	0.74
8:D:146:LYS:NZ	17:N:107:ASN:HD21	1.85	0.74
28:Y:187:VAL:HG23	28:Y:192:ASP:CB	2.18	0.74
24:U:14:GLU:OE1	24:U:15:PRO:HD2	1.86	0.74
1:0:2534:C:H1'	39:0:3787:HOH:O	1.87	0.74
1:0:1116:U:O2'	1:0:1118:A:H2	1.70	0.74
14:K:74:VAL:HG13	14:K:113:ILE:HG12	1.68	0.74
16:M:28:GLN:O	16:M:32:ARG:HG3	1.88	0.74
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.17	0.74
33:I:125:ALA:O	33:I:129:VAL:HG23	1.89	0.73
12:H:166:SER:CB	12:H:167:PRO:HD3	2.18	0.73
15:L:37:LYS:HG2	39:L:9338:HOH:O	1.89	0.73
26:W:13:MET:HE1	26:W:17:ILE:HG22	1.70	0.73
12:H:9:ILE:HG23	12:H:126:ARG:CZ	2.19	0.73
5:A:191:GLY:HA2	5:A:194:MET:CE	2.18	0.73
25:V:39:ALA:N	25:V:40:PRO:HD2	2.04	0.73
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.71	0.73
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.70	0.73
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.18	0.73
7:C:78:ARG:HG3	7:C:78:ARG:HH11	1.54	0.73
17:N:47:LEU:HD11	17:N:127:LEU:HD21	1.70	0.73
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.89	0.72
12:H:27:LYS:H	12:H:59:HIS:HD2	1.36	0.72
15:L:133:VAL:HA	39:L:9378:HOH:O	1.88	0.72
1:0:1244:U:OP1	13:J:18:ILE:HD13	1.89	0.72
6:B:254:GLN:HG2	6:B:255:GLY:N	2.03	0.72
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.22	0.72
13:J:131:THR:HB	13:J:134:GLU:HG3	1.71	0.72
1:0:182:G:H5'	39:0:5407:HOH:O	1.88	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.20	0.72
13:J:93:ARG:HH11	13:J:93:ARG:HB3	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:115:LEU:HD21	7:C:243:VAL:HG13	1.72	0.72
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.72	0.72
39:O:7627:HOH:O	6:B:211:THR:HG21	1.89	0.72
1:O:447:A:OP2	23:T:1:SER:HB2	1.89	0.72
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.72	0.72
1:O:2679:G:H2'	1:O:2681:A:OP2	1.90	0.71
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.71	0.71
1:O:380:A:H2'	39:O:7405:HOH:O	1.89	0.71
1:O:2878:U:H2'	1:O:2879:A:O4'	1.89	0.71
1:O:130:C:H2'	39:O:3454:HOH:O	1.90	0.71
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.71	0.71
1:O:1666:C:O2'	1:O:1667:A:H5''	1.90	0.71
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.73	0.71
1:O:450:C:OP1	7:C:184:ARG:NH2	2.23	0.71
17:N:169:PRO:O	17:N:172:PHE:HB3	1.91	0.71
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.55	0.71
1:O:2862:G:H4'	6:B:336:GLN:O	1.91	0.71
18:O:32:ARG:HD3	18:O:32:ARG:O	1.91	0.71
2:9:3006:C:C5'	17:N:37:ARG:HH12	2.00	0.71
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.72	0.70
15:L:143:THR:HG22	15:L:145:LEU:H	1.55	0.70
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.54	0.70
21:R:99:ALA:HB1	21:R:109:MET:CE	2.20	0.70
16:M:24:GLN:NE2	16:M:27:ARG:HH11	1.89	0.70
1:O:1751:G:C2'	1:O:1752:G:H5''	2.21	0.70
1:O:2768:A:H2'	1:O:2769:C:O4'	1.90	0.70
27:X:43:VAL:HG12	27:X:44:ASP:H	1.56	0.70
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.73	0.70
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.74	0.70
27:X:25:ARG:HD3	27:X:64:ALA:O	1.92	0.70
1:O:1206:U:H5'	1:O:1206:U:H6	1.57	0.70
1:O:56:G:H5''	25:V:50:ARG:HH12	1.56	0.70
10:F:21:GLU:O	10:F:24:ARG:HG3	1.92	0.70
1:O:506:G:H22	1:O:509:A:C5'	2.03	0.70
13:J:52:GLN:HG3	13:J:53:ILE:N	2.06	0.70
2:9:3029:C:H2'	2:9:3030:C:H5'	1.72	0.70
26:W:21:LEU:HD21	26:W:48:VAL:CG1	2.22	0.70
16:M:164:THR:HG22	16:M:167:GLY:N	2.07	0.70
1:O:1667:A:C8	1:O:1667:A:H5'	2.24	0.70
1:O:2533:C:C6	1:O:2533:C:H5'	2.25	0.70
26:W:84:VAL:HG12	39:W:6679:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:6:GLU:HA	9:E:46:THR:HG22	1.72	0.70
2:9:3092:G:H2'	2:9:3093:A:C8	2.27	0.70
1:0:1372:A:H3'	39:0:7367:HOH:O	1.92	0.69
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.72	0.69
7:C:140:VAL:HB	39:C:9249:HOH:O	1.92	0.69
22:S:57:THR:HG22	22:S:59:ASP:N	2.06	0.69
2:9:3056:A:C2'	2:9:3057:A:H5''	2.22	0.69
1:0:2769:C:C2'	1:0:2770:G:H5'	2.22	0.69
7:C:242:GLU:HG3	39:C:9182:HOH:O	1.92	0.69
8:D:25:MET:CE	8:D:37:ALA:HB1	2.22	0.69
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.27	0.69
5:A:33:GLU:O	5:A:34:ASP:HB2	1.92	0.69
2:9:3006:C:C5'	17:N:37:ARG:NH1	2.55	0.69
1:0:289:G:N2	1:0:363:A:H2	1.90	0.69
1:0:1118:A:C8	1:0:1118:A:H3'	2.28	0.69
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.75	0.69
1:0:56:G:H5''	25:V:50:ARG:NH1	2.08	0.69
8:D:99:ASP:HA	39:D:5675:HOH:O	1.91	0.69
10:F:91:VAL:HG12	10:F:92:GLY:N	2.08	0.69
1:0:272:A:H5'	1:0:273:G:OP2	1.93	0.69
1:0:544:G:H2'	1:0:545:G:H5''	1.74	0.69
24:U:9:CYS:HA	24:U:52:THR:HG23	1.73	0.69
22:S:73:ASP:OD1	22:S:76:GLU:HG3	1.93	0.68
28:Y:189:ASN:HD22	28:Y:189:ASN:C	1.95	0.68
33:I:75:THR:N	33:I:112:LYS:HZ1	1.91	0.68
17:N:164:ASP:OD1	17:N:167:ASP:HA	1.94	0.68
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.94	0.68
2:9:3014:G:C8	2:9:3014:G:H5'	2.28	0.68
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.93	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.68
1:0:1118:A:H8	1:0:1119:G:H5''	1.59	0.68
1:0:1118:A:H62	1:0:1244:U:H3	1.40	0.68
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.59	0.68
39:0:5098:HOH:O	13:J:47:THR:HB	1.94	0.68
1:0:1159:G:H21	1:0:1189:A:H8	1.40	0.68
1:0:157:G:H4'	16:M:95:LYS:HE3	1.76	0.68
33:I:99:ASP:OD1	33:I:138:THR:HB	1.94	0.68
6:B:98:THR:HG22	6:B:99:GLU:N	2.09	0.68
26:W:88:THR:HG23	26:W:110:GLN:NE2	2.08	0.68
7:C:236:THR:H	7:C:239:ALA:HB3	1.59	0.67
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.33	0.67
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.76	0.67
7:C:236:THR:CG2	7:C:239:ALA:H	1.99	0.67
26:W:122:ARG:HH11	26:W:122:ARG:HG2	1.58	0.67
18:O:73:ASP:HA	18:O:92:VAL:O	1.95	0.67
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.77	0.67
12:H:46:GLN:HG3	12:H:137:TYR:CE2	2.29	0.67
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.10	0.67
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.77	0.67
8:D:99:ASP:HB3	8:D:103:ASN:H	1.60	0.67
13:J:107:ASN:ND2	13:J:109:TYR:H	1.92	0.67
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.30	0.67
1:O:1701:A:H5'	39:O:6499:HOH:O	1.95	0.67
8:D:135:VAL:HG22	8:D:136:ARG:N	2.08	0.67
23:T:52:ARG:HB2	23:T:95:ASN:HB3	1.76	0.67
39:O:6500:HOH:O	28:Y:158:LYS:HD3	1.95	0.67
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.75	0.67
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	1.75	0.67
1:O:506:G:H22	1:O:509:A:H5''	1.59	0.66
1:O:1593:C:H5'	19:P:116:SER:O	1.95	0.66
1:O:1299:G:O6	15:L:6:ARG:HD3	1.95	0.66
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.76	0.66
7:C:139:VAL:HG13	39:C:9247:HOH:O	1.93	0.66
1:O:111:C:O2'	30:1:20:ARG:HG2	1.96	0.66
17:N:15:GLU:HB3	17:N:17:ARG:HG3	1.76	0.66
1:O:656:G:OP2	18:O:37:ARG:HD2	1.94	0.66
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.31	0.66
7:C:2:GLN:HB3	39:C:9185:HOH:O	1.95	0.66
27:X:43:VAL:HG12	27:X:44:ASP:N	2.11	0.66
12:H:99:LYS:HD3	12:H:119:LYS:HD3	1.78	0.66
1:O:1684:A:H1'	31:2:43:ARG:HH22	1.60	0.66
6:B:275:GLY:O	6:B:291:ASP:HA	1.96	0.66
1:O:1205:U:H2'	1:O:1206:U:H5''	1.78	0.66
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.96	0.66
33:I:118:SER:HB2	33:I:123:ASN:HB2	1.77	0.66
2:9:3039:U:H1'	2:9:3044:A:H61	1.61	0.66
24:U:14:GLU:O	24:U:17:THR:HB	1.95	0.66
18:O:47:ARG:HG3	18:O:47:ARG:HH11	1.61	0.66
16:M:24:GLN:HE21	16:M:27:ARG:HH11	1.42	0.65
1:O:871:G:C8	1:O:871:G:C5'	2.72	0.65
1:O:1701:A:H4'	1:O:1702:U:C5'	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2426:G:H1'	39:0:6311:HOH:O	1.95	0.65
1:0:1427:A:H61	1:0:1440:U:H1'	1.60	0.65
1:0:1166:A:H1'	1:0:1192:A:C2	2.31	0.65
1:0:558:C:H2'	1:0:559:U:H5'	1.77	0.65
6:B:139:ASP:HB2	6:B:165:ARG:HE	1.61	0.65
28:Y:186:ARG:HG2	28:Y:186:ARG:HH11	1.62	0.65
6:B:87:TYR:CE2	6:B:96:PRO:HG3	2.31	0.65
1:0:138:U:H5''	1:0:139:C:OP2	1.96	0.65
1:0:1819:G:H2'	1:0:1820:G:H4'	1.77	0.65
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.27	0.65
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.26	0.65
1:0:188:C:H5''	16:M:163:LEU:HD21	1.78	0.65
19:P:20:ARG:NH1	19:P:54:LYS:HD3	2.11	0.65
6:B:62:ARG:HA	6:B:65:MET:CE	2.25	0.65
13:J:74:ARG:CB	13:J:74:ARG:HH11	2.10	0.65
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.79	0.65
25:V:55:ARG:O	25:V:59:ILE:HG12	1.96	0.65
31:2:40:ARG:HD2	31:2:47:THR:HG22	1.78	0.65
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.78	0.65
23:T:48:VAL:HG23	23:T:98:VAL:HA	1.79	0.65
26:W:35:VAL:HG23	26:W:41:TYR:CD2	2.32	0.65
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.78	0.65
5:A:32:VAL:HG22	5:A:38:ILE:HG13	1.79	0.65
8:D:136:ARG:HD2	8:D:155:HIS:O	1.96	0.65
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.79	0.65
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.79	0.65
1:0:1205:U:H2'	1:0:1206:U:C5'	2.27	0.65
10:F:26:THR:HG21	10:F:103:GLU:HB2	1.79	0.65
1:0:2827:A:H2'	1:0:2828:G:O4'	1.97	0.65
1:0:1441:G:O2'	1:0:1442:A:H5'	1.96	0.65
1:0:21:G:H5''	21:R:1:GLY:O	1.96	0.65
13:J:19:MET:HE1	13:J:132:LEU:HD11	1.79	0.65
1:0:1209:C:H2'	1:0:1210:G:H8	1.61	0.65
26:W:88:THR:HG22	26:W:89:ASP:H	1.61	0.65
1:0:1535:G:H2'	1:0:1536:C:C6	2.32	0.65
6:B:238:ASN:ND2	6:B:240:GLY:H	1.94	0.64
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.79	0.64
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.26	0.64
1:0:1632:A:H2'	1:0:1633:C:H5'	1.79	0.64
2:9:3069:U:OP1	17:N:4:PRO:HG3	1.97	0.64
1:0:2504:A:H4'	12:H:71:ARG:HH11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.80	0.64
1:0:1116:U:H3	1:0:1246:A:H62	1.43	0.64
8:D:50:VAL:O	8:D:71:ALA:HA	1.97	0.64
30:1:10:LYS:HG3	39:1:2979:HOH:O	1.97	0.64
1:0:2578:G:H5'	1:0:2578:G:H8	1.61	0.64
6:B:279:THR:OG1	6:B:290:VAL:HB	1.98	0.64
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.78	0.64
1:0:1667:A:H2'	1:0:1668:U:C6	2.32	0.64
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.28	0.64
33:I:106:LYS:O	33:I:110:GLU:HG3	1.96	0.64
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.79	0.64
26:W:119:HIS:HD2	26:W:120:PRO:O	1.79	0.64
10:F:58:GLU:HA	10:F:61:MET:HG3	1.80	0.64
26:W:38:THR:HG22	26:W:39:ASP:N	2.13	0.64
1:0:1654:U:H2'	5:A:47:HIS:HD2	1.61	0.64
16:M:60:VAL:C	16:M:61:ILE:HD12	2.18	0.64
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.64
26:W:4:LEU:HD22	26:W:52:VAL:CG2	2.27	0.64
17:N:152:GLU:C	17:N:154:LEU:H	2.02	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.98	0.64
1:0:564:G:H1'	39:0:6525:HOH:O	1.98	0.64
9:E:69:ILE:HA	9:E:72:MET:CE	2.28	0.64
6:B:55:ASN:HB3	6:B:63:GLU:HA	1.78	0.64
2:9:3006:C:OP1	17:N:37:ARG:NH1	2.31	0.64
5:A:36:ASP:HA	5:A:83:GLY:HA3	1.79	0.64
1:0:1119:G:N2	1:0:1246:A:C2	2.62	0.64
1:0:656:G:H5'	18:O:3:THR:HB	1.80	0.64
32:3:17:HIS:O	32:3:18:GLN:HG3	1.98	0.64
1:0:560:C:H42	1:0:597:A:H61	1.44	0.63
2:9:3028:U:H5''	17:N:40:ASN:ND2	2.13	0.63
31:2:5:LYS:O	31:2:9:LYS:HG3	1.97	0.63
10:F:38:LYS:NZ	16:M:3:SER:HA	2.13	0.63
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.79	0.63
11:G:64:ASN:N	11:G:64:ASN:HD22	1.94	0.63
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.33	0.63
15:L:79:ASP:HB3	39:L:9365:HOH:O	1.98	0.63
30:1:28:HIS:HD2	30:1:30:LYS:H	1.44	0.63
7:C:16:VAL:HG12	7:C:17:ASP:N	2.13	0.63
33:I:111:GLN:O	33:I:114:PRO:HD2	1.98	0.63
1:0:1213:C:O2'	1:0:1214:G:H5'	1.99	0.63
1:0:338:C:H4'	7:C:174:ILE:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:40:ARG:HG3	31:2:45:ASN:HB3	1.80	0.63
8:D:64:ARG:HB3	8:D:67:ASP:OD2	1.98	0.63
1:0:2748:G:H2'	39:0:7711:HOH:O	1.99	0.63
25:V:12:THR:CG2	25:V:15:GLU:HG3	2.19	0.63
33:I:138:THR:HG22	33:I:139:ILE:N	2.14	0.63
6:B:41:PHE:HA	6:B:79:MET:HE2	1.81	0.63
1:0:88:G:H5'	1:0:88:G:H8	1.63	0.63
6:B:305:ASP:O	6:B:306:LYS:HB2	1.99	0.63
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.80	0.63
1:0:316:A:H5'	23:T:54:ASP:OD2	1.99	0.62
1:0:447:A:P	23:T:1:SER:HB2	2.39	0.62
13:J:107:ASN:HD21	13:J:109:TYR:HB2	1.64	0.62
17:N:100:ALA:O	17:N:129:ILE:HG23	1.99	0.62
1:0:1086:A:C6	26:W:11:VAL:HG11	2.34	0.62
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.97	0.62
7:C:127:ARG:HH21	7:C:225:PRO:HG2	1.65	0.62
13:J:52:GLN:HG3	13:J:53:ILE:H	1.64	0.62
1:0:1165:G:H1'	1:0:1174:A:H1'	1.81	0.62
1:0:1973:A:H8	1:0:1973:A:H5'	1.63	0.62
6:B:248:ARG:O	6:B:251:VAL:HG13	1.99	0.62
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.81	0.62
7:C:16:VAL:HG12	7:C:17:ASP:H	1.63	0.62
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.34	0.62
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.14	0.62
1:0:2851:G:O2'	1:0:2852:A:H5'	1.99	0.62
1:0:2054:A:N3	21:R:128:ARG:NH2	2.47	0.62
1:0:2524:G:H21	1:0:2526:C:N4	1.98	0.62
27:X:71:ARG:HD3	39:X:2171:HOH:O	2.00	0.62
5:A:51:ARG:HB2	39:A:9403:HOH:O	2.00	0.62
9:E:9:GLU:HG3	9:E:10:ASP:N	2.14	0.62
1:0:2265:U:H2'	1:0:2266:A:C8	2.35	0.62
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.81	0.62
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.30	0.62
31:2:40:ARG:HA	31:2:45:ASN:ND2	2.15	0.62
6:B:198:GLU:HA	39:B:9466:HOH:O	2.00	0.62
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.81	0.62
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.82	0.62
1:0:2769:C:O2'	1:0:2770:G:H5'	2.00	0.62
1:0:2524:G:H21	1:0:2526:C:H41	1.48	0.62
1:0:2524:G:N2	1:0:2526:C:H41	1.97	0.62
33:I:101:SER:H	33:I:104:GLN:NE2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:43:VAL:HG12	27:X:47:ALA:HB3	1.81	0.61
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.82	0.61
7:C:200:PRO:HB3	7:C:212:VAL:HG23	1.82	0.61
32:3:3:MET:HG3	32:3:4:PRO:HD2	1.82	0.61
1:0:1175:G:H1'	1:0:1193:A:H2'	1.82	0.61
21:R:9:ASP:O	21:R:13:THR:HB	1.99	0.61
10:F:61:MET:HB3	16:M:19:GLN:OE1	1.99	0.61
27:X:78:GLU:HG2	27:X:79:GLU:H	1.65	0.61
5:A:121:ALA:O	5:A:124:VAL:HG22	2.00	0.61
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.30	0.61
1:0:31:C:H2'	39:0:7853:HOH:O	1.98	0.61
1:0:2720:C:O2	14:K:87:ARG:NH2	2.32	0.61
1:0:1803:C:H2'	1:0:1804:A:C8	2.36	0.61
21:R:132:ARG:HG2	21:R:133:ALA:N	2.14	0.61
1:0:2676:C:H4'	13:J:70:PHE:CE1	2.35	0.61
1:0:282:C:O2'	1:0:283:U:H5'	2.00	0.61
25:V:39:ALA:C	25:V:41:GLU:H	2.04	0.61
21:R:39:THR:HG23	21:R:107:GLU:O	2.00	0.61
2:9:3035:C:H5''	39:9:4078:HOH:O	2.01	0.61
7:C:77:ALA:O	7:C:78:ARG:HG3	2.01	0.61
13:J:19:MET:CE	13:J:132:LEU:HD21	2.30	0.61
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.33	0.61
1:0:2491:G:H1'	39:0:7055:HOH:O	1.99	0.61
39:0:7211:HOH:O	5:A:211:LYS:HG2	2.01	0.61
8:D:146:LYS:NZ	17:N:107:ASN:ND2	2.48	0.61
6:B:62:ARG:HA	6:B:65:MET:HE2	1.82	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.00	0.61
2:9:3064:C:H2'	2:9:3065:A:H5'	1.83	0.61
1:0:553:G:P	28:Y:204:ARG:HH22	2.23	0.61
5:A:199:HIS:HD2	5:A:201:PHE:H	1.47	0.61
13:J:133:GLY:O	13:J:137:GLU:HG3	2.00	0.61
1:0:2036:C:O4'	14:K:44:LEU:HG	2.00	0.61
19:P:134:VAL:O	19:P:137:LEU:HB3	2.00	0.61
5:A:211:LYS:CB	5:A:212:PRO:HD2	2.28	0.61
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.83	0.61
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.16	0.61
1:0:1182:C:H1'	1:0:1192:A:H8	1.65	0.60
1:0:1189:A:H1'	1:0:1209:C:O4'	2.00	0.60
9:E:11:VAL:HG12	9:E:12:ASP:N	2.15	0.60
17:N:164:ASP:CG	17:N:167:ASP:HA	2.20	0.60
2:9:3049:G:O2'	2:9:3050:G:H5'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:43:GLU:HB3	39:S:9144:HOH:O	2.01	0.60
1:0:2004:U:H4'	39:0:5552:HOH:O	2.00	0.60
1:0:870:G:OP2	5:A:3:ARG:HD3	2.01	0.60
7:C:1:MET:HG2	7:C:2:GLN:N	2.09	0.60
1:0:1187:U:O2'	1:0:1189:A:H2	1.81	0.60
6:B:108:GLU:HB3	6:B:111:ARG:HD2	1.83	0.60
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.60
12:H:27:LYS:H	12:H:59:HIS:CD2	2.18	0.60
19:P:64:GLU:HG2	39:P:169:HOH:O	2.00	0.60
39:E:2512:HOH:O	13:J:127:ILE:HD11	2.02	0.60
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.75	0.60
17:N:154:LEU:O	17:N:155:GLU:HB3	2.02	0.60
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.00	0.60
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.32	0.60
11:G:64:ASN:O	11:G:68:GLU:HG3	2.02	0.60
6:B:103:ASP:HB2	39:B:9398:HOH:O	2.01	0.60
29:Z:22:SER:O	29:Z:26:VAL:HG23	2.01	0.60
21:R:39:THR:HG22	21:R:42:GLU:N	2.07	0.60
33:I:92:PRO:O	33:I:94:GLU:HG3	2.00	0.60
5:A:211:LYS:HB3	5:A:212:PRO:CD	2.30	0.60
23:T:35:TYR:CD2	23:T:112:LEU:HD22	2.36	0.60
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
1:0:1058:A:H2'	1:0:1060:C:H5''	1.82	0.60
5:A:109:GLU:HG2	5:A:116:GLY:N	2.16	0.60
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.84	0.60
13:J:131:THR:HG22	13:J:133:GLY:H	1.66	0.60
1:0:1060:C:H6	1:0:1060:C:H5'	1.67	0.60
1:0:848:C:H5'	39:0:7450:HOH:O	2.02	0.60
19:P:103:THR:O	19:P:107:GLU:HG3	2.02	0.60
1:0:2755:G:H1'	39:0:4950:HOH:O	2.01	0.60
1:0:1634:G:H2'	1:0:1635:U:C6	2.37	0.60
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.60
1:0:185:G:O3'	1:0:186:A:H4'	2.02	0.60
13:J:131:THR:HG22	13:J:133:GLY:N	2.16	0.60
17:N:23:ARG:HH11	17:N:23:ARG:HG2	1.67	0.60
15:L:77:ALA:HB3	39:L:9330:HOH:O	2.00	0.60
1:0:544:G:C2'	1:0:545:G:H5''	2.31	0.59
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.82	0.59
1:0:1441:G:H1'	39:0:7929:HOH:O	2.00	0.59
33:I:72:VAL:HG13	33:I:73:PRO:HD2	1.83	0.59
1:0:2630:G:O6	5:A:206:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:4883:HOH:O	18:O:39:THR:HB	2.01	0.59
1:O:542:A:H5'	1:O:542:A:C8	2.32	0.59
1:O:797:A:C4'	29:Z:10:ARG:N	2.65	0.59
6:B:7:ARG:CZ	6:B:11:LEU:HD21	2.32	0.59
13:J:19:MET:HE2	13:J:79:PHE:HA	1.84	0.59
11:G:12:ILE:HG22	11:G:17:GLN:NE2	2.16	0.59
1:O:470:U:O2'	30:1:16:HIS:HD2	1.84	0.59
1:O:1167:G:H4'	33:I:135:LEU:HD22	1.83	0.59
29:Z:10:ARG:HA	39:Z:9214:HOH:O	2.02	0.59
1:O:136:C:H2'	1:O:137:U:O4'	2.02	0.59
1:O:1979:G:H2'	39:O:3588:HOH:O	2.00	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.16	0.59
13:J:47:THR:HG22	13:J:48:GLY:H	1.66	0.59
12:H:28:ILE:HG23	39:H:9179:HOH:O	2.03	0.59
10:F:38:LYS:HZ1	16:M:3:SER:HA	1.67	0.59
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.32	0.59
1:O:1527:A:H1'	1:O:1528:A:C8	2.37	0.59
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.37	0.59
22:S:37:VAL:O	22:S:41:VAL:HG23	2.02	0.59
1:O:2769:C:H2'	1:O:2770:G:H5'	1.84	0.59
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.32	0.59
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.84	0.59
1:O:1333:U:H2'	1:O:1334:C:C6	2.37	0.59
15:L:67:ARG:O	15:L:71:GLU:HG3	2.02	0.59
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.85	0.59
10:F:96:ALA:HA	39:F:3111:HOH:O	2.03	0.59
7:C:214:THR:HG23	39:C:9237:HOH:O	2.02	0.59
12:H:166:SER:CB	12:H:167:PRO:CD	2.79	0.59
17:N:47:LEU:HD12	17:N:92:ALA:HB1	1.85	0.59
21:R:119:VAL:O	21:R:119:VAL:HG12	2.03	0.59
1:O:396:U:O2'	1:O:418:C:H4'	2.02	0.59
1:O:475:G:H5'	7:C:73:LEU:HD23	1.85	0.59
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.33	0.59
12:H:66:ARG:HD3	39:H:9179:HOH:O	2.03	0.59
1:O:244:C:OP2	10:F:38:LYS:HE3	2.03	0.59
17:N:80:SER:HB2	39:N:9334:HOH:O	2.02	0.59
1:O:2890:A:H1'	24:U:56:ARG:NH2	2.18	0.59
21:R:44:VAL:O	21:R:48:GLU:HG3	2.02	0.59
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.85	0.59
6:B:36:PRO:HA	6:B:168:GLY:CA	2.25	0.59
17:N:73:ALA:HB1	17:N:74:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:16:LEU:HA	23:T:19:ARG:HG3	1.85	0.59
9:E:69:ILE:HA	9:E:72:MET:HE3	1.83	0.58
1:0:1377:C:H6	1:0:1377:C:H5'	1.68	0.58
16:M:57:LYS:HE2	16:M:140:ALA:O	2.02	0.58
39:O:4280:HOH:O	7:C:188:ARG:HD3	2.02	0.58
6:B:238:ASN:HD22	6:B:240:GLY:N	1.95	0.58
1:0:90:A:H2'	1:0:91:G:O4'	2.03	0.58
1:0:902:G:N7	15:L:18:HIS:HD2	2.01	0.58
9:E:137:ASP:O	9:E:141:VAL:HG23	2.04	0.58
9:E:81:GLU:O	9:E:172:PRO:HD3	2.03	0.58
28:Y:144:ARG:CZ	39:Y:9409:HOH:O	2.50	0.58
9:E:100:ASP:HB2	39:E:2789:HOH:O	2.03	0.58
5:A:200:PRO:HG2	5:A:225:VAL:HG21	1.85	0.58
15:L:136:ALA:HB3	39:L:9378:HOH:O	2.03	0.58
23:T:73:HIS:CD2	23:T:88:PRO:HG3	2.38	0.58
8:D:36:ASN:HA	39:D:7500:HOH:O	2.03	0.58
6:B:147:VAL:HG12	6:B:150:ALA:H	1.68	0.58
11:G:16:LYS:O	11:G:20:VAL:HG23	2.03	0.58
17:N:12:ARG:HD3	17:N:18:THR:OG1	2.03	0.58
1:0:1164:U:H3	1:0:1192:A:H2	1.51	0.58
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.85	0.58
30:1:8:GLN:HE22	30:1:11:LYS:NZ	2.01	0.58
9:E:77:THR:OG1	9:E:78:GLU:N	2.34	0.58
15:L:134:GLU:HA	15:L:138:GLY:O	2.03	0.58
1:0:380:A:OP2	16:M:9:ARG:HD2	2.03	0.58
1:0:95:A:H5''	1:0:97:G:O4'	2.02	0.58
2:9:3001:U:H5''	2:9:3003:A:OP1	2.04	0.58
6:B:307:ARG:CB	6:B:307:ARG:HH11	2.13	0.58
14:K:55:VAL:HG12	14:K:56:SER:N	2.19	0.58
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.86	0.58
9:E:8:PRO:HB2	9:E:11:VAL:HG23	1.85	0.58
7:C:246:ARG:HH11	7:C:246:ARG:HB3	1.69	0.58
8:D:101:THR:O	8:D:157:LEU:HB3	2.03	0.58
20:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.04	0.58
1:0:31:C:H4'	39:O:7597:HOH:O	2.04	0.58
1:0:1666:C:C2'	1:0:1667:A:H5''	2.34	0.58
17:N:47:LEU:HD13	17:N:97:VAL:HG11	1.85	0.58
13:J:108:PRO:HG2	13:J:109:TYR:HD1	1.67	0.58
8:D:51:ARG:HD3	39:D:7636:HOH:O	2.03	0.58
6:B:154:VAL:HG12	6:B:156:LYS:HG2	1.85	0.58
1:0:1008:C:H5''	12:H:16:ARG:HH12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:45:VAL:HG23	13:J:130:VAL:O	2.04	0.58
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.85	0.58
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.85	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.86	0.58
1:O:818:A:O2'	29:Z:13:ARG:HD3	2.02	0.58
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.04	0.58
16:M:99:ARG:CD	16:M:167:GLY:HA2	2.30	0.57
16:M:99:ARG:HD2	16:M:167:GLY:CA	2.29	0.57
39:O:7597:HOH:O	23:T:9:LYS:HB2	2.04	0.57
19:P:10:ALA:O	19:P:13:VAL:HG12	2.04	0.57
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.68	0.57
1:O:2690:U:O2'	9:E:111:LYS:HE3	2.04	0.57
1:O:2502:C:C2'	1:O:2503:A:H5'	2.34	0.57
17:N:132:ASN:O	17:N:135:VAL:HG12	2.04	0.57
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.86	0.57
1:O:1942:A:O2'	1:O:1943:C:H5'	2.05	0.57
1:O:2780:C:H1'	9:E:143:GLN:NE2	2.18	0.57
23:T:24:ARG:HH21	23:T:39:ASN:HD22	1.52	0.57
21:R:39:THR:HB	21:R:42:GLU:HG3	1.84	0.57
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.34	0.57
1:O:1234:U:N3	6:B:244:PRO:HB3	2.19	0.57
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.34	0.57
31:2:41:HIS:N	31:2:45:ASN:HD22	1.92	0.57
1:O:2896:A:H5''	39:O:6318:HOH:O	2.04	0.57
1:O:2769:C:H2'	1:O:2770:G:C5'	2.34	0.57
21:R:14:ALA:HB3	21:R:147:LEU:HB2	1.84	0.57
1:O:1406:A:H4'	1:O:1407:A:H5''	1.86	0.57
6:B:16:ARG:HD3	39:B:9417:HOH:O	2.04	0.57
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.86	0.57
8:D:23:VAL:O	8:D:23:VAL:HG23	2.03	0.57
8:D:154:LYS:H	8:D:154:LYS:CD	2.10	0.57
1:O:2505:G:O2'	1:O:2506:A:H5'	2.05	0.57
17:N:17:ARG:NH1	17:N:17:ARG:HB3	2.18	0.57
5:A:88:ILE:HG22	5:A:88:ILE:O	2.03	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.02	0.57
22:S:56:ASN:O	31:2:8:LYS:NZ	2.36	0.57
7:C:236:THR:HA	39:C:9249:HOH:O	2.05	0.57
1:O:1666:C:H2'	1:O:1667:A:C5'	2.35	0.57
24:U:52:THR:HG22	24:U:54:THR:N	2.19	0.57
6:B:132:HIS:NE2	6:B:171:VAL:HG23	2.19	0.57
19:P:115:SER:O	19:P:117:SER:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.86	0.57
8:D:64:ARG:HG2	8:D:67:ASP:HB3	1.86	0.57
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.86	0.57
23:T:32:ARG:NH1	23:T:38:ARG:HH12	2.03	0.57
1:0:820:G:H3'	39:0:3345:HOH:O	2.04	0.57
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.20	0.57
13:J:108:PRO:HG2	13:J:109:TYR:CD1	2.39	0.57
2:9:3041:C:H4'	8:D:48:MET:HB2	1.86	0.57
13:J:51:GLU:O	13:J:55:GLU:HG3	2.04	0.57
6:B:140:LEU:HA	39:B:9384:HOH:O	2.04	0.57
16:M:164:THR:CG2	16:M:167:GLY:H	2.15	0.57
26:W:18:GLN:O	26:W:22:GLU:HG3	2.04	0.57
1:0:1189:A:H1'	1:0:1209:C:C1'	2.33	0.57
27:X:15:ARG:HB3	27:X:15:ARG:HH11	1.70	0.57
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.70	0.57
9:E:43:ASP:HA	39:E:5864:HOH:O	2.05	0.57
1:0:1787:C:H4'	1:0:2883:A:O4'	2.05	0.57
1:0:1596:U:H2'	1:0:1598:A:OP2	2.05	0.57
2:9:3020:G:O2'	2:9:3021:G:H5'	2.05	0.57
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.35	0.57
1:0:2629:C:N4	5:A:206:ARG:HH21	2.03	0.57
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.87	0.57
17:N:115:VAL:HG23	39:N:9356:HOH:O	2.05	0.56
8:D:159:PRO:O	8:D:163:VAL:HG23	2.05	0.56
2:9:3039:U:H1'	2:9:3044:A:N6	2.19	0.56
6:B:42:ALA:HB1	6:B:308:LEU:HD11	1.86	0.56
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.05	0.56
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.18	0.56
1:0:316:A:N3	1:0:336:G:O2'	2.36	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
5:A:232:ARG:NH2	5:A:236:GLY:O	2.37	0.56
8:D:138:GLY:N	39:D:7597:HOH:O	2.38	0.56
1:0:2301:A:H5''	1:0:2302:A:H5'	1.86	0.56
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.56
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.86	0.56
33:I:107:GLN:HA	33:I:110:GLU:OE2	2.05	0.56
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.34	0.56
1:0:1506:U:H5'	1:0:1506:U:H6	1.70	0.56
6:B:109:LEU:HG	6:B:113:LEU:HD12	1.87	0.56
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.56
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:775:G:OP1	30:1:16:HIS:HE1	1.89	0.56
1:0:952:G:H4'	39:0:6927:HOH:O	2.05	0.56
5:A:179:MET:HG2	5:A:186:TRP:CG	2.41	0.56
17:N:42:HIS:CG	17:N:62:HIS:HE1	2.24	0.56
13:J:47:THR:HG22	13:J:48:GLY:N	2.21	0.56
1:0:2781:U:H1'	9:E:139:GLU:OE2	2.04	0.56
26:W:151:GLU:O	26:W:154:ARG:HB2	2.05	0.56
15:L:133:VAL:HB	39:L:9363:HOH:O	2.05	0.56
9:E:84:MET:HG2	9:E:168:ILE:HD13	1.87	0.56
1:0:1333:U:H2'	1:0:1334:C:H6	1.71	0.56
1:0:2414:A:H2'	1:0:2415:A:C8	2.39	0.56
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.70	0.56
1:0:1835:U:C5	1:0:1840:A:N7	2.64	0.56
17:N:151:ASP:HB3	39:N:9324:HOH:O	2.05	0.56
13:J:19:MET:HE1	13:J:132:LEU:HD21	1.87	0.56
1:0:2897:C:H2'	1:0:2898:G:H8	1.69	0.56
25:V:39:ALA:N	25:V:40:PRO:CD	2.69	0.56
6:B:24:PRO:HG2	6:B:204:GLY:HA2	1.86	0.56
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
1:0:2712:G:H5'	39:K:4183:HOH:O	2.06	0.56
12:H:56:GLN:HE21	12:H:126:ARG:NE	2.00	0.56
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.41	0.56
1:0:960:G:H2'	1:0:960:G:N3	2.21	0.56
6:B:88:GLU:HG3	6:B:88:GLU:O	2.04	0.56
29:Z:56:GLN:HA	29:Z:62:TYR:O	2.05	0.56
1:0:21:G:H4'	21:R:2:ILE:HG22	1.87	0.56
5:A:132:ASP:OD1	5:A:133:ARG:N	2.39	0.56
15:L:143:THR:HG22	15:L:144:ASP:N	2.20	0.56
24:U:46:ALA:HB1	24:U:52:THR:HG21	1.88	0.56
2:9:3064:C:C2'	2:9:3065:A:H5'	2.36	0.56
7:C:194:PHE:HA	7:C:234:VAL:HG13	1.88	0.56
17:N:179:LEU:HD23	17:N:184:ILE:CD1	2.36	0.56
17:N:116:PHE:HB3	17:N:136:LEU:HD23	1.87	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:396:U:OP2	32:3:38:ARG:HD2	2.05	0.56
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.41	0.56
1:0:2508:C:H2'	39:0:6948:HOH:O	2.06	0.56
1:0:2506:A:O2'	1:0:2507:G:O5'	2.23	0.55
6:B:27:ASN:N	6:B:27:ASN:HD22	1.96	0.55
30:1:37:CYS:SG	30:1:39:PHE:HB2	2.46	0.55
1:0:2266:A:OP2	16:M:90:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:12:ILE:HG22	11:G:17:GLN:HE21	1.70	0.55
8:D:94:ALA:HB3	8:D:97:GLN:HE21	1.71	0.55
6:B:82:VAL:HG12	6:B:82:VAL:O	2.06	0.55
26:W:107:LEU:O	26:W:112:LEU:HB2	2.06	0.55
9:E:2:ARG:HH21	9:E:48:VAL:HG21	1.71	0.55
26:W:130:HIS:O	26:W:136:GLY:HA3	2.05	0.55
9:E:107:PHE:CE2	9:E:108:LEU:HD13	2.41	0.55
28:Y:189:ASN:ND2	28:Y:192:ASP:H	2.03	0.55
33:I:131:THR:O	33:I:135:LEU:HG	2.06	0.55
1:0:1181:A:H5'	33:I:94:GLU:OE2	2.06	0.55
20:Q:26:PRO:O	20:Q:30:VAL:HG22	2.05	0.55
6:B:138:GLY:O	6:B:139:ASP:O	2.24	0.55
1:0:2769:C:H2'	1:0:2770:G:O4'	2.07	0.55
1:0:1130:U:H2'	1:0:1131:G:O4'	2.06	0.55
6:B:30:PRO:HB2	6:B:39:GLN:HE21	1.72	0.55
17:N:43:VAL:HG13	17:N:118:ILE:HD11	1.87	0.55
6:B:294:TYR:HE2	39:B:9459:HOH:O	1.87	0.55
5:A:131:HIS:O	5:A:132:ASP:HB2	2.06	0.55
26:W:122:ARG:HH22	26:W:154:ARG:HB3	1.72	0.55
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.20	0.55
33:I:102:VAL:CG1	33:I:106:LYS:HE3	2.36	0.55
1:0:1299:G:N7	15:L:6:ARG:NH1	2.54	0.55
1:0:1679:C:H5'	39:0:9638:HOH:O	2.07	0.55
8:D:67:ASP:O	8:D:69:ILE:HG13	2.07	0.55
25:V:39:ALA:O	25:V:41:GLU:N	2.40	0.55
24:U:52:THR:CG2	24:U:54:THR:HB	2.36	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.06	0.55
25:V:58:THR:O	25:V:62:GLU:HG3	2.07	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.28	0.55
10:F:91:VAL:HG12	10:F:92:GLY:H	1.70	0.55
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.40	0.55
9:E:108:LEU:HD11	9:E:164:ASP:HB2	1.89	0.55
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.88	0.55
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.35	0.55
17:N:170:GLU:O	17:N:174:GLU:HG3	2.07	0.55
1:0:1636:G:O2'	1:0:1637:A:H5'	2.06	0.55
5:A:164:ARG:CZ	39:A:9385:HOH:O	2.55	0.55
8:D:23:VAL:HG12	8:D:130:VAL:HG22	1.87	0.55
22:S:33:SER:OG	22:S:36:GLU:HG3	2.07	0.55
8:D:86:THR:C	8:D:89:PRO:HD2	2.27	0.55
17:N:18:THR:HG21	39:N:9344:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:162:MET:HE1	6:B:308:LEU:HD21	1.87	0.55
39:0:7725:HOH:O	32:3:60:LYS:HG3	2.06	0.55
1:0:1120:U:H5'	1:0:1120:U:C6	2.41	0.55
10:F:48:VAL:HG23	10:F:74:PHE:CB	2.36	0.55
14:K:125:ALA:C	14:K:127:ALA:H	2.10	0.55
6:B:175:LEU:O	6:B:175:LEU:HD23	2.06	0.55
2:9:3044:A:O4'	8:D:76:ARG:NE	2.38	0.55
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.87	0.55
1:0:2846:C:OP1	6:B:158:LYS:HD3	2.07	0.55
1:0:2472:C:O2'	1:0:2634:G:H4'	2.07	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.22	0.55
1:0:1666:C:H2'	1:0:1667:A:H5'	1.88	0.55
1:0:1183:C:N4	1:0:1184:C:H41	2.05	0.55
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.89	0.55
26:W:41:TYR:O	26:W:45:VAL:HG13	2.07	0.55
9:E:24:GLY:HA3	9:E:76:VAL:HB	1.89	0.55
1:0:2241:C:O2'	1:0:2242:U:H5'	2.07	0.55
7:C:218:VAL:HG12	39:C:9227:HOH:O	2.07	0.55
7:C:19:PRO:HG2	7:C:22:PHE:CE1	2.42	0.55
23:T:47:THR:HB	23:T:100:ASP:HB3	1.89	0.55
24:U:13:ILE:HG12	24:U:32:CYS:HB3	1.88	0.55
21:R:39:THR:HB	21:R:42:GLU:CG	2.37	0.55
5:A:94:LEU:N	5:A:94:LEU:HD23	2.22	0.55
14:K:98:VAL:CG1	14:K:99:ASP:N	2.70	0.55
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.88	0.55
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.07	0.55
21:R:39:THR:HB	21:R:42:GLU:CD	2.26	0.54
26:W:88:THR:HG22	26:W:89:ASP:N	2.22	0.54
1:0:1183:C:H2'	39:0:6463:HOH:O	2.05	0.54
15:L:143:THR:HG21	39:L:9340:HOH:O	2.07	0.54
33:I:113:HIS:N	33:I:114:PRO:HD2	2.22	0.54
17:N:64:SER:C	17:N:66:LEU:H	2.11	0.54
39:0:5756:HOH:O	6:B:298:LYS:HD3	2.07	0.54
1:0:1834:C:H2'	1:0:1840:A:N6	2.21	0.54
31:2:10:ARG:HH11	31:2:49:GLU:CD	2.11	0.54
31:2:10:ARG:HD2	31:2:49:GLU:OE2	2.07	0.54
1:0:1972:U:H2'	1:0:1973:A:C5'	2.37	0.54
12:H:21:THR:O	12:H:120:ILE:HD12	2.07	0.54
1:0:1236:A:C8	13:J:63:ILE:HD11	2.41	0.54
1:0:285:A:H2'	1:0:286:U:O4'	2.07	0.54
1:0:280:C:H2'	1:0:281:U:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.36	0.54
2:9:3029:C:C2'	2:9:3030:C:H5'	2.37	0.54
1:0:1500:U:P	19:P:41:ARG:HH22	2.30	0.54
7:C:129:HIS:HE1	7:C:231:ARG:HA	1.72	0.54
1:0:2524:G:H21	1:0:2526:C:H5	1.54	0.54
39:0:4937:HOH:O	6:B:300:SER:HB3	2.07	0.54
39:0:9671:HOH:O	30:1:1:THR:HA	2.07	0.54
1:0:2453:G:H4'	15:L:50:GLY:C	2.28	0.54
15:L:104:ASP:O	15:L:105:TYR:HB3	2.07	0.54
1:0:2064:U:H5'	1:0:2652:U:H4'	1.89	0.54
1:0:790:A:H2'	1:0:791:A:O4'	2.07	0.54
7:C:168:ARG:NH2	7:C:190:ALA:O	2.40	0.54
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.88	0.54
17:N:37:ARG:NE	39:N:9331:HOH:O	2.41	0.54
13:J:6:PHE:HB3	13:J:109:TYR:OH	2.07	0.54
1:0:1632:A:C2'	1:0:1633:C:H5'	2.37	0.54
5:A:52:SER:HB2	5:A:164:ARG:HH11	1.72	0.54
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
15:L:54:PRO:HG2	15:L:57:VAL:HG21	1.89	0.54
19:P:141:ILE:C	19:P:143:ALA:H	2.11	0.54
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.36	0.54
19:P:83:LYS:O	19:P:86:ALA:HB3	2.08	0.54
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.54
1:0:1419:U:H5'	1:0:1420:C:OP2	2.06	0.54
20:Q:61:GLY:HA2	39:Q:6286:HOH:O	2.08	0.54
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.22	0.54
10:F:46:GLU:O	10:F:73:PRO:HD2	2.08	0.54
39:C:9167:HOH:O	23:T:2:LYS:HE2	2.08	0.54
1:0:2837:U:H1'	6:B:307:ARG:HH12	1.71	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
8:D:146:LYS:HZ3	17:N:107:ASN:HD21	1.55	0.54
13:J:39:VAL:HG13	13:J:106:GLY:O	2.07	0.54
11:G:12:ILE:N	11:G:13:PRO:HD3	2.22	0.54
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.22	0.54
1:0:2256:G:H2'	1:0:2257:G:H5'	1.90	0.54
24:U:5:GLU:HG3	24:U:10:GLY:O	2.07	0.54
1:0:827:A:H2'	1:0:828:G:O4'	2.06	0.54
5:A:55:VAL:HG23	5:A:68:ILE:O	2.08	0.54
8:D:146:LYS:HZ1	17:N:107:ASN:HD21	1.53	0.54
1:0:2502:C:H2'	1:0:2503:A:H5'	1.90	0.54
1:0:644:G:N3	1:0:644:G:H5'	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:30:MET:CE	27:X:55:ASN:HA	2.34	0.54
6:B:52:VAL:O	6:B:53:LEU:HD12	2.08	0.54
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.38	0.54
1:0:2748:G:H1'	39:0:8169:HOH:O	2.07	0.54
1:0:1677:U:OP2	31:2:8:LYS:NZ	2.40	0.54
20:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.07	0.54
1:0:1236:A:H2'	1:0:1237:U:O4'	2.08	0.54
33:I:76:ALA:O	33:I:80:LYS:HG3	2.08	0.54
26:W:13:MET:HE2	26:W:18:GLN:CA	2.35	0.54
6:B:139:ASP:CB	6:B:165:ARG:HE	2.20	0.54
1:0:119:A:H2'	1:0:120:A:H5''	1.90	0.54
1:0:1477:C:O2'	1:0:1478:U:H5'	2.08	0.54
15:L:148:GLU:HA	39:L:9377:HOH:O	2.07	0.54
1:0:462:A:C2	31:2:37:HIS:HB3	2.43	0.54
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.23	0.54
19:P:13:VAL:HG21	19:P:41:ARG:HG2	1.89	0.54
1:0:1342:C:C2'	1:0:1343:C:H5'	2.38	0.54
1:0:1904:A:H2'	1:0:1905:U:O4'	2.08	0.54
1:0:1287:A:O4'	26:W:117:ARG:HD3	2.08	0.54
1:0:545:G:H2'	1:0:546:C:O4'	2.08	0.53
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.90	0.53
13:J:75:PRO:HA	13:J:132:LEU:HD12	1.90	0.53
6:B:71:VAL:HG11	6:B:296:LEU:HB3	1.90	0.53
1:0:947:U:H2'	1:0:948:G:C8	2.43	0.53
18:O:42:GLU:HB2	39:O:2176:HOH:O	2.08	0.53
7:C:219:ASN:O	7:C:222:ASP:HB2	2.07	0.53
18:O:96:VAL:HA	39:O:4258:HOH:O	2.07	0.53
12:H:167:PRO:O	12:H:168:ALA:HB2	2.08	0.53
5:A:35:GLY:O	5:A:36:ASP:CB	2.47	0.53
26:W:6:GLN:HG2	26:W:29:VAL:HA	1.90	0.53
1:0:1634:G:H3'	39:0:4181:HOH:O	2.08	0.53
1:0:1528:A:H2'	1:0:1529:G:O4'	2.08	0.53
1:0:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.53
2:9:3013:A:O2'	2:9:3014:G:H5''	2.08	0.53
5:A:199:HIS:CD2	5:A:201:PHE:H	2.24	0.53
15:L:134:GLU:HG3	39:L:9363:HOH:O	2.07	0.53
26:W:65:VAL:HA	26:W:68:THR:HG22	1.90	0.53
7:C:7:ASP:OD2	7:C:9:ASP:HB2	2.08	0.53
6:B:214:PRO:HD2	39:B:9322:HOH:O	2.08	0.53
1:0:2044:G:OP1	27:X:23:HIS:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.43	0.53
8:D:64:ARG:CD	8:D:67:ASP:HB3	2.38	0.53
18:O:105:ASN:ND2	18:O:109:SER:H	2.03	0.53
5:A:105:VAL:HG13	5:A:155:THR:O	2.08	0.53
6:B:81:ALA:O	6:B:186:GLY:HA3	2.07	0.53
1:0:1380:U:O4	1:0:2043:U:H4'	2.08	0.53
1:0:10:U:O4	1:0:532:A:OP2	2.24	0.53
14:K:75:ARG:O	14:K:93:ASN:HA	2.09	0.53
5:A:192:VAL:HG13	39:A:9352:HOH:O	2.09	0.53
6:B:30:PRO:HB2	6:B:39:GLN:NE2	2.23	0.53
1:0:2468:A:H61	32:3:48:ASN:HD21	1.56	0.53
1:0:1097:A:H5''	26:W:125:HIS:NE2	2.24	0.53
33:I:98:ALA:O	33:I:137:VAL:HA	2.09	0.53
17:N:143:ARG:HA	17:N:172:PHE:CD2	2.43	0.53
17:N:38:LYS:HE2	17:N:107:ASN:ND2	2.23	0.53
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.89	0.53
6:B:297:VAL:HB	39:B:9413:HOH:O	2.09	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.43	0.53
1:0:2748:G:H5'	39:0:7711:HOH:O	2.08	0.53
19:P:131:PHE:CD1	19:P:137:LEU:HD13	2.43	0.53
1:0:1014:A:H2'	1:0:1015:C:H5'	1.90	0.53
1:0:671:A:O2'	1:0:672:G:H2'	2.09	0.53
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.89	0.53
33:I:134:SER:O	33:I:135:LEU:HD23	2.09	0.53
1:0:2521:A:OP2	12:H:3:ALA:HB3	2.08	0.53
13:J:45:VAL:HG21	13:J:129:PHE:CD1	2.44	0.53
9:E:10:ASP:HA	39:E:6017:HOH:O	2.08	0.53
19:P:103:THR:HA	19:P:106:ARG:NH1	2.23	0.53
8:D:153:THR:O	8:D:156:ARG:HB2	2.08	0.53
5:A:36:ASP:O	5:A:38:ILE:N	2.42	0.53
5:A:192:VAL:HB	39:A:9391:HOH:O	2.07	0.53
15:L:120:LEU:HD12	15:L:133:VAL:HG21	1.91	0.53
1:0:952:G:N3	1:0:2302:A:H2'	2.23	0.53
7:C:45:ASP:OD2	7:C:98:ARG:HD2	2.09	0.53
22:S:6:LYS:O	22:S:7:HIS:HB3	2.08	0.53
7:C:5:ILE:HD11	7:C:16:VAL:CG2	2.38	0.53
7:C:76:ARG:HD3	39:C:9165:HOH:O	2.08	0.53
26:W:64:THR:O	26:W:68:THR:HG22	2.09	0.53
5:A:76:VAL:HG23	29:Z:63:LYS:HB3	1.91	0.53
25:V:56:ILE:O	25:V:60:GLN:HG3	2.09	0.53
5:A:36:ASP:HB2	5:A:85:SER:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:315:VAL:HG23	6:B:316:ARG:HG2	1.91	0.53
24:U:17:THR:HG22	24:U:18:GLY:N	2.23	0.53
33:I:122:THR:HG22	33:I:126:LYS:HE3	1.89	0.53
27:X:71:ARG:HB3	27:X:88:GLU:OE1	2.08	0.53
1:O:2064:U:H4'	1:O:2653:A:OP1	2.09	0.53
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.89	0.53
1:O:2894:C:O2'	1:O:2895:C:H5'	2.09	0.53
1:O:1352:A:N1	7:C:48:SER:HB3	2.23	0.53
28:Y:112:GLU:CD	28:Y:115:ARG:HH12	2.12	0.53
26:W:122:ARG:HG2	26:W:152:ALA:O	2.09	0.52
16:M:9:ARG:HB2	16:M:47:ASP:OD2	2.08	0.52
1:O:1086:A:N6	26:W:11:VAL:HG11	2.24	0.52
32:3:3:MET:O	32:3:90:PHE:HA	2.09	0.52
8:D:170:TYR:O	8:D:171:ASP:HB3	2.09	0.52
1:O:2132:C:H1'	16:M:124:GLY:HA3	1.91	0.52
24:U:49:LEU:HD13	24:U:51:TRP:HE1	1.73	0.52
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.42	0.52
13:J:93:ARG:NH1	13:J:93:ARG:HB3	2.23	0.52
23:T:9:LYS:CE	23:T:13:ARG:NH1	2.64	0.52
1:O:2533:C:H6	1:O:2533:C:C5'	2.21	0.52
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.90	0.52
6:B:150:ALA:O	6:B:152:PRO:HD3	2.08	0.52
18:O:96:VAL:HG12	18:O:100:GLN:HB2	1.91	0.52
39:O:7531:HOH:O	5:A:177:HIS:HE1	1.92	0.52
18:O:38:ARG:NH1	39:O:7674:HOH:O	2.43	0.52
21:R:39:THR:CG2	21:R:42:GLU:HG3	2.39	0.52
33:I:92:PRO:C	33:I:94:GLU:H	2.11	0.52
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.92	0.52
1:O:1419:U:H2'	1:O:1685:A:C2	2.44	0.52
10:F:37:THR:O	10:F:41:GLU:HG3	2.09	0.52
1:O:383:A:H4'	39:O:5573:HOH:O	2.10	0.52
1:O:270:U:H1'	39:O:4014:HOH:O	2.08	0.52
1:O:2840:A:OP1	6:B:211:THR:HG23	2.10	0.52
1:O:317:A:OP1	23:T:52:ARG:O	2.26	0.52
5:A:217:ARG:HG2	5:A:229:ALA:HB2	1.89	0.52
19:P:38:GLU:HA	19:P:41:ARG:NH1	2.24	0.52
1:O:776:A:OP1	30:1:28:HIS:HE1	1.93	0.52
2:9:3114:G:O6	17:N:11:ARG:HD3	2.10	0.52
1:O:947:U:H2'	1:O:948:G:H8	1.72	0.52
7:C:95:GLU:N	7:C:95:GLU:OE1	2.32	0.52
7:C:13:ASP:OD1	7:C:13:ASP:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:46:ILE:HA	25:V:49:LEU:HD12	1.91	0.52
14:K:22:ASP:HB2	39:K:5264:HOH:O	2.09	0.52
13:J:41:ALA:HB3	39:J:5907:HOH:O	2.09	0.52
1:0:1878:G:H1'	39:0:6340:HOH:O	2.09	0.52
23:T:43:ASN:ND2	23:T:108:ARG:CZ	2.73	0.52
6:B:171:VAL:HG12	6:B:174:ARG:NH2	2.25	0.52
1:0:2504:A:H4'	12:H:71:ARG:NH1	2.25	0.52
17:N:143:ARG:NH1	17:N:173:ASP:OD1	2.43	0.52
1:0:1157:C:H2'	1:0:1158:G:H8	1.74	0.52
10:F:58:GLU:HA	10:F:61:MET:HE2	1.91	0.52
1:0:447:A:O2'	1:0:448:G:H5'	2.09	0.52
27:X:43:VAL:HG22	27:X:76:ARG:NH1	2.24	0.52
6:B:41:PHE:HA	6:B:79:MET:CE	2.38	0.52
15:L:54:PRO:HG2	15:L:57:VAL:CG2	2.40	0.52
1:0:1853:C:O2'	5:A:217:ARG:NH2	2.43	0.52
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.74	0.52
13:J:42:GLU:HG3	13:J:145:TRP:CD1	2.44	0.52
1:0:1778:A:H2'	1:0:1779:A:H5'	1.92	0.52
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.91	0.52
8:D:167:GLU:OE2	8:D:173:GLU:HG2	2.09	0.52
25:V:57:LYS:HA	25:V:60:GLN:HE21	1.74	0.52
29:Z:81:ARG:O	29:Z:82:SER:C	2.47	0.52
22:S:77:VAL:O	22:S:80:ARG:HG2	2.09	0.52
6:B:144:THR:HB	39:B:9433:HOH:O	2.09	0.52
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.92	0.52
1:0:2740:G:H2'	1:0:2741:A:O4'	2.10	0.52
1:0:288:A:H61	1:0:364:C:H42	1.58	0.52
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.52
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.91	0.52
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.40	0.52
6:B:280:VAL:HG13	6:B:334:SER:HA	1.92	0.52
1:0:162:C:H2'	1:0:163:U:H5'	1.92	0.52
17:N:114:LYS:O	17:N:117:ALA:HB3	2.09	0.52
25:V:12:THR:HG22	25:V:15:GLU:CG	2.19	0.52
26:W:139:GLY:O	26:W:141:HIS:CD2	2.63	0.52
25:V:38:GLY:C	25:V:40:PRO:HD2	2.30	0.52
2:9:3091:C:H2'	2:9:3092:G:O4'	2.10	0.52
27:X:78:GLU:HG2	27:X:79:GLU:N	2.24	0.52
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.52
1:0:1015:C:H2'	1:0:1016:U:C6	2.44	0.52
8:D:153:THR:HA	8:D:156:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:20:ARG:HG2	31:2:21:VAL:N	2.25	0.52
1:0:2719:A:C2	6:B:70:PRO:HG3	2.45	0.52
26:W:1:MET:N	26:W:37:GLU:HG3	2.25	0.52
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.92	0.52
1:0:1123:A:C6	1:0:1238:C:H5'	2.45	0.52
6:B:177:HIS:O	6:B:181:ILE:HG13	2.10	0.52
11:G:71:LEU:C	11:G:73:ASP:H	2.13	0.52
1:0:2718:C:H6	1:0:2718:C:H5'	1.75	0.51
23:T:71:VAL:CG1	23:T:90:PRO:HB3	2.34	0.51
14:K:75:ARG:CZ	39:K:4172:HOH:O	2.58	0.51
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.51
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.10	0.51
24:U:6:CYS:C	24:U:8:TYR:H	2.14	0.51
19:P:94:TRP:CZ2	19:P:98:ILE:HG13	2.46	0.51
1:0:485:A:O2'	1:0:487:G:H5'	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51
1:0:1331:A:OP2	28:Y:142:SER:OG	2.27	0.51
7:C:156:LEU:O	7:C:160:LEU:HG	2.09	0.51
13:J:95:ARG:O	13:J:99:GLU:HG3	2.10	0.51
1:0:2392:C:H4'	39:Q:2875:HOH:O	2.09	0.51
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.22	0.51
1:0:506:G:H22	1:0:509:A:H5'	1.73	0.51
1:0:1015:C:H2'	1:0:1016:U:H6	1.74	0.51
1:0:2300:A:H4'	1:0:2301:A:O5'	2.11	0.51
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.91	0.51
12:H:169:GLY:HA3	39:H:9189:HOH:O	2.10	0.51
2:9:3039:U:H3'	2:9:3040:C:H5''	1.92	0.51
19:P:103:THR:HB	39:P:181:HOH:O	2.09	0.51
26:W:1:MET:HB2	26:W:103:GLU:HG2	1.91	0.51
5:A:81:GLN:HB2	5:A:92:ASN:ND2	2.25	0.51
23:T:41:ARG:NH1	23:T:42:VAL:O	2.43	0.51
1:0:1462:C:H2'	1:0:1463:A:C8	2.46	0.51
26:W:48:VAL:HG12	26:W:52:VAL:HB	1.93	0.51
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.39	0.51
1:0:475:G:OP1	7:C:73:LEU:HD22	2.11	0.51
14:K:118:ALA:HA	14:K:125:ALA:HB2	1.93	0.51
1:0:1878:G:O2'	1:0:1879:U:OP2	2.28	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.92	0.51
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.10	0.51
1:0:603:A:H5''	1:0:604:G:OP1	2.10	0.51
1:0:1624:A:H5'	1:0:1626:A:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1029:U:O2'	1:0:1273:C:OP1	2.25	0.51
2:9:3057:A:O2'	8:D:152:PRO:HD2	2.10	0.51
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.44	0.51
23:T:48:VAL:HG22	23:T:97:ARG:C	2.31	0.51
1:0:1010:C:H4'	17:N:4:PRO:HB2	1.93	0.51
1:0:1803:C:H2'	1:0:1804:A:H8	1.74	0.51
2:9:3034:A:H2'	2:9:3035:C:O4'	2.10	0.51
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.51
1:0:1495:C:H1'	1:0:1573:A:H1'	1.92	0.51
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.41	0.51
1:0:1614:G:H2'	39:0:4895:HOH:O	2.11	0.51
15:L:73:VAL:HG11	15:L:118:LEU:HD21	1.91	0.51
1:0:1278:A:H4'	1:0:1279:U:C4	2.45	0.51
2:9:3055:U:H4'	2:9:3056:A:C8	2.45	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.51
23:T:35:TYR:CG	23:T:112:LEU:HD22	2.46	0.51
1:0:588:G:O6	26:W:154:ARG:NH1	2.42	0.51
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.74	0.51
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.10	0.51
11:G:64:ASN:N	11:G:64:ASN:ND2	2.57	0.51
1:0:2676:C:H4'	13:J:70:PHE:HE1	1.76	0.51
1:0:2256:G:H2'	1:0:2257:G:C5'	2.40	0.51
1:0:2335:C:H2'	1:0:2336:G:C8	2.46	0.51
15:L:30:ARG:NH2	39:L:9320:HOH:O	2.40	0.51
1:0:92:G:H4'	25:V:44:GLY:HA3	1.93	0.51
10:F:110:ASP:O	10:F:114:LYS:HG3	2.11	0.51
1:0:1849:G:H1'	1:0:2011:A:N1	2.26	0.51
12:H:45:VAL:HG21	12:H:140:VAL:HA	1.91	0.51
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.76	0.51
7:C:127:ARG:HG2	7:C:127:ARG:NH1	2.26	0.51
14:K:14:LYS:HG3	14:K:32:ILE:O	2.11	0.51
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.24	0.51
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.76	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.10	0.51
16:M:64:ARG:HD2	39:M:9385:HOH:O	2.10	0.51
9:E:93:MET:HE1	9:E:165:GLY:N	2.25	0.51
25:V:12:THR:HG23	25:V:14:ALA:H	1.76	0.51
8:D:63:ILE:HG13	8:D:64:ARG:N	2.26	0.51
1:0:2909:G:H2'	1:0:2910:A:H8	1.74	0.51
1:0:2265:U:H2'	1:0:2266:A:H8	1.75	0.51
1:0:1741:U:O2'	1:0:2723:G:H4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:144:ARG:NH1	39:Y:9376:HOH:O	2.44	0.51
6:B:175:LEU:C	6:B:175:LEU:HD23	2.30	0.51
6:B:128:ILE:O	6:B:131:ALA:HB3	2.11	0.51
1:O:1923:G:H4'	32:3:31:THR:O	2.10	0.51
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.25	0.51
1:O:328:U:O4'	7:C:202:THR:HG22	2.11	0.51
1:O:449:A:N7	7:C:43:LYS:HG2	2.26	0.51
1:O:2487:C:O4'	3:4:77:HFA:HB2	2.10	0.51
12:H:63:GLU:HA	39:H:9179:HOH:O	2.10	0.51
1:O:1342:C:O2'	1:O:1343:C:H5'	2.11	0.51
26:W:108:ARG:HE	26:W:114:PRO:CG	2.22	0.51
14:K:62:PRO:HG3	14:K:65:ARG:NH2	2.26	0.51
15:L:125:PHE:CE1	15:L:140:VAL:HG13	2.46	0.51
1:O:2717:C:O2'	1:O:2718:C:H5''	2.11	0.51
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.25	0.51
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.11	0.51
6:B:202:VAL:HG11	6:B:301:VAL:HG13	1.91	0.51
1:O:2081:A:H4'	13:J:69:TYR:CE1	2.46	0.51
6:B:232:TRP:CD1	6:B:235:ARG:HD2	2.46	0.51
7:C:153:VAL:O	7:C:157:LEU:HG	2.11	0.51
1:O:263:U:O4'	10:F:59:ILE:HD13	2.11	0.51
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.40	0.50
1:O:1132:A:N6	1:O:1229:C:H2'	2.27	0.50
17:N:176:ARG:O	17:N:180:LEU:HD13	2.12	0.50
6:B:314:ALA:CB	6:B:317:PRO:HG3	2.41	0.50
13:J:46:ILE:O	13:J:46:ILE:HG12	2.11	0.50
17:N:67:ALA:C	17:N:69:TYR:H	2.13	0.50
31:2:20:ARG:CG	31:2:21:VAL:N	2.74	0.50
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.74	0.50
1:O:2821:C:H4'	6:B:116:PRO:HB3	1.93	0.50
9:E:21:THR:HG23	9:E:30:THR:OG1	2.11	0.50
21:R:99:ALA:HB1	21:R:109:MET:HE3	1.91	0.50
8:D:94:ALA:CB	8:D:97:GLN:HE21	2.25	0.50
10:F:48:VAL:CG2	10:F:74:PHE:HB3	2.41	0.50
9:E:15:GLN:HB2	9:E:20:ILE:HG12	1.93	0.50
12:H:148:GLU:HA	12:H:148:GLU:OE1	2.11	0.50
27:X:70:ILE:HG23	27:X:70:ILE:O	2.11	0.50
7:C:236:THR:HG22	7:C:239:ALA:CB	2.42	0.50
17:N:77:ASN:OD1	17:N:79:PRO:HD2	2.12	0.50
9:E:68:HIS:O	9:E:72:MET:HG3	2.11	0.50
20:Q:32:GLU:O	20:Q:93:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:119:HIS:O	6:B:121:PRO:HD3	2.11	0.50
1:0:958:G:H2'	1:0:959:C:C6	2.46	0.50
7:C:150:THR:HA	7:C:203:ALA:O	2.11	0.50
31:2:41:HIS:O	31:2:45:ASN:HB2	2.11	0.50
15:L:114:VAL:HG11	39:L:9378:HOH:O	2.10	0.50
6:B:147:VAL:O	6:B:147:VAL:HG12	2.11	0.50
8:D:25:MET:CE	8:D:41:LEU:HG	2.31	0.50
28:Y:187:VAL:HB	39:Y:9372:HOH:O	2.10	0.50
2:9:3055:U:H4'	2:9:3056:A:H8	1.74	0.50
1:0:2072:G:C6	1:0:2533:C:H1'	2.47	0.50
5:A:51:ARG:NH1	5:A:120:ARG:O	2.44	0.50
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.76	0.50
28:Y:155:ARG:NH1	39:Y:9359:HOH:O	2.44	0.50
8:D:105:SER:HB2	8:D:131:THR:HG23	1.92	0.50
1:0:2372:A:H2'	1:0:2373:U:C6	2.47	0.50
16:M:46:LEU:HG	39:M:9419:HOH:O	2.12	0.50
14:K:45:PRO:HB2	39:K:7169:HOH:O	2.11	0.50
1:0:797:A:H4'	29:Z:10:ARG:N	2.26	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.47	0.50
1:0:2054:A:C2	21:R:128:ARG:NH2	2.80	0.50
6:B:5:ARG:HD2	6:B:8:LYS:NZ	2.27	0.50
19:P:105:LEU:HD21	19:P:137:LEU:HD21	1.94	0.50
5:A:109:GLU:HG2	5:A:116:GLY:H	1.76	0.50
1:0:2256:G:C2'	1:0:2257:G:H5'	2.42	0.50
1:0:67:A:H5''	1:0:69:A:C8	2.47	0.50
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.75	0.50
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.12	0.50
1:0:820:G:H5''	39:0:3345:HOH:O	2.12	0.50
1:0:926:A:O2'	15:L:41:HIS:CD2	2.65	0.50
1:0:1423:C:O2'	1:0:1424:A:H5'	2.12	0.50
20:Q:64:GLU:HG3	20:Q:74:ASP:OD2	2.10	0.50
21:R:72:VAL:CG1	21:R:75:TRP:HB3	2.42	0.50
6:B:7:ARG:HG2	6:B:7:ARG:HH11	1.77	0.50
25:V:1:THR:O	25:V:4:HIS:CE1	2.65	0.50
6:B:52:VAL:C	6:B:53:LEU:HD12	2.31	0.50
1:0:1881:A:OP1	5:A:199:HIS:HE1	1.95	0.50
21:R:96:VAL:O	21:R:99:ALA:HB3	2.11	0.50
9:E:84:MET:HB2	9:E:131:LEU:HB2	1.93	0.50
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.41	0.50
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.26	0.50
18:O:38:ARG:HD3	39:O:7674:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2834:G:OP1	27:X:39:LYS:HE2	2.11	0.50
26:W:88:THR:CG2	26:W:110:GLN:NE2	2.74	0.49
29:Z:26:VAL:O	29:Z:30:GLU:HG3	2.12	0.49
25:V:64:GLY:O	25:V:65:ASP:CB	2.59	0.49
23:T:43:ASN:HD22	23:T:108:ARG:NH2	2.09	0.49
1:0:292:G:H2'	1:0:358:G:N2	2.27	0.49
1:0:1087:G:H4'	1:0:1088:A:OP1	2.13	0.49
1:0:2670:G:O2'	1:0:2671:U:H5'	2.12	0.49
1:0:1189:A:H1'	1:0:1209:C:H1'	1.94	0.49
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.93	0.49
1:0:1819:G:H2'	1:0:1820:G:C4'	2.43	0.49
26:W:38:THR:HG22	26:W:39:ASP:H	1.77	0.49
39:O:5696:HOH:O	11:G:12:ILE:HA	2.13	0.49
1:0:474:C:O3'	7:C:73:LEU:CD2	2.60	0.49
1:0:159:G:OP1	16:M:74:LYS:HE3	2.12	0.49
1:0:705:C:H2'	1:0:705:C:O2	2.12	0.49
1:0:2588:OMG:H3'	1:0:2589:U:H5''	1.94	0.49
1:0:1242:A:H5'	13:J:82:THR:CG2	2.26	0.49
33:I:92:PRO:HG3	39:I:6825:HOH:O	2.13	0.49
1:0:2270:G:C4'	5:A:223:ARG:HH12	2.21	0.49
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.94	0.49
17:N:47:LEU:CD1	17:N:97:VAL:HG11	2.42	0.49
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.47	0.49
1:0:1114:A:H2'	1:0:1115:U:C6	2.48	0.49
1:0:1114:A:H2'	1:0:1115:U:H6	1.77	0.49
16:M:159:VAL:HG13	16:M:160:PHE:N	2.27	0.49
7:C:145:GLU:OE1	7:C:198:ASP:HB2	2.12	0.49
1:0:1559:A:OP2	1:0:1559:A:H8	1.96	0.49
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.95	0.49
7:C:76:ARG:HG2	7:C:78:ARG:NH1	2.27	0.49
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.93	0.49
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.26	0.49
16:M:61:ILE:CG2	16:M:62:VAL:N	2.75	0.49
16:M:122:GLN:OE1	16:M:127:LYS:HE2	2.12	0.49
1:0:512:G:O3'	1:0:513:A:H8	1.96	0.49
1:0:2385:G:H2'	1:0:2386:U:C6	2.48	0.49
28:Y:219:GLU:HG3	28:Y:220:GLU:N	2.27	0.49
12:H:9:ILE:HD12	12:H:54:THR:CG2	2.43	0.49
8:D:163:VAL:HA	39:D:6326:HOH:O	2.13	0.49
7:C:111:VAL:HB	39:C:9120:HOH:O	2.12	0.49
12:H:88:ARG:NH1	12:H:135:THR:OG1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:34:GLU:HG2	21:R:46:TYR:OH	2.12	0.49
39:O:4494:HOH:O	14:K:2:GLU:HG3	2.12	0.49
1:O:1191:A:H3'	1:O:1192:A:H5''	1.93	0.49
12:H:9:ILE:O	12:H:9:ILE:HG22	2.11	0.49
6:B:321:PRO:HA	39:B:9466:HOH:O	2.12	0.49
1:O:1972:U:H2'	1:O:1973:A:H5'	1.95	0.49
6:B:80:ARG:O	6:B:82:VAL:HG23	2.12	0.49
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.28	0.49
1:O:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.49
1:O:1138:G:H4'	39:O:5940:HOH:O	2.13	0.49
21:R:47:LEU:O	21:R:51:ILE:HG13	2.12	0.49
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.78	0.49
5:A:33:GLU:OE1	5:A:33:GLU:N	2.45	0.49
26:W:21:LEU:O	26:W:26:ILE:HG12	2.13	0.49
12:H:9:ILE:HG12	12:H:56:GLN:CG	2.43	0.49
1:O:1205:U:C2'	1:O:1206:U:H5''	2.42	0.49
17:N:163:PHE:O	17:N:164:ASP:OD1	2.30	0.49
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.28	0.49
23:T:19:ARG:NH1	23:T:68:ASP:O	2.46	0.49
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.77	0.49
18:O:21:SER:OG	18:O:106:PRO:HB2	2.13	0.49
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.93	0.49
1:O:2346:C:O5'	1:O:2346:C:H6	1.95	0.49
27:X:31:ILE:O	27:X:35:GLU:HG3	2.12	0.49
12:H:162:ARG:HD3	39:H:9182:HOH:O	2.13	0.49
1:O:621:C:H5'	28:Y:132:ASP:OD2	2.13	0.49
22:S:42:GLU:HG2	22:S:49:VAL:HG23	1.95	0.49
14:K:115:ARG:HG3	14:K:116:GLU:N	2.28	0.49
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.27	0.49
1:O:1666:C:C2'	1:O:1667:A:C5'	2.91	0.49
1:O:2506:A:H1'	39:O:4039:HOH:O	2.11	0.49
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.48	0.49
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.95	0.49
1:O:553:G:OP2	28:Y:204:ARG:NH2	2.44	0.49
1:O:303:C:H2'	1:O:304:G:O4'	2.13	0.49
1:O:602:A:O2'	1:O:605:C:H4'	2.13	0.49
17:N:110:THR:HB	17:N:113:SER:OG	2.13	0.49
17:N:154:LEU:HD12	17:N:156:GLU:O	2.13	0.49
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.43	0.49
23:T:64:ASN:HB3	23:T:73:HIS:HB2	1.94	0.49
1:O:1202:A:H2'	1:O:1203:G:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.76	0.49
1:O:1313:A:H5'	28:Y:208:LYS:O	2.12	0.49
7:C:20:ASP:O	7:C:23:GLU:HB2	2.12	0.49
11:G:23:ILE:O	11:G:27:ILE:HG13	2.12	0.49
7:C:142:ASP:OD1	7:C:237:GLU:HB3	2.13	0.49
1:O:1181:A:N1	1:O:1192:A:O2'	2.46	0.49
5:A:36:ASP:C	5:A:38:ILE:H	2.16	0.49
26:W:4:LEU:O	26:W:32:CYS:HA	2.12	0.49
1:O:1189:A:H3'	39:O:7845:HOH:O	2.11	0.49
7:C:72:LYS:HG2	7:C:77:ALA:HA	1.94	0.49
27:X:76:ARG:NH1	27:X:76:ARG:HG3	2.22	0.49
18:O:32:ARG:HH21	18:O:35:LYS:HD2	1.78	0.49
1:O:1766:U:O2	1:O:1778:A:H5'	2.13	0.49
1:O:485:A:N3	1:O:487:G:H5''	2.27	0.49
5:A:97:ALA:HB2	5:A:150:PRO:HB2	1.95	0.49
1:O:74:A:H2'	1:O:75:U:C6	2.47	0.49
1:O:2251:G:H2'	1:O:2252:A:C8	2.47	0.49
1:O:2815:G:N7	13:J:80:LYS:NZ	2.59	0.49
26:W:90:TYR:CE2	26:W:99:ALA:HB2	2.48	0.48
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.23	0.48
19:P:14:LEU:HD13	19:P:51:ALA:HB2	1.94	0.48
2:9:3054:A:H2	39:9:3535:HOH:O	1.96	0.48
1:O:1158:G:O2'	1:O:1159:G:H5'	2.13	0.48
23:T:48:VAL:HG22	23:T:97:ARG:O	2.13	0.48
6:B:62:ARG:HA	6:B:65:MET:HE3	1.93	0.48
10:F:26:THR:HG21	10:F:103:GLU:CB	2.41	0.48
6:B:112:THR:OG1	6:B:158:LYS:HG2	2.12	0.48
1:O:1406:A:H4'	1:O:1407:A:C5'	2.43	0.48
17:N:82:TYR:C	17:N:82:TYR:CD2	2.87	0.48
26:W:19:ASP:O	26:W:23:MET:HG3	2.13	0.48
1:O:660:A:H4'	1:O:661:G:O5'	2.13	0.48
1:O:669:G:O2'	1:O:670:G:H5'	2.13	0.48
26:W:34:LEU:CD1	26:W:100:LEU:HD13	2.43	0.48
18:O:26:TRP:HA	18:O:26:TRP:CE3	2.48	0.48
1:O:1119:G:H8	13:J:52:GLN:HE22	1.61	0.48
1:O:2780:C:H2'	1:O:2781:U:C6	2.48	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
17:N:33:ARG:NH2	39:N:9351:HOH:O	2.46	0.48
24:U:39:ASN:HD22	24:U:44:ARG:HH11	1.61	0.48
1:O:1028:U:H1'	39:O:3938:HOH:O	2.12	0.48
19:P:135:ALA:HB1	19:P:139:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:133:HIS:HD2	39:Y:9383:HOH:O	1.95	0.48
1:0:2730:G:O2'	1:0:2731:G:H5'	2.13	0.48
26:W:139:GLY:O	26:W:141:HIS:HD2	1.96	0.48
33:I:123:ASN:HA	33:I:126:LYS:HD2	1.93	0.48
19:P:143:ALA:HA	39:P:192:HOH:O	2.12	0.48
1:0:1839:A:H5'	1:0:2643:G:H4'	1.95	0.48
1:0:2076:U:H5''	39:0:3991:HOH:O	2.12	0.48
1:0:1555:G:H4'	1:0:1630:A:H2	1.78	0.48
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.48
33:I:139:ILE:HG22	33:I:140:GLU:N	2.27	0.48
25:V:1:THR:HG23	25:V:2:VAL:N	2.24	0.48
9:E:45:ASP:OD2	9:E:46:THR:HG23	2.12	0.48
13:J:130:VAL:HG12	13:J:131:THR:N	2.28	0.48
2:9:3044:A:H1'	8:D:76:ARG:NH2	2.29	0.48
27:X:78:GLU:CG	27:X:79:GLU:H	2.26	0.48
9:E:119:HIS:O	9:E:140:ALA:HB1	2.13	0.48
16:M:81:ARG:HG3	16:M:85:ARG:HB2	1.95	0.48
1:0:289:G:O2'	1:0:290:C:H5'	2.14	0.48
8:D:64:ARG:CG	8:D:67:ASP:HB3	2.44	0.48
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.95	0.48
1:0:2896:A:OP1	27:X:15:ARG:NH1	2.47	0.48
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.48
9:E:132:THR:O	9:E:132:THR:HG23	2.13	0.48
1:0:581:G:O2'	1:0:582:C:H5'	2.13	0.48
1:0:349:U:O2'	1:0:350:C:H5'	2.14	0.48
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.49	0.48
1:0:1189:A:O2'	1:0:1208:C:H2'	2.12	0.48
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.59	0.48
6:B:162:MET:CE	6:B:308:LEU:HD21	2.43	0.48
1:0:821:U:H2'	1:0:822:C:H6	1.78	0.48
6:B:280:VAL:CG1	6:B:334:SER:HA	2.43	0.48
1:0:2793:A:H2'	1:0:2794:G:H5'	1.96	0.48
1:0:503:G:H2'	1:0:504:G:H8	1.78	0.48
32:3:69:TYR:HB2	32:3:78:HIS:CE1	2.48	0.48
26:W:126:ASP:HB3	26:W:135:GLY:O	2.13	0.48
39:0:7597:HOH:O	23:T:9:LYS:HD2	2.14	0.48
28:Y:189:ASN:ND2	28:Y:189:ASN:C	2.66	0.48
21:R:8:ALA:CB	21:R:13:THR:HG21	2.35	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.95	0.48
7:C:246:ARG:NH1	7:C:246:ARG:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.48
12:H:73:LEU:HD21	12:H:146:VAL:HA	1.96	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.14	0.48
1:0:2728:C:H2'	1:0:2729:C:H6	1.78	0.48
28:Y:216:ARG:HD3	39:Y:9371:HOH:O	2.14	0.48
17:N:154:LEU:O	17:N:155:GLU:CB	2.62	0.48
33:I:75:THR:OG1	33:I:112:LYS:NZ	2.46	0.48
6:B:41:PHE:HB3	6:B:190:MET:HE3	1.95	0.48
2:9:3051:A:H5'	17:N:160:SER:HB3	1.96	0.48
8:D:172:VAL:HG12	8:D:173:GLU:N	2.28	0.48
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.96	0.48
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.44	0.48
25:V:49:LEU:O	25:V:53:ILE:HG13	2.14	0.48
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.96	0.48
21:R:114:VAL:HA	21:R:144:GLU:O	2.13	0.48
1:0:1398:G:H2'	1:0:1399:A:C8	2.48	0.48
1:0:2325:C:O2'	1:0:2411:C:H1'	2.12	0.48
27:X:10:VAL:HG12	27:X:11:THR:N	2.28	0.48
1:0:204:A:H2'	1:0:205:U:H5'	1.95	0.48
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.96	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.48
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.96	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.29	0.48
10:F:58:GLU:HG3	10:F:61:MET:HE1	1.96	0.48
32:3:16:GLU:HG3	32:3:18:GLN:HE21	1.79	0.48
5:A:164:ARG:HA	29:Z:69:TYR:CE1	2.49	0.48
9:E:20:ILE:HD11	9:E:40:VAL:CG1	2.44	0.48
1:0:1525:G:H5'	1:0:1526:A:OP2	2.14	0.48
1:0:343:C:O2'	1:0:344:C:H5'	2.13	0.48
17:N:44:ARG:HG3	17:N:45:ALA:N	2.29	0.48
1:0:797:A:H5'	29:Z:10:ARG:N	2.28	0.47
1:0:506:G:N2	1:0:508:A:H3'	2.29	0.47
33:I:112:LYS:O	33:I:116:LEU:HG	2.13	0.47
19:P:16:VAL:HG13	19:P:20:ARG:HB2	1.96	0.47
5:A:179:MET:HA	5:A:179:MET:CE	2.44	0.47
1:0:2898:G:H4'	6:B:288:GLY:HA2	1.96	0.47
1:0:702:G:O2'	1:0:703:G:H5'	2.14	0.47
17:N:119:GLN:O	17:N:123:ILE:HG13	2.14	0.47
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.61	0.47
1:0:1565:C:O4'	1:0:2738:G:H1'	2.14	0.47
1:0:894:A:C2	7:C:87:ARG:NH2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:25:ARG:O	29:Z:29:ILE:HG13	2.14	0.47
17:N:32:PRO:HD2	17:N:99:GLU:O	2.14	0.47
14:K:99:ASP:OD2	14:K:103:ASP:HB2	2.14	0.47
22:S:76:GLU:HB3	39:S:9145:HOH:O	2.12	0.47
11:G:71:LEU:O	11:G:73:ASP:N	2.47	0.47
1:O:2050:G:OP1	21:R:79:ARG:HB3	2.14	0.47
1:O:1940:C:H4'	39:O:7519:HOH:O	2.14	0.47
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.78	0.47
6:B:254:GLN:HG2	6:B:255:GLY:H	1.78	0.47
1:O:657:G:H2'	1:O:658:C:C6	2.49	0.47
26:W:11:VAL:O	26:W:12:ASN:HB2	2.14	0.47
8:D:94:ALA:HA	8:D:174:VAL:O	2.14	0.47
1:O:1787:C:O2'	1:O:1788:U:H5'	2.14	0.47
1:O:790:A:H1'	1:O:1710:A:H2'	1.96	0.47
1:O:1904:A:C2	1:O:1905:U:H1'	2.49	0.47
29:Z:80:ARG:O	29:Z:81:ARG:O	2.33	0.47
26:W:108:ARG:HE	26:W:114:PRO:HG3	1.80	0.47
1:O:2604:A:H5'	39:O:6019:HOH:O	2.13	0.47
1:O:598:C:H2'	1:O:599:G:H8	1.78	0.47
1:O:407:A:H2'	1:O:408:A:C8	2.49	0.47
1:O:538:C:OP2	28:Y:134:HIS:HE1	1.97	0.47
1:O:42:C:H1'	39:O:4943:HOH:O	2.14	0.47
1:O:1160:G:O2'	1:O:1190:G:H1'	2.14	0.47
1:O:2807:U:P	6:B:27:ASN:HD21	2.37	0.47
1:O:1120:U:H5'	1:O:1121:G:OP2	2.13	0.47
7:C:7:ASP:C	7:C:9:ASP:H	2.18	0.47
14:K:34:VAL:HG21	14:K:46:LYS:O	2.15	0.47
1:O:2243:C:H5''	39:O:4043:HOH:O	2.14	0.47
1:O:228:C:H2'	1:O:229:G:H5'	1.97	0.47
12:H:45:VAL:HA	12:H:167:PRO:O	2.14	0.47
1:O:121:U:OP2	31:2:10:ARG:NH2	2.38	0.47
1:O:2073:G:OP2	1:O:2490:A:H5'	2.14	0.47
1:O:1205:U:H2'	1:O:1206:U:H5'	1.96	0.47
1:O:440:C:O2'	1:O:441:A:H5'	2.14	0.47
1:O:1477:C:H5'	1:O:1868:G:C5'	2.44	0.47
1:O:945:U:O2'	26:W:43:GLY:HA3	2.14	0.47
1:O:2563:U:H2'	1:O:2565:C:O5'	2.14	0.47
1:O:1185:U:H2'	1:O:1186:C:C6	2.49	0.47
23:T:71:VAL:HG12	23:T:72:ILE:N	2.29	0.47
1:O:2507:G:H2'	1:O:2510:C:H42	1.79	0.47
9:E:137:ASP:OD1	9:E:139:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:255:GLY:O	6:B:257:THR:HG23	2.15	0.47
8:D:166:ILE:HB	39:D:6326:HOH:O	2.15	0.47
10:F:91:VAL:CG1	10:F:92:GLY:N	2.76	0.47
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.15	0.47
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.47
1:0:485:A:HO2'	1:0:487:G:H8	1.63	0.47
5:A:72:GLU:HG3	29:Z:66:GLY:HA2	1.97	0.47
8:D:22:VAL:HA	8:D:73:VAL:O	2.14	0.47
20:Q:16:ASN:HB2	39:Q:6597:HOH:O	2.13	0.47
1:0:1250:C:O2'	1:0:1251:C:H5'	2.15	0.47
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.97	0.47
5:A:65:ARG:C	5:A:66:ARG:HG3	2.34	0.47
33:I:135:LEU:HA	39:I:7210:HOH:O	2.15	0.47
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.38	0.47
27:X:30:MET:CE	27:X:58:ALA:HB3	2.44	0.47
6:B:195:ARG:NH1	6:B:324:ASP:OD1	2.47	0.47
1:0:1450:C:O2'	1:0:1494:A:H5'	2.15	0.47
17:N:47:LEU:HD12	17:N:92:ALA:CB	2.44	0.47
1:0:1427:A:N6	1:0:1440:U:H1'	2.29	0.47
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.48	0.47
6:B:152:PRO:HD2	39:B:9439:HOH:O	2.13	0.47
1:0:816:G:H5'	1:0:1598:A:H4'	1.96	0.47
39:0:3892:HOH:O	5:A:236:GLY:HA3	2.14	0.47
1:0:2241:C:H2'	1:0:2242:U:C6	2.49	0.47
32:3:48:ASN:ND2	32:3:50:GLY:H	2.12	0.47
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.68	0.47
9:E:20:ILE:O	9:E:30:THR:HA	2.15	0.47
9:E:15:GLN:HB3	9:E:42:VAL:HG23	1.96	0.47
18:O:26:TRP:HA	18:O:26:TRP:HE3	1.79	0.47
22:S:8:PRO:HD2	25:V:32:ALA:HA	1.96	0.47
7:C:196:THR:HG23	39:C:9200:HOH:O	2.14	0.47
39:0:4995:HOH:O	17:N:21:HIS:HD2	1.97	0.47
1:0:1537:C:H1'	39:0:6789:HOH:O	2.14	0.47
1:0:2387:U:H2'	1:0:2388:C:C6	2.49	0.47
28:Y:103:THR:HG22	28:Y:104:GLU:OE2	2.14	0.47
1:0:1930:A:H2'	1:0:1931:A:C8	2.50	0.47
1:0:1597:A:O4'	19:P:95:GLU:HG2	2.15	0.47
2:9:3061:C:H2'	2:9:3062:A:H8	1.80	0.47
1:0:1418:U:OP1	31:2:42:TRP:HB3	2.15	0.47
1:0:1252:A:H2'	1:0:1253:C:O4'	2.15	0.47
20:Q:77:ASP:HB3	20:Q:82:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:32:VAL:O	5:A:33:GLU:C	2.53	0.47
5:A:192:VAL:HG12	5:A:192:VAL:O	2.15	0.47
1:0:1206:U:H2'	1:0:1207:A:O4'	2.15	0.47
1:0:1071:G:H4'	28:Y:154:ARG:NH2	2.30	0.47
1:0:1427:A:H61	1:0:1440:U:C1'	2.27	0.47
9:E:69:ILE:HA	9:E:72:MET:HE2	1.97	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47
1:0:2005:G:H3'	1:0:2005:G:OP2	2.15	0.47
5:A:82:VAL:HG13	5:A:93:THR:HB	1.97	0.47
16:M:166:ALA:CA	16:M:169:ARG:HH21	2.28	0.47
1:0:968:G:O2'	1:0:969:G:H5'	2.15	0.47
1:0:1625:U:H4'	39:0:4933:HOH:O	2.14	0.47
5:A:211:LYS:CB	5:A:212:PRO:CD	2.91	0.47
26:W:48:VAL:HG12	26:W:48:VAL:O	2.15	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.30	0.47
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.45	0.47
1:0:952:G:OP1	20:Q:42:LYS:HE2	2.15	0.47
7:C:22:PHE:HA	7:C:116:ALA:HA	1.96	0.47
1:0:120:A:H2'	1:0:120:A:N3	2.30	0.47
7:C:7:ASP:OD1	7:C:11:ASN:O	2.33	0.47
7:C:40:ALA:O	7:C:43:LYS:HB2	2.15	0.47
1:0:703:G:O2'	1:0:704:C:H5'	2.15	0.47
1:0:661:G:C5	1:0:686:A:C2	3.03	0.47
1:0:204:A:C2'	1:0:205:U:H5'	2.44	0.47
32:3:70:ARG:HG2	32:3:70:ARG:HH11	1.79	0.47
31:2:40:ARG:HG2	31:2:40:ARG:HH11	1.80	0.47
33:I:92:PRO:HB3	33:I:135:LEU:CA	2.45	0.47
13:J:74:ARG:O	13:J:78:ILE:HG12	2.15	0.47
30:1:25:LYS:CD	31:2:48:ASP:HA	2.45	0.47
39:0:6967:HOH:O	17:N:4:PRO:HD2	2.15	0.47
1:0:1972:U:C2'	1:0:1973:A:H5''	2.45	0.47
9:E:166:VAL:HG12	39:E:3134:HOH:O	2.14	0.47
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.47
15:L:40:PHE:O	15:L:43:HIS:HB2	2.15	0.47
32:3:65:THR:CG2	32:3:67:LEU:HG	2.45	0.47
33:I:92:PRO:C	33:I:94:GLU:N	2.68	0.46
1:0:793:A:C5'	19:P:83:LYS:HG2	2.40	0.46
24:U:6:CYS:HA	24:U:13:ILE:HD11	1.97	0.46
14:K:66:ARG:HD3	39:K:2777:HOH:O	2.14	0.46
18:O:25:VAL:HG23	18:O:26:TRP:N	2.30	0.46
16:M:166:ALA:N	16:M:169:ARG:HH21	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2783:A:H2'	1:0:2784:A:C8	2.50	0.46
1:0:1304:U:H2'	1:0:1305:C:C6	2.50	0.46
1:0:1507:C:H4'	39:0:3895:HOH:O	2.15	0.46
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.15	0.46
20:Q:66:LYS:HB2	20:Q:70:ALA:O	2.15	0.46
1:0:2281:C:C2'	1:0:2282:U:H5'	2.44	0.46
1:0:2520:G:H5'	12:H:61:SER:OG	2.14	0.46
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.46
39:0:4890:HOH:O	5:A:6:GLY:HA3	2.14	0.46
28:Y:117:LEU:HD12	28:Y:174:VAL:HG11	1.95	0.46
1:0:282:C:H1'	1:0:368:C:H42	1.77	0.46
8:D:135:VAL:CG2	8:D:136:ARG:N	2.78	0.46
27:X:18:ARG:HA	39:X:5356:HOH:O	2.14	0.46
9:E:64:THR:HG22	9:E:68:HIS:CD2	2.50	0.46
7:C:200:PRO:HB3	7:C:212:VAL:CG2	2.45	0.46
1:0:1334:C:O2'	1:0:1335:C:H5'	2.16	0.46
1:0:2455:A:H2'	1:0:2456:A:O4'	2.15	0.46
6:B:132:HIS:HD1	6:B:132:HIS:C	2.18	0.46
6:B:141:ARG:HB3	6:B:164:THR:O	2.15	0.46
26:W:65:VAL:CG1	26:W:116:LEU:HD13	2.46	0.46
24:U:52:THR:HG21	24:U:54:THR:HB	1.97	0.46
1:0:2690:U:H4'	9:E:111:LYS:CE	2.46	0.46
7:C:165:ASP:O	7:C:168:ARG:HB3	2.15	0.46
1:0:1135:G:H5'	39:0:6153:HOH:O	2.15	0.46
1:0:792:G:H4'	39:0:3711:HOH:O	2.16	0.46
1:0:333:G:O2'	1:0:334:G:H5'	2.16	0.46
10:F:101:ALA:HA	39:F:5413:HOH:O	2.16	0.46
14:K:121:PHE:N	14:K:121:PHE:CD1	2.84	0.46
16:M:49:ALA:C	16:M:54:TYR:HB3	2.36	0.46
21:R:124:GLY:HA3	21:R:136:TRP:O	2.16	0.46
1:0:2314:G:C2'	1:0:2315:C:H5'	2.45	0.46
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.42	0.46
33:I:132:CYS:C	33:I:134:SER:H	2.16	0.46
6:B:304:PRO:HD2	6:B:307:ARG:HD2	1.97	0.46
5:A:212:PRO:HB2	39:A:9355:HOH:O	2.15	0.46
1:0:2036:C:C1'	14:K:44:LEU:HG	2.46	0.46
7:C:246:ARG:HD2	39:C:9170:HOH:O	2.15	0.46
27:X:27:ASP:OD2	27:X:27:ASP:N	2.48	0.46
12:H:170:ASN:HD22	12:H:170:ASN:N	2.12	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
6:B:277:GLU:N	6:B:278:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2765:C:H2'	1:0:2766:A:C8	2.51	0.46
17:N:37:ARG:NH2	39:N:9331:HOH:O	2.48	0.46
8:D:135:VAL:CG2	8:D:136:ARG:H	2.23	0.46
6:B:41:PHE:HB3	6:B:190:MET:CE	2.45	0.46
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.50	0.46
10:F:48:VAL:HG23	10:F:74:PHE:HB3	1.97	0.46
23:T:43:ASN:HD22	23:T:108:ARG:CZ	2.28	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.50	0.46
1:0:1211:G:O2'	1:0:1212:C:H5'	2.15	0.46
1:0:1180:U:H2'	1:0:1181:A:C8	2.50	0.46
1:0:1820:G:C6	1:0:2030:A:C2	3.03	0.46
1:0:553:G:P	28:Y:204:ARG:NH2	2.89	0.46
6:B:146:THR:C	6:B:148:PRO:HD3	2.36	0.46
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.98	0.46
1:0:236:A:H8	1:0:236:A:OP1	1.98	0.46
1:0:589:U:H2'	1:0:590:A:H8	1.80	0.46
1:0:2529:G:H3'	39:0:7362:HOH:O	2.15	0.46
21:R:33:ARG:NH1	39:R:9342:HOH:O	2.49	0.46
1:0:399:C:H5'	16:M:179:GLY:O	2.16	0.46
5:A:173:GLY:O	5:A:176:HIS:HB3	2.16	0.46
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.31	0.46
1:0:622:G:O2'	1:0:623:U:H5'	2.16	0.46
5:A:1:GLY:HA2	5:A:197:VAL:HG23	1.98	0.46
5:A:8:ARG:HG2	39:A:9347:HOH:O	2.15	0.46
1:0:542:A:H2'	1:0:543:G:O4'	2.16	0.46
23:T:69:LYS:O	23:T:71:VAL:HG23	2.15	0.46
1:0:1268:C:O2'	1:0:1269:G:H5'	2.16	0.46
17:N:34:LEU:HA	17:N:47:LEU:HD23	1.97	0.46
30:1:28:HIS:O	30:1:32:LYS:N	2.47	0.46
30:1:8:GLN:HE22	30:1:11:LYS:HZ2	1.63	0.46
1:0:2708:G:N2	14:K:1:MET:O	2.44	0.46
1:0:247:A:H2'	39:0:4210:HOH:O	2.16	0.46
23:T:53:GLY:HA3	39:T:6384:HOH:O	2.15	0.46
16:M:167:GLY:O	16:M:171:ARG:HG3	2.16	0.46
24:U:17:THR:CG2	24:U:18:GLY:N	2.78	0.46
12:H:27:LYS:N	12:H:59:HIS:HD2	2.07	0.46
24:U:9:CYS:CA	24:U:52:THR:HG23	2.41	0.46
33:I:123:ASN:HA	33:I:126:LYS:CD	2.45	0.46
1:0:1972:U:H2'	1:0:1973:A:H5'	1.97	0.46
1:0:2715:G:N2	6:B:264:GLU:OE1	2.48	0.46
20:Q:75:ILE:HA	39:Q:6286:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.38	0.46
6:B:235:ARG:HA	39:B:9400:HOH:O	2.15	0.46
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.15	0.46
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.46	0.46
17:N:72:GLU:H	17:N:171:HIS:CE1	2.33	0.46
16:M:107:ARG:HD2	39:M:9378:HOH:O	2.16	0.46
1:O:825:U:H5''	1:O:826:U:OP1	2.16	0.46
31:2:40:ARG:CD	31:2:47:THR:HG22	2.43	0.46
13:J:47:THR:O	13:J:53:ILE:HD11	2.16	0.46
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.43	0.46
1:O:2782:G:O6	1:O:2790:C:H5''	2.16	0.46
1:O:1268:C:O2'	28:Y:169:ARG:HB2	2.16	0.46
6:B:62:ARG:NH2	6:B:66:GLU:O	2.49	0.46
1:O:2421:G:H3'	1:O:2422:U:H5''	1.98	0.46
2:9:3051:A:H5'	17:N:160:SER:CB	2.46	0.46
1:O:816:G:C6	1:O:817:G:N1	2.84	0.46
29:Z:20:ARG:O	29:Z:21:VAL:C	2.54	0.46
1:O:1926:G:H2'	1:O:1927:A:C8	2.51	0.46
6:B:312:ARG:HG2	6:B:313:PRO:N	2.28	0.46
1:O:241:A:C2	1:O:378:A:H4'	2.51	0.46
1:O:1500:U:P	19:P:41:ARG:NH2	2.89	0.46
6:B:41:PHE:CG	6:B:190:MET:HE3	2.51	0.46
5:A:105:VAL:HG12	5:A:106:CYS:N	2.30	0.46
1:O:1973:A:H5'	1:O:1973:A:C8	2.49	0.46
16:M:157:ASP:HB3	16:M:160:PHE:HD1	1.81	0.46
28:Y:165:GLU:HB3	39:Y:9394:HOH:O	2.16	0.46
1:O:468:U:H3'	39:O:7737:HOH:O	2.15	0.46
6:B:54:VAL:HB	39:B:9421:HOH:O	2.16	0.46
16:M:99:ARG:HE	16:M:170:ASN:HD22	1.64	0.45
1:O:1168:C:H5''	33:I:87:THR:HG23	1.97	0.45
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.45
23:T:48:VAL:CG2	23:T:98:VAL:HA	2.46	0.45
1:O:700:A:C2	15:L:71:GLU:HG2	2.51	0.45
1:O:2415:A:O2'	17:N:29:SER:HB3	2.17	0.45
1:O:1120:U:H6	1:O:1120:U:H5''	1.80	0.45
9:E:22:VAL:HG12	9:E:76:VAL:HG11	1.99	0.45
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.16	0.45
1:O:581:G:H5'	39:O:7847:HOH:O	2.16	0.45
1:O:2039:A:OP2	6:B:234:ARG:NH2	2.50	0.45
1:O:2684:A:H2'	1:O:2685:C:C6	2.51	0.45
1:O:1167:G:H2'	1:O:1168:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:559:U:H2'	1:0:560:C:O4'	2.16	0.45
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.46	0.45
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.45
6:B:80:ARG:HA	6:B:186:GLY:O	2.16	0.45
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.98	0.45
16:M:5:TYR:HE2	16:M:46:LEU:HD13	1.82	0.45
1:0:721:A:H5''	18:O:51:TYR:CE2	2.51	0.45
1:0:200:U:H2'	39:0:3737:HOH:O	2.16	0.45
1:0:2706:A:H2'	1:0:2707:C:O4'	2.16	0.45
7:C:25:PRO:HG2	39:C:9121:HOH:O	2.16	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.45
17:N:154:LEU:HD11	17:N:157:PRO:HA	1.99	0.45
6:B:141:ARG:HG2	6:B:165:ARG:CA	2.44	0.45
27:X:18:ARG:NH1	39:X:4132:HOH:O	2.48	0.45
24:U:52:THR:HG22	24:U:54:THR:HB	1.97	0.45
39:0:9866:HOH:O	26:W:119:HIS:HE1	1.99	0.45
1:0:2428:G:N7	32:3:60:LYS:NZ	2.62	0.45
1:0:2897:C:H2'	1:0:2898:G:C8	2.50	0.45
6:B:84:LEU:HD23	6:B:142:LEU:HD23	1.98	0.45
9:E:13:ALA:CB	9:E:22:VAL:HG22	2.46	0.45
1:0:2649:A:C8	1:0:2649:A:H5'	2.52	0.45
1:0:539:G:H2'	1:0:540:A:C8	2.51	0.45
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.98	0.45
8:D:84:LEU:HA	8:D:87:ALA:HB3	1.98	0.45
1:0:2478:U:O2'	1:0:2479:A:H5'	2.16	0.45
7:C:236:THR:O	7:C:237:GLU:C	2.55	0.45
1:0:2270:G:H4'	5:A:223:ARG:NH1	2.23	0.45
13:J:45:VAL:HG22	13:J:46:ILE:N	2.31	0.45
19:P:10:ALA:CA	19:P:13:VAL:HG12	2.43	0.45
5:A:53:ALA:HB3	39:A:9403:HOH:O	2.16	0.45
1:0:2036:C:C4'	14:K:44:LEU:HG	2.47	0.45
1:0:2451:G:O2'	32:3:38:ARG:NH2	2.48	0.45
6:B:25:ARG:HA	6:B:310:ARG:HH21	1.82	0.45
1:0:106:A:H2'	1:0:107:U:O4'	2.17	0.45
12:H:84:LYS:NZ	12:H:84:LYS:HB2	2.31	0.45
7:C:84:VAL:O	7:C:85:LYS:HB2	2.16	0.45
1:0:612:U:H2'	1:0:613:C:C6	2.51	0.45
39:0:6934:HOH:O	6:B:1:PRO:HD2	2.16	0.45
1:0:1119:G:H8	13:J:52:GLN:NE2	2.14	0.45
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.47	0.45
19:P:13:VAL:HG13	19:P:14:LEU:N	2.32	0.45
13:J:107:ASN:HD22	13:J:108:PRO:N	2.15	0.45
9:E:131:LEU:HD12	9:E:166:VAL:HG11	1.99	0.45
9:E:23:GLU:HG2	9:E:28:SER:CB	2.47	0.45
1:0:407:A:H8	39:0:4736:HOH:O	1.98	0.45
4:5:77:PHE:N	4:5:77:PHE:HD2	2.15	0.45
1:0:2067:A:H2'	1:0:2068:G:O4'	2.17	0.45
1:0:1805:G:O2'	1:0:1806:G:H5'	2.17	0.45
1:0:1044:C:H5''	39:0:9343:HOH:O	2.16	0.45
1:0:170:U:H2'	1:0:171:C:H5'	1.97	0.45
1:0:2403:C:H2'	1:0:2404:G:O5'	2.16	0.45
26:W:4:LEU:CD2	26:W:54:PHE:HB3	2.43	0.45
1:0:777:U:O2'	30:1:11:LYS:HG2	2.17	0.45
23:T:38:ARG:NH1	23:T:38:ARG:HG3	2.32	0.45
6:B:109:LEU:CG	6:B:113:LEU:HD12	2.46	0.45
17:N:67:ALA:C	17:N:69:TYR:N	2.70	0.45
15:L:121:ILE:HA	15:L:141:GLU:O	2.17	0.45
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.51	0.45
6:B:85:ARG:NH1	6:B:163:GLU:OE1	2.47	0.45
1:0:1919:A:H4'	39:0:5112:HOH:O	2.17	0.45
1:0:189:A:OP1	16:M:171:ARG:NH2	2.49	0.45
1:0:1209:C:H2'	1:0:1210:G:C8	2.47	0.45
1:0:558:C:H2'	1:0:559:U:C5'	2.44	0.45
6:B:88:GLU:HB3	6:B:97:LEU:HG	1.99	0.45
1:0:709:G:O2'	18:O:25:VAL:CG1	2.65	0.45
1:0:2724:U:H2'	1:0:2725:G:O4'	2.16	0.45
32:3:8:ASN:O	32:3:9:THR:HB	2.17	0.45
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	1.99	0.45
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.00	0.45
8:D:35:ALA:HB1	39:D:7502:HOH:O	2.17	0.45
5:A:194:MET:CE	5:A:199:HIS:HB2	2.47	0.45
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.99	0.45
12:H:28:ILE:HA	12:H:63:GLU:OE1	2.17	0.45
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.52	0.45
2:9:3049:G:C2'	2:9:3050:G:H5'	2.47	0.45
6:B:175:LEU:O	6:B:178:ALA:HB3	2.17	0.45
31:2:20:ARG:CG	31:2:21:VAL:H	2.30	0.45
1:0:1855:G:H4'	1:0:1856:C:O5'	2.16	0.45
1:0:1309:U:O2'	1:0:1310:U:H5'	2.16	0.45
1:0:2438:G:H2'	1:0:2439:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.61	0.45
16:M:99:ARG:HE	16:M:170:ASN:ND2	2.14	0.45
1:0:2812:A:C2	1:0:2814:A:N6	2.72	0.45
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.97	0.45
2:9:3050:G:H2'	2:9:3051:A:C8	2.52	0.45
23:T:73:HIS:CD2	23:T:88:PRO:CG	3.00	0.45
6:B:154:VAL:CG1	6:B:156:LYS:HG2	2.47	0.45
1:0:1845:A:O3'	5:A:187:PRO:HB2	2.17	0.45
1:0:2089:A:O2'	1:0:2090:G:H5'	2.17	0.45
1:0:709:G:O2'	18:O:25:VAL:HG12	2.16	0.45
18:O:50:ARG:HD2	18:O:51:TYR:CE1	2.52	0.45
1:0:2135:A:O2'	1:0:2136:G:H5'	2.17	0.45
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.45
1:0:1497:G:H4'	1:0:1627:G:O2'	2.17	0.45
1:0:886:A:OP2	1:0:2113:G:H5'	2.15	0.45
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.99	0.45
15:L:65:ASP:OD1	15:L:109:LEU:HB2	2.16	0.45
1:0:1815:A:H2'	1:0:1816:C:O4'	2.17	0.45
25:V:7:GLU:O	25:V:11:MET:HG3	2.17	0.45
13:J:77:GLY:O	13:J:78:ILE:C	2.56	0.45
39:0:4351:HOH:O	6:B:27:ASN:HB2	2.17	0.45
5:A:135:VAL:CG2	5:A:147:ARG:HG2	2.40	0.45
26:W:122:ARG:NH1	26:W:152:ALA:O	2.50	0.45
1:0:553:G:O4'	1:0:1325:G:H5'	2.17	0.45
2:9:3001:U:H4'	2:9:3003:A:OP1	2.17	0.45
17:N:183:ASP:O	17:N:184:ILE:O	2.35	0.45
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.47	0.45
1:0:1878:G:O2'	1:0:1879:U:P	2.74	0.45
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.52	0.45
1:0:128:A:O2'	1:0:129:A:H5'	2.17	0.45
6:B:226:LYS:NZ	39:B:9327:HOH:O	2.42	0.45
5:A:123:GLY:HA2	5:A:159:VAL:O	2.16	0.45
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.45
1:0:2274:A:O2'	1:0:2275:G:H5'	2.16	0.45
7:C:140:VAL:HG12	7:C:141:SER:N	2.32	0.44
33:I:132:CYS:C	33:I:134:SER:N	2.70	0.44
1:0:2272:G:H5'	5:A:223:ARG:HB2	1.99	0.44
17:N:143:ARG:NH1	17:N:173:ASP:OD2	2.51	0.44
1:0:1165:G:O3'	1:0:1174:A:H4'	2.17	0.44
1:0:271:C:H41	1:0:378:A:H2	1.64	0.44
6:B:41:PHE:CE1	6:B:79:MET:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1631:A:H2'	1:0:1632:A:C8	2.52	0.44
32:3:74:CYS:N	39:3:9362:HOH:O	2.49	0.44
1:0:704:C:H2'	1:0:705:C:H6	1.82	0.44
5:A:134:ASN:O	5:A:150:PRO:HD3	2.17	0.44
1:0:2252:A:C5	1:0:2253:G:H1'	2.53	0.44
4:5:77:PHE:CD2	4:5:77:PHE:N	2.84	0.44
1:0:2344:G:N3	1:0:2344:G:H2'	2.33	0.44
1:0:941:G:C5	1:0:942:U:C4	3.05	0.44
1:0:1687:C:O2	30:1:9:GLY:HA2	2.17	0.44
1:0:154:C:H2'	1:0:155:C:H6	1.82	0.44
1:0:1067:A:H5'	39:0:4628:HOH:O	2.17	0.44
9:E:83:GLY:O	9:E:169:THR:N	2.43	0.44
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.17	0.44
22:S:57:THR:CG2	22:S:58:MET:N	2.80	0.44
1:0:282:C:H2'	1:0:283:U:O4'	2.17	0.44
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.98	0.44
9:E:102:VAL:HG13	9:E:116:THR:HG23	1.98	0.44
1:0:1625:U:H3'	1:0:1625:U:H6	1.82	0.44
7:C:8:LEU:HD11	7:C:143:ASP:O	2.17	0.44
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.16	0.44
1:0:2365:G:H4'	20:Q:45:PRO:O	2.18	0.44
27:X:74:ALA:CB	27:X:85:VAL:HG22	2.47	0.44
1:0:1116:U:O2'	1:0:1118:A:C2	2.56	0.44
26:W:65:VAL:HG12	26:W:116:LEU:HD13	1.98	0.44
15:L:143:THR:CG2	15:L:144:ASP:N	2.79	0.44
1:0:2578:G:H5'	1:0:2578:G:C8	2.48	0.44
21:R:61:GLN:CD	39:R:9339:HOH:O	2.55	0.44
1:0:2524:G:N2	1:0:2526:C:H5	2.14	0.44
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.86	0.44
1:0:1226:G:H5'	39:0:4805:HOH:O	2.18	0.44
39:0:3450:HOH:O	9:E:57:LYS:HE2	2.17	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.17	0.44
1:0:2486:A:H2	4:5:78:ACA:O1	2.01	0.44
1:0:1415:G:H5'	30:1:12:ASN:O	2.17	0.44
12:H:26:SER:HA	12:H:59:HIS:CD2	2.53	0.44
9:E:80:TRP:O	9:E:134:SER:HA	2.18	0.44
16:M:61:ILE:N	16:M:61:ILE:HD12	2.32	0.44
1:0:1130:U:H5'	39:0:7837:HOH:O	2.18	0.44
12:H:154:TYR:C	12:H:154:TYR:CD1	2.91	0.44
6:B:75:GLU:C	6:B:77:PRO:HD3	2.38	0.44
1:0:1311:G:C2	1:0:1312:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:29:ASP:OD1	22:S:31:ARG:HG3	2.17	0.44
1:0:24:G:N2	1:0:518:G:H1'	2.32	0.44
13:J:135:ILE:O	13:J:139:LEU:HG	2.18	0.44
1:0:2473:U:O3'	1:0:2474:A:H3'	2.18	0.44
1:0:1180:U:H4'	33:I:91:GLU:HG2	2.00	0.44
6:B:304:PRO:HD2	6:B:307:ARG:NH1	2.33	0.44
6:B:87:TYR:HE2	6:B:96:PRO:HG3	1.82	0.44
1:0:2904:U:H4'	27:X:8:ARG:HH12	1.81	0.44
1:0:1747:A:C8	14:K:44:LEU:HD13	2.53	0.44
1:0:2629:C:H41	5:A:206:ARG:HH21	1.64	0.44
6:B:16:ARG:NH1	39:B:9425:HOH:O	2.51	0.44
1:0:926:A:O2'	15:L:41:HIS:HD2	2.00	0.44
1:0:2589:U:H2'	1:0:2590:U:C6	2.52	0.44
1:0:1422:U:H4'	39:0:7914:HOH:O	2.16	0.44
1:0:517:U:H1'	39:0:7746:HOH:O	2.17	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.44
22:S:22:ASN:ND2	22:S:68:LEU:HB2	2.33	0.44
3:4:75:C:H2'	3:4:76:5AA:O4'	2.18	0.44
1:0:558:C:C2'	1:0:559:U:C5'	2.95	0.44
16:M:61:ILE:HG22	16:M:62:VAL:N	2.31	0.44
32:3:73:GLU:HB3	39:3:9362:HOH:O	2.17	0.44
29:Z:19:GLY:O	29:Z:23:ARG:HG2	2.17	0.44
6:B:148:PRO:HD2	39:B:9385:HOH:O	2.18	0.44
23:T:40:VAL:HG22	23:T:41:ARG:N	2.33	0.44
1:0:263:U:C4	10:F:54:VAL:HG13	2.53	0.44
1:0:2664:A:OP1	1:0:2664:A:H8	2.01	0.44
1:0:1785:G:OP1	19:P:76:GLY:HA3	2.18	0.44
1:0:2638:G:H1'	39:0:4852:HOH:O	2.18	0.44
1:0:2591:C:H2'	1:0:2592:G:O4'	2.18	0.44
1:0:1173:A:H4'	1:0:1174:A:C8	2.53	0.44
13:J:131:THR:HB	13:J:134:GLU:CG	2.45	0.44
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.26	0.44
1:0:2728:C:H2'	1:0:2729:C:C6	2.52	0.44
28:Y:108:ASP:N	28:Y:108:ASP:OD1	2.51	0.44
18:O:44:ASN:CG	18:O:67:SER:HB2	2.38	0.44
9:E:1:PRO:HG2	9:E:59:MET:SD	2.58	0.44
1:0:2831:C:H2'	1:0:2832:C:H5'	1.98	0.44
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.44
1:0:1375:A:C2'	1:0:1376:G:H5'	2.47	0.44
25:V:12:THR:HB	25:V:15:GLU:OE2	2.18	0.44
28:Y:189:ASN:CA	28:Y:217:ILE:HD11	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:74:VAL:HG21	14:K:96:VAL:HG23	1.99	0.44
17:N:15:GLU:HB3	17:N:17:ARG:CG	2.46	0.44
1:0:657:G:H2'	1:0:658:C:H6	1.82	0.44
27:X:76:ARG:O	27:X:77:PHE:HB3	2.18	0.44
1:0:364:C:H2'	1:0:365:G:C8	2.53	0.44
32:3:69:TYR:CZ	32:3:80:ARG:HD2	2.53	0.44
8:D:18:ILE:HD13	8:D:84:LEU:CD1	2.48	0.44
1:0:105:G:O2'	1:0:106:A:H5'	2.18	0.44
2:9:3059:C:O5'	2:9:3059:C:H6	2.00	0.44
1:0:2786:G:H2'	39:0:7365:HOH:O	2.17	0.44
1:0:1482:A:O2'	1:0:1483:C:H5'	2.18	0.44
21:R:17:MET:HE3	21:R:19:ARG:HH21	1.83	0.44
18:O:113:VAL:O	18:O:114:ILE:HD13	2.18	0.44
2:9:3072:C:O2'	2:9:3073:G:H5'	2.18	0.44
22:S:51:GLN:HB3	22:S:67:ARG:NH1	2.33	0.44
24:U:23:HIS:HB2	24:U:27:ALA:HB3	2.00	0.44
12:H:50:ILE:HG23	12:H:131:GLU:O	2.18	0.44
1:0:1943:C:H4'	5:A:211:LYS:O	2.18	0.44
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.38	0.44
1:0:1641:A:H2'	1:0:1642:A:C5'	2.42	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.44
33:I:112:LYS:C	33:I:114:PRO:HD2	2.38	0.44
13:J:107:ASN:HD22	13:J:107:ASN:C	2.20	0.44
6:B:84:LEU:HD23	6:B:178:ALA:HB1	1.98	0.44
1:0:598:C:H2'	1:0:599:G:C8	2.53	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.53	0.44
5:A:114:ASP:C	5:A:114:ASP:OD1	2.56	0.44
16:M:147:LEU:O	16:M:150:ILE:HG22	2.18	0.44
10:F:28:ALA:CB	10:F:99:THR:HG23	2.47	0.44
16:M:184:ARG:HG3	16:M:185:PRO:HA	2.00	0.44
22:S:52:VAL:C	22:S:53:ASN:HD22	2.21	0.44
6:B:274:GLU:HA	6:B:292:GLY:O	2.18	0.44
1:0:2717:C:H2'	1:0:2718:C:C5'	2.32	0.43
1:0:1589:G:H22	1:0:1605:G:H1'	1.83	0.43
1:0:2419:U:H5''	1:0:2420:G:H5'	2.00	0.43
1:0:1741:U:H3'	39:0:3068:HOH:O	2.18	0.43
1:0:790:A:H1'	1:0:1710:A:O2'	2.18	0.43
18:O:77:ALA:HB1	18:O:98:LEU:HD12	2.00	0.43
6:B:232:TRP:HD1	6:B:235:ARG:HD2	1.83	0.43
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.38	0.43
7:C:136:VAL:HA	7:C:137:PRO:C	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1069:C:H2'	1:0:1070:A:O4'	2.18	0.43
18:O:24:ALA:O	18:O:28:ASP:HB2	2.18	0.43
8:D:66:GLY:O	8:D:67:ASP:HB3	2.18	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
7:C:162:VAL:CG2	7:C:232:LEU:HD21	2.48	0.43
7:C:174:ILE:HG12	7:C:186:TYR:CE2	2.53	0.43
1:0:664:U:O4	1:0:681:G:H5''	2.18	0.43
12:H:20:ILE:HG23	12:H:120:ILE:HD11	2.00	0.43
7:C:7:ASP:O	7:C:9:ASP:N	2.51	0.43
39:O:3249:HOH:O	27:X:23:HIS:HD2	2.00	0.43
7:C:132:ASP:O	7:C:133:ARG:HB2	2.18	0.43
12:H:170:ASN:ND2	12:H:170:ASN:N	2.64	0.43
7:C:118:THR:O	7:C:136:VAL:HG13	2.17	0.43
8:D:169:THR:O	8:D:169:THR:HG22	2.18	0.43
1:0:2601:A:N1	14:K:38:SER:HB2	2.33	0.43
1:0:745:G:H5''	1:0:746:A:OP1	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.53	0.43
12:H:54:THR:HA	12:H:127:VAL:O	2.18	0.43
6:B:51:VAL:HG13	6:B:53:LEU:CD1	2.48	0.43
6:B:41:PHE:CB	6:B:190:MET:HE3	2.48	0.43
30:1:28:HIS:CD2	30:1:30:LYS:HB2	2.54	0.43
19:P:59:ARG:HH22	19:P:66:GLN:NE2	2.17	0.43
24:U:6:CYS:HB2	24:U:32:CYS:HB3	2.00	0.43
1:0:2281:C:H2'	1:0:2282:U:H5'	2.01	0.43
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.99	0.43
18:O:7:LEU:HD22	39:O:5650:HOH:O	2.18	0.43
1:0:2362:A:H2'	1:0:2363:G:C8	2.53	0.43
2:9:3094:G:O2'	2:9:3095:C:H5'	2.18	0.43
1:0:451:C:O2'	1:0:452:G:H5'	2.18	0.43
12:H:9:ILE:HG12	12:H:56:GLN:HG3	2.00	0.43
6:B:7:ARG:HD3	6:B:9:GLY:O	2.17	0.43
1:0:2716:G:C5'	6:B:206:THR:HG21	2.43	0.43
5:A:132:ASP:HB3	5:A:135:VAL:O	2.18	0.43
9:E:81:GLU:HG2	9:E:134:SER:CB	2.45	0.43
1:0:1746:A:O4'	1:0:1747:A:C2	2.71	0.43
1:0:1203:G:O2'	1:0:1204:C:H5'	2.18	0.43
19:P:141:ILE:O	19:P:143:ALA:N	2.41	0.43
14:K:82:ARG:NH2	14:K:115:ARG:HG2	2.33	0.43
1:0:1483:C:O2'	1:0:1484:G:H5'	2.18	0.43
10:F:79:GLN:HB2	39:F:5498:HOH:O	2.18	0.43
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
5:A:48:ASP:HB3	39:A:9403:HOH:O	2.19	0.43
1:0:677:C:H4'	7:C:246:ARG:NH2	2.33	0.43
8:D:51:ARG:HA	39:D:7636:HOH:O	2.18	0.43
6:B:90:THR:C	6:B:92:TYR:H	2.21	0.43
1:0:1761:U:H5'	19:P:81:LYS:O	2.19	0.43
1:0:1434:A:H2'	1:0:1436:C:C5	2.53	0.43
1:0:1433:G:O2'	1:0:1434:A:H5'	2.19	0.43
5:A:96:LEU:HD22	5:A:128:LEU:HD13	2.00	0.43
26:W:90:TYR:N	26:W:90:TYR:CD1	2.86	0.43
8:D:142:ALA:HA	8:D:149:ARG:O	2.19	0.43
5:A:88:ILE:HD13	5:A:100:PRO:CD	2.46	0.43
14:K:87:ARG:NH1	39:K:4066:HOH:O	2.51	0.43
7:C:129:HIS:CE1	7:C:232:LEU:H	2.37	0.43
11:G:71:LEU:C	11:G:73:ASP:N	2.70	0.43
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.43
18:O:1:SER:HA	39:O:7521:HOH:O	2.18	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.18	0.43
1:0:1498:G:O2'	1:0:1499:U:H5'	2.18	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.19	0.43
6:B:223:ARG:O	6:B:228:ALA:HB2	2.18	0.43
14:K:12:LEU:CD1	14:K:18:ILE:HG21	2.48	0.43
1:0:1825:U:O2'	1:0:1826:C:H5'	2.18	0.43
17:N:49:THR:HG23	17:N:56:ASP:HB2	1.99	0.43
1:0:466:A:H2'	1:0:467:G:O4'	2.18	0.43
15:L:93:VAL:HG21	15:L:122:ALA:HB2	2.01	0.43
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.43
1:0:2717:C:OP1	6:B:207:LYS:HG3	2.19	0.43
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.34	0.43
26:W:63:GLU:HG2	26:W:93:ILE:HG22	2.00	0.43
1:0:2909:G:H2'	1:0:2910:A:C8	2.52	0.43
6:B:51:VAL:HG22	6:B:53:LEU:CD1	2.49	0.43
1:0:2851:G:C2'	1:0:2852:A:H5'	2.49	0.43
1:0:1634:G:H2'	1:0:1635:U:H6	1.82	0.43
1:0:820:G:O2'	1:0:856:G:H4'	2.18	0.43
1:0:1202:A:C2'	1:0:1203:G:H5'	2.48	0.43
2:9:3047:A:C2	2:9:3048:C:C2	3.07	0.43
9:E:13:ALA:HB1	9:E:22:VAL:HG22	2.01	0.43
15:L:73:VAL:HG23	15:L:74:THR:N	2.34	0.43
1:0:625:U:H5''	1:0:1044:C:N4	2.33	0.43
1:0:2361:A:H8	1:0:2361:A:H5'	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:0:9430:HOH:O	7:C:103:ASN:HB3	2.17	0.43
1:0:1021:G:O2'	1:0:1022:A:H5'	2.18	0.43
1:0:949:U:H4'	20:Q:95:GLU:HA	2.00	0.43
8:D:75:LEU:HD22	8:D:79:MET:HB3	2.00	0.43
15:L:128:GLY:O	15:L:132:LYS:HG3	2.18	0.43
11:G:63:ARG:N	39:G:2569:HOH:O	2.52	0.43
30:1:25:LYS:HD2	31:2:49:GLU:N	2.34	0.43
1:0:1293:U:H5'	28:Y:154:ARG:HH21	1.83	0.43
19:P:16:VAL:HG22	19:P:20:ARG:CZ	2.48	0.43
28:Y:106:THR:HG22	28:Y:107:PRO:O	2.19	0.43
1:0:821:U:H2'	1:0:822:C:C6	2.54	0.43
1:0:820:G:C6	5:A:171:LYS:HB2	2.54	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:2346:C:O2'	8:D:52:THR:HG21	2.18	0.43
32:3:69:TYR:CE1	32:3:80:ARG:HD2	2.54	0.43
25:V:42:ASN:HB3	39:V:7247:HOH:O	2.18	0.43
1:0:2329:C:O2'	1:0:2330:U:H5'	2.19	0.43
1:0:1508:C:H5'	22:S:21:GLN:NE2	2.34	0.43
32:3:57:GLY:HA2	39:3:9325:HOH:O	2.18	0.43
1:0:2379:G:N7	1:0:2408:A:N1	2.66	0.43
7:C:49:ASP:HB3	7:C:52:ALA:HB2	2.01	0.43
5:A:36:ASP:CG	5:A:85:SER:HB2	2.38	0.43
10:F:58:GLU:HG3	10:F:61:MET:CE	2.48	0.43
6:B:51:VAL:HG23	6:B:329:TYR:O	2.18	0.43
1:0:378:A:OP1	16:M:9:ARG:NH2	2.39	0.43
1:0:1095:U:O2	26:W:120:PRO:HG2	2.18	0.43
1:0:474:C:O2'	7:C:73:LEU:HD21	2.19	0.43
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.53	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.43
27:X:75:ALA:O	27:X:83:ALA:HA	2.19	0.43
26:W:84:VAL:HG21	26:W:93:ILE:HG12	2.01	0.43
1:0:2781:U:H2'	1:0:2782:G:H5'	2.00	0.43
26:W:38:THR:CG2	26:W:39:ASP:N	2.80	0.43
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.48	0.43
1:0:284:C:H4'	1:0:285:A:O5'	2.19	0.43
32:3:70:ARG:HB3	39:3:9371:HOH:O	2.19	0.43
10:F:111:ILE:O	10:F:115:VAL:HG23	2.18	0.43
1:0:2271:G:H2'	1:0:2271:G:N3	2.33	0.43
30:1:45:ARG:HB3	39:1:988:HOH:O	2.19	0.43
1:0:2488:A:H2	39:0:7453:HOH:O	2.01	0.43
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:65:VAL:HG21	16:M:105:ALA:HB2	2.01	0.43
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.82	0.42
26:W:122:ARG:HH11	26:W:122:ARG:CG	2.27	0.42
10:F:91:VAL:CG1	10:F:92:GLY:H	2.32	0.42
5:A:81:GLN:HG3	5:A:92:ASN:HD21	1.84	0.42
21:R:114:VAL:HG13	21:R:114:VAL:O	2.18	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.34	0.42
1:0:2637:A:H4'	1:0:2638:G:C5'	2.49	0.42
23:T:75:GLU:O	23:T:76:ASP:HB2	2.19	0.42
1:0:488:U:O2'	23:T:82:THR:HG21	2.19	0.42
1:0:587:A:H5''	39:0:7462:HOH:O	2.19	0.42
19:P:55:LYS:CG	19:P:56:GLY:N	2.81	0.42
15:L:21:ARG:N	39:L:9331:HOH:O	2.51	0.42
1:0:2092:G:H2'	1:0:2613:G:OP1	2.19	0.42
39:0:4323:HOH:O	7:C:149:LYS:HE3	2.18	0.42
39:K:1387:HOH:O	24:U:20:MET:HE3	2.18	0.42
8:D:11:HIS:CG	8:D:12:GLU:N	2.87	0.42
1:0:290:C:O2'	1:0:291:C:H5'	2.18	0.42
39:0:3941:HOH:O	18:O:3:THR:HG21	2.18	0.42
17:N:42:HIS:HA	17:N:75:THR:O	2.19	0.42
1:0:2698:G:H2'	1:0:2699:A:O4'	2.19	0.42
12:H:31:HIS:HD2	12:H:87:LEU:O	2.02	0.42
15:L:149:ARG:O	15:L:150:GLN:HB2	2.19	0.42
6:B:153:SER:HB2	6:B:287:TYR:CZ	2.54	0.42
8:D:23:VAL:HG11	8:D:83:PHE:CZ	2.54	0.42
26:W:21:LEU:HD13	26:W:26:ILE:HD11	2.01	0.42
27:X:44:ASP:HB3	27:X:46:ASP:OD1	2.20	0.42
6:B:74:ILE:HG13	39:B:9413:HOH:O	2.19	0.42
5:A:48:ASP:HA	5:A:49:PRO:HD3	1.82	0.42
9:E:9:GLU:CG	9:E:10:ASP:N	2.82	0.42
2:9:3034:A:O5'	2:9:3034:A:H8	2.02	0.42
6:B:310:ARG:HD2	39:B:9457:HOH:O	2.17	0.42
8:D:173:GLU:HG3	8:D:174:VAL:N	2.34	0.42
6:B:175:LEU:C	6:B:175:LEU:CD2	2.87	0.42
1:0:1517:U:C2	1:0:1670:G:N2	2.87	0.42
15:L:24:ALA:HB2	15:L:30:ARG:HD2	2.02	0.42
1:0:154:C:H2'	1:0:155:C:C6	2.54	0.42
1:0:2607:U:H4'	39:0:9750:HOH:O	2.18	0.42
1:0:324:G:O2'	1:0:325:U:H5'	2.19	0.42
6:B:270:ILE:O	6:B:271:ASP:HB2	2.19	0.42
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:39:THR:CB	21:R:42:GLU:HG3	2.49	0.42
6:B:265:LEU:HD21	6:B:316:ARG:HD3	2.01	0.42
9:E:7:ILE:HD11	9:E:11:VAL:C	2.40	0.42
13:J:39:VAL:HG11	13:J:107:ASN:HB2	2.01	0.42
1:O:338:C:H4'	7:C:174:ILE:HD12	1.99	0.42
22:S:39:ASP:HB3	22:S:43:GLU:OE2	2.19	0.42
1:O:2846:C:H4'	6:B:156:LYS:HB3	2.01	0.42
6:B:24:PRO:HG3	6:B:204:GLY:HA2	2.01	0.42
6:B:280:VAL:HG13	6:B:333:GLU:O	2.18	0.42
1:O:2821:C:O2'	6:B:114:ASP:O	2.37	0.42
1:O:2821:C:H4'	6:B:116:PRO:CB	2.50	0.42
1:O:2724:U:H6	1:O:2724:U:O5'	2.03	0.42
1:O:1311:G:O6	7:C:173:LYS:HE3	2.19	0.42
15:L:10:SER:O	15:L:11:ARG:HB3	2.19	0.42
1:O:653:C:H2'	1:O:654:A:C8	2.53	0.42
1:O:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.42
24:U:33:SER:O	24:U:37:GLU:HG3	2.18	0.42
24:U:37:GLU:O	24:U:40:ALA:HB3	2.20	0.42
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.55	0.42
5:A:36:ASP:C	5:A:38:ILE:N	2.72	0.42
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	2.01	0.42
20:Q:18:PRO:O	20:Q:21:ARG:HB2	2.20	0.42
18:O:105:ASN:HD21	18:O:109:SER:N	2.08	0.42
6:B:139:ASP:HB2	6:B:165:ARG:NE	2.31	0.42
12:H:29:ALA:HB3	12:H:66:ARG:NH1	2.26	0.42
6:B:305:ASP:O	6:B:306:LYS:CB	2.65	0.42
1:O:474:C:O3'	7:C:73:LEU:HD21	2.18	0.42
9:E:24:GLY:CA	9:E:76:VAL:HB	2.50	0.42
15:L:104:ASP:HB3	39:L:9370:HOH:O	2.20	0.42
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.89	0.42
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.35	0.42
1:O:2564:G:OP2	1:O:2565:C:H5''	2.19	0.42
14:K:120:ARG:HB3	14:K:121:PHE:CE1	2.55	0.42
1:O:949:U:O2'	20:Q:40:HIS:HE1	2.01	0.42
12:H:77:LEU:O	12:H:81:GLY:HA3	2.20	0.42
2:9:3031:C:H2'	2:9:3032:G:O4'	2.18	0.42
23:T:80:GLU:HG2	39:T:2885:HOH:O	2.20	0.42
1:O:806:A:H2'	1:O:807:A:O4'	2.20	0.42
1:O:2842:G:H2'	1:O:2843:A:H5'	2.01	0.42
26:W:5:VAL:HG11	26:W:153:MET:CE	2.50	0.42
17:N:79:PRO:O	17:N:83:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1543:G:N1	1:0:1641:A:OP2	2.39	0.42
5:A:192:VAL:CG1	5:A:192:VAL:O	2.66	0.42
1:0:396:U:H1'	39:0:7795:HOH:O	2.19	0.42
1:0:2690:U:H4'	9:E:111:LYS:NZ	2.34	0.42
1:0:820:G:H5'	1:0:821:U:H5'	2.01	0.42
1:0:1130:U:H4'	39:0:6345:HOH:O	2.18	0.42
5:A:164:ARG:NE	39:A:9385:HOH:O	2.51	0.42
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.42
1:0:514:G:H2'	1:0:514:G:OP1	2.20	0.42
14:K:90:PHE:N	14:K:90:PHE:CD1	2.88	0.42
1:0:1006:A:N1	1:0:2311:A:H1'	2.35	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42
12:H:97:GLU:HB3	12:H:121:VAL:HG11	2.00	0.42
1:0:2433:A:H2'	1:0:2434:A:C8	2.54	0.42
1:0:1568:G:O2'	1:0:1569:U:H5'	2.19	0.42
9:E:118:ILE:CG2	9:E:122:THR:HB	2.50	0.42
15:L:64:ILE:HG13	15:L:68:GLU:OE1	2.19	0.42
21:R:69:LYS:HE2	21:R:78:GLY:O	2.19	0.42
17:N:108:SER:HA	17:N:109:PRO:HD3	1.79	0.42
1:0:1943:C:O4'	5:A:212:PRO:HA	2.19	0.42
1:0:797:A:H2'	1:0:798:G:O4'	2.19	0.42
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.48	0.42
21:R:113:HIS:O	21:R:145:LEU:HD12	2.19	0.42
8:D:170:TYR:CD1	8:D:170:TYR:N	2.88	0.42
26:W:108:ARG:HE	26:W:114:PRO:HG2	1.85	0.42
1:0:2091:G:O3'	6:B:235:ARG:HD3	2.20	0.42
1:0:2764:C:H2'	1:0:2765:C:H6	1.84	0.42
1:0:589:U:H2'	1:0:590:A:C8	2.54	0.42
7:C:85:LYS:HA	7:C:85:LYS:HD2	1.90	0.42
15:L:10:SER:O	15:L:12:THR:N	2.50	0.42
1:0:2326:U:H4'	1:0:2412:G:H4'	2.02	0.42
7:C:107:ARG:NE	39:C:9256:HOH:O	2.46	0.42
1:0:772:G:H2'	1:0:773:A:O4'	2.19	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.20	0.42
33:I:91:GLU:O	33:I:94:GLU:HB2	2.20	0.42
12:H:3:ALA:HA	12:H:58:ARG:HH12	1.84	0.42
7:C:16:VAL:CG1	7:C:17:ASP:N	2.82	0.42
8:D:159:PRO:O	8:D:162:ALA:HB3	2.20	0.42
14:K:99:ASP:OD1	14:K:101:ASN:N	2.50	0.42
1:0:2419:U:H5''	1:0:2420:G:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:84:MET:HE3	9:E:131:LEU:HD13	2.02	0.42
27:X:12:ILE:CD1	27:X:36:HIS:ND1	2.83	0.42
16:M:80:GLY:O	16:M:81:ARG:HD3	2.19	0.42
27:X:10:VAL:CG1	27:X:11:THR:N	2.82	0.42
18:O:44:ASN:OD1	18:O:65:LEU:HB2	2.20	0.42
9:E:16:ASP:O	9:E:17:HIS:HB2	2.20	0.42
1:0:424:C:H2'	1:0:425:U:C6	2.55	0.42
9:E:92:PRO:HB2	39:E:4917:HOH:O	2.19	0.42
1:0:737:A:H2'	1:0:738:G:O4'	2.20	0.42
1:0:1373:G:H4'	39:0:5530:HOH:O	2.20	0.42
7:C:187:ARG:NH2	39:C:9163:HOH:O	2.52	0.42
1:0:870:G:C3'	1:0:871:G:H5''	2.49	0.42
31:2:40:ARG:HG3	31:2:45:ASN:CB	2.49	0.42
26:W:4:LEU:HA	26:W:4:LEU:HD23	1.83	0.42
2:9:3092:G:C6	2:9:3093:A:C6	3.08	0.42
19:P:37:ARG:O	19:P:41:ARG:HG3	2.20	0.42
6:B:190:MET:CE	6:B:194:PHE:CD1	3.03	0.42
1:0:1213:C:C2'	1:0:1214:G:H5'	2.50	0.42
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.01	0.42
1:0:795:G:N3	1:0:817:G:C2	2.88	0.42
26:W:125:HIS:CD2	26:W:127:GLY:H	2.38	0.42
31:2:25:VAL:O	31:2:29:THR:HG23	2.20	0.42
1:0:2894:C:H2'	1:0:2895:C:H6	1.84	0.42
5:A:217:ARG:CG	5:A:217:ARG:HH11	2.32	0.42
1:0:68:U:O2'	1:0:69:A:H5''	2.20	0.42
1:0:2274:A:H1'	16:M:86:GLN:NE2	2.35	0.42
1:0:2379:G:H5'	1:0:2381:C:O4'	2.20	0.42
1:0:571:C:H6	1:0:571:C:O5'	2.03	0.42
5:A:87:GLU:HB3	39:A:9419:HOH:O	2.19	0.42
1:0:392:U:O2'	16:M:182:LYS:HE2	2.20	0.42
1:0:1515:A:H2'	1:0:1516:C:C6	2.55	0.42
1:0:522:U:O2'	1:0:1366:C:H5'	2.19	0.42
1:0:1196:C:H2'	1:0:1197:G:O4'	2.20	0.42
33:I:131:THR:O	33:I:131:THR:HG22	2.20	0.42
1:0:1244:U:H2'	13:J:47:THR:HG21	2.02	0.42
17:N:73:ALA:HB2	17:N:163:PHE:CE2	2.55	0.42
26:W:35:VAL:HA	26:W:36:PRO:HD3	1.84	0.42
5:A:105:VAL:CG1	5:A:106:CYS:N	2.83	0.42
39:0:6882:HOH:O	23:T:38:ARG:NH1	2.52	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.42
14:K:22:ASP:C	14:K:22:ASP:OD1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2831:C:C2'	1:0:2832:C:H5'	2.50	0.42
1:0:1391:G:H2'	1:0:1392:A:H5'	2.02	0.42
5:A:70:ALA:HA	5:A:71:PRO:HD3	1.82	0.42
1:0:1470:A:OP1	16:M:93:ARG:HD2	2.19	0.42
1:0:1051:C:H2'	1:0:1052:G:O4'	2.20	0.42
1:0:1790:C:H2'	1:0:1791:U:C6	2.54	0.42
1:0:794:U:H3	1:0:819:A:H61	1.67	0.42
21:R:59:PHE:O	21:R:63:ASN:HB3	2.20	0.42
1:0:533:U:H3'	39:0:4041:HOH:O	2.20	0.42
10:F:13:GLU:OE2	10:F:78:GLU:HG2	2.20	0.42
23:T:50:VAL:HG12	23:T:56:ALA:HA	2.02	0.42
28:Y:212:ARG:HD2	39:Y:9400:HOH:O	2.20	0.42
6:B:132:HIS:NE2	6:B:171:VAL:CG2	2.82	0.41
31:2:41:HIS:HD2	31:2:44:ARG:H	1.68	0.41
14:K:55:VAL:CG1	14:K:56:SER:N	2.83	0.41
1:0:1702:U:H5'	39:0:3719:HOH:O	2.19	0.41
13:J:39:VAL:HG12	13:J:40:ASN:ND2	2.35	0.41
21:R:29:LYS:NZ	39:R:9339:HOH:O	2.53	0.41
2:9:3114:G:H2'	2:9:3115:C:C6	2.55	0.41
6:B:149:ASP:HB2	39:B:9385:HOH:O	2.19	0.41
9:E:114:ARG:HB3	9:E:151:LEU:HD11	2.02	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.58	0.41
13:J:42:GLU:HG2	13:J:43:ARG:HG3	2.02	0.41
27:X:36:HIS:CE1	27:X:40:HIS:CD2	3.08	0.41
1:0:332:G:O2'	1:0:333:G:H5'	2.20	0.41
17:N:72:GLU:HG2	17:N:72:GLU:O	2.20	0.41
1:0:1790:C:H2'	1:0:1791:U:H6	1.84	0.41
1:0:834:G:H3'	1:0:835:U:H4'	2.02	0.41
1:0:2824:C:H5''	1:0:2825:C:H5'	2.02	0.41
1:0:1355:A:H2'	39:0:4409:HOH:O	2.19	0.41
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.41
7:C:236:THR:HG21	39:C:9174:HOH:O	2.19	0.41
1:0:2509:A:H2'	1:0:2510:C:O4'	2.20	0.41
17:N:152:GLU:C	17:N:154:LEU:N	2.72	0.41
27:X:43:VAL:CG1	27:X:44:ASP:H	2.31	0.41
24:U:6:CYS:O	24:U:8:TYR:N	2.54	0.41
26:W:73:LEU:HD22	26:W:111:GLY:HA2	2.02	0.41
1:0:1579:C:H4'	1:0:1580:A:OP1	2.20	0.41
1:0:2032:U:H2'	1:0:2033:G:C5'	2.50	0.41
31:2:39:ARG:HG2	39:2:3143:HOH:O	2.20	0.41
18:O:112:ARG:HA	39:O:1484:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1873:G:H3'	39:0:5457:HOH:O	2.20	0.41
28:Y:197:ASP:OD1	28:Y:199:ASP:N	2.48	0.41
28:Y:187:VAL:HG13	28:Y:187:VAL:O	2.20	0.41
1:0:1180:U:H2'	1:0:1181:A:O4'	2.20	0.41
26:W:60:GLU:O	26:W:63:GLU:HB2	2.20	0.41
7:C:76:ARG:HG2	7:C:78:ARG:HH12	1.85	0.41
1:0:1205:U:C2'	1:0:1206:U:C5'	2.97	0.41
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.02	0.41
1:0:1592:G:O2'	1:0:1593:C:O5'	2.38	0.41
24:U:39:ASN:HB3	39:U:3805:HOH:O	2.20	0.41
14:K:125:ALA:O	14:K:127:ALA:N	2.52	0.41
15:L:53:ARG:O	15:L:58:GLN:NE2	2.51	0.41
1:0:2831:C:H2'	1:0:2832:C:C5'	2.50	0.41
1:0:1217:G:H2'	1:0:1218:U:C6	2.55	0.41
1:0:1771:U:O2'	1:0:1773:G:N7	2.50	0.41
16:M:123:ASP:OD1	16:M:126:GLN:HG2	2.20	0.41
5:A:213:LYS:NZ	39:A:9358:HOH:O	2.51	0.41
6:B:14:GLY:HA2	6:B:15:PRO:C	2.40	0.41
7:C:37:ALA:O	7:C:41:ASN:ND2	2.53	0.41
5:A:215:ILE:HG13	5:A:216:SER:N	2.35	0.41
25:V:11:MET:HB3	25:V:15:GLU:HB2	2.02	0.41
8:D:23:VAL:HG21	8:D:45:THR:CG2	2.49	0.41
8:D:64:ARG:HD3	8:D:67:ASP:HB3	2.01	0.41
17:N:15:GLU:CB	17:N:17:ARG:HG3	2.48	0.41
9:E:11:VAL:HG12	9:E:12:ASP:H	1.81	0.41
27:X:25:ARG:NH1	39:X:3861:HOH:O	2.53	0.41
6:B:55:ASN:HB3	6:B:63:GLU:CA	2.49	0.41
1:0:2421:G:H3'	1:0:2422:U:C5'	2.50	0.41
13:J:70:PHE:CD2	13:J:70:PHE:O	2.73	0.41
1:0:1234:U:C4	6:B:244:PRO:HB3	2.55	0.41
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.82	0.41
1:0:622:G:P	28:Y:148:GLY:HA3	2.60	0.41
1:0:2361:A:H2'	1:0:2362:A:C8	2.54	0.41
1:0:2699:A:H2'	1:0:2700:G:O4'	2.20	0.41
27:X:32:LEU:HD23	27:X:32:LEU:HA	1.93	0.41
1:0:2324:G:H4'	1:0:2418:G:O2'	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
1:0:308:U:C4	1:0:342:C:H1'	2.55	0.41
1:0:2353:A:H4'	1:0:2354:A:O5'	2.20	0.41
28:Y:100:ARG:NH1	28:Y:215:GLU:HA	2.35	0.41
1:0:1080:C:H4'	1:0:1081:A:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2575:C:H2'	1:0:2576:A:O4'	2.20	0.41
2:9:3106:C:O2'	2:9:3107:C:H5'	2.20	0.41
28:Y:187:VAL:HG13	28:Y:205:ILE:HA	2.01	0.41
27:X:41:PHE:CZ	27:X:74:ALA:HB3	2.55	0.41
28:Y:234:VAL:HG12	28:Y:235:GLU:N	2.35	0.41
6:B:254:GLN:NE2	39:B:9395:HOH:O	2.53	0.41
8:D:149:ARG:NH2	17:N:15:GLU:O	2.53	0.41
27:X:15:ARG:HB3	27:X:15:ARG:NH1	2.34	0.41
6:B:57:GLU:O	6:B:63:GLU:HB2	2.20	0.41
6:B:152:PRO:HA	39:B:9373:HOH:O	2.20	0.41
23:T:24:ARG:HH21	23:T:39:ASN:ND2	2.17	0.41
1:0:2413:A:H2'	1:0:2414:A:O4'	2.20	0.41
14:K:65:ARG:O	14:K:66:ARG:HB2	2.21	0.41
15:L:125:PHE:CZ	15:L:140:VAL:HG13	2.55	0.41
27:X:12:ILE:HB	27:X:70:ILE:HG22	2.01	0.41
1:0:2045:G:H2'	1:0:2046:G:O4'	2.21	0.41
7:C:51:TYR:CE2	30:1:53:LYS:HB3	2.55	0.41
1:0:419:A:H1'	1:0:1921:A:C2	2.55	0.41
1:0:899:C:H5'	39:0:3496:HOH:O	2.21	0.41
1:0:1289:C:O2'	1:0:1290:G:H5'	2.20	0.41
6:B:168:GLY:O	6:B:169:GLY:O	2.39	0.41
23:T:71:VAL:HG12	23:T:72:ILE:H	1.85	0.41
17:N:83:LEU:HD11	17:N:172:PHE:HD1	1.85	0.41
30:1:25:LYS:CG	31:2:49:GLU:H	2.25	0.41
1:0:1299:G:N2	39:0:4951:HOH:O	2.52	0.41
1:0:2823:G:H4'	1:0:2827:A:O4'	2.21	0.41
9:E:166:VAL:HB	39:E:6341:HOH:O	2.20	0.41
9:E:73:PHE:O	9:E:76:VAL:HG22	2.20	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.19	0.41
24:U:49:LEU:HD12	24:U:51:TRP:CZ2	2.56	0.41
1:0:2456:A:H2'	1:0:2457:U:C6	2.55	0.41
14:K:120:ARG:HB3	14:K:121:PHE:CD1	2.55	0.41
1:0:2613:G:O2'	1:0:2614:C:H5'	2.20	0.41
1:0:2825:C:H4'	1:0:2826:G:O5'	2.21	0.41
11:G:19:GLU:HG2	11:G:66:LEU:HD13	2.03	0.41
7:C:88:SER:O	7:C:91:PRO:HD3	2.20	0.41
1:0:2001:G:O2'	1:0:2002:C:H5'	2.20	0.41
5:A:39:ALA:O	5:A:61:GLU:HG3	2.20	0.41
8:D:37:ALA:O	8:D:40:ILE:HG12	2.21	0.41
5:A:186:TRP:CG	5:A:187:PRO:HA	2.56	0.41
25:V:6:GLN:O	25:V:9:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:228:C:C2'	1:0:229:G:H5'	2.50	0.41
14:K:12:LEU:HD13	14:K:18:ILE:HG21	2.03	0.41
1:0:1827:G:C6	1:0:1828:G:C6	3.09	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.89	0.41
1:0:2787:C:H2'	1:0:2788:A:O4'	2.20	0.41
1:0:1409:G:H5'	39:0:4018:HOH:O	2.19	0.41
1:0:413:G:H2'	1:0:414:C:C6	2.55	0.41
1:0:415:A:O2'	1:0:416:G:H5'	2.21	0.41
1:0:1056:U:H2'	1:0:1057:A:O4'	2.20	0.41
9:E:106:ASN:ND2	9:E:109:GLY:HA2	2.36	0.41
1:0:2735:U:H2'	1:0:2736:U:C6	2.55	0.41
32:3:62:THR:HB	39:3:9350:HOH:O	2.21	0.41
1:0:1759:A:N3	1:0:1818:C:H2'	2.36	0.41
1:0:731:U:H2'	1:0:732:C:C6	2.55	0.41
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.34	0.41
5:A:34:ASP:OD1	5:A:35:GLY:N	2.48	0.41
23:T:65:VAL:HG22	23:T:72:ILE:HG22	2.03	0.41
1:0:1157:C:H2'	1:0:1158:G:C8	2.53	0.41
1:0:187:A:H3'	1:0:188:C:H6	1.84	0.41
17:N:11:ARG:HA	17:N:14:ARG:CZ	2.51	0.41
1:0:1334:C:H2'	1:0:1335:C:H6	1.85	0.41
26:W:108:ARG:HG3	26:W:114:PRO:HG3	2.02	0.41
9:E:88:TYR:HB2	9:E:91:PHE:O	2.21	0.41
11:G:27:ILE:HD12	11:G:70:ALA:HB1	2.03	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.21	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.41
1:0:1052:G:N3	1:0:1052:G:H2'	2.36	0.41
1:0:876:A:H2'	1:0:876:A:N3	2.36	0.41
1:0:240:C:O2	1:0:240:C:H2'	2.21	0.41
1:0:585:C:H2'	1:0:586:C:O4'	2.21	0.41
1:0:2248:C:H2'	1:0:2249:G:H8	1.86	0.41
9:E:35:TYR:CD2	9:E:36:PRO:HD2	2.56	0.41
23:T:23:VAL:C	23:T:93:THR:HG21	2.41	0.41
1:0:1160:G:HO2'	1:0:1190:G:H8	1.65	0.41
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.50	0.41
1:0:1942:A:H3'	39:0:7519:HOH:O	2.20	0.41
2:9:3056:A:C3'	2:9:3057:A:H5''	2.49	0.41
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.86	0.41
14:K:113:ILE:HG22	14:K:114:ALA:O	2.21	0.41
26:W:122:ARG:HG2	26:W:122:ARG:H	1.71	0.41
16:M:27:ARG:HH22	16:M:44:THR:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1733:A:H4'	6:B:212:GLN:HA	2.01	0.41
17:N:154:LEU:C	17:N:156:GLU:H	2.23	0.41
1:0:907:A:H4'	1:0:1328:A:C2	2.55	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.02	0.41
16:M:134:ILE:O	16:M:136:PRO:HD3	2.21	0.41
2:9:3028:U:H2'	2:9:3029:C:C6	2.56	0.41
24:U:53:ASP:O	24:U:54:THR:C	2.59	0.41
24:U:52:THR:HG22	24:U:54:THR:H	1.84	0.41
1:0:1298:U:H2'	1:0:1299:G:C8	2.56	0.41
6:B:62:ARG:O	6:B:63:GLU:C	2.59	0.41
32:3:14:CYS:HB3	32:3:16:GLU:HG2	2.02	0.41
1:0:1972:U:C2'	1:0:1973:A:C5'	2.99	0.41
28:Y:182:PHE:HD2	28:Y:200:THR:O	2.04	0.41
1:0:1874:U:OP1	5:A:51:ARG:HD2	2.21	0.41
21:R:119:VAL:O	21:R:119:VAL:CG1	2.68	0.41
1:0:903:U:O4	15:L:18:HIS:HB2	2.21	0.41
1:0:902:G:N7	15:L:18:HIS:CD2	2.86	0.41
9:E:107:PHE:CD2	9:E:108:LEU:HD13	2.56	0.41
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.86	0.41
18:O:77:ALA:HA	18:O:96:VAL:O	2.21	0.41
8:D:153:THR:HA	8:D:156:ARG:CG	2.51	0.41
1:0:1279:U:O2	1:0:1279:U:H2'	2.21	0.41
1:0:69:A:H5'	1:0:69:A:C8	2.55	0.41
1:0:2795:C:O2'	1:0:2796:U:H5'	2.20	0.41
7:C:54:LEU:HD23	7:C:79:ARG:HG3	2.03	0.41
1:0:2050:G:H5''	21:R:80:TYR:O	2.21	0.41
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.86	0.41
12:H:36:LYS:HA	12:H:84:LYS:NZ	2.36	0.41
1:0:1855:G:H8	5:A:144:GLU:OE2	2.03	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
8:D:20:LYS:HA	8:D:75:LEU:O	2.21	0.41
1:0:569:A:H5''	1:0:587:A:N1	2.36	0.41
15:L:12:THR:HG21	15:L:16:GLY:O	2.20	0.41
1:0:1697:G:O2'	1:0:1698:U:H5'	2.20	0.41
1:0:2816:A:H5''	1:0:2817:G:H5'	2.03	0.41
1:0:1846:U:O2'	5:A:172:ALA:HB2	2.21	0.41
2:9:3011:A:O2'	2:9:3012:C:H3'	2.20	0.41
27:X:45:GLU:HG3	39:X:6178:HOH:O	2.20	0.41
1:0:1794:G:P	19:P:133:SER:HB2	2.60	0.41
21:R:83:LYS:HD3	39:R:9312:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:132:HIS:HB2	6:B:137:LEU:HD22	2.02	0.41
6:B:98:THR:CG2	6:B:99:GLU:H	2.22	0.41
26:W:119:HIS:CD2	26:W:120:PRO:HD2	2.56	0.41
1:0:336:G:H5''	39:0:4017:HOH:O	2.21	0.41
1:0:795:G:H4'	39:0:6718:HOH:O	2.19	0.41
9:E:26:ASN:HB3	9:E:76:VAL:O	2.21	0.41
12:H:87:LEU:HD13	12:H:134:PHE:CE2	2.55	0.41
12:H:77:LEU:O	12:H:81:GLY:CA	2.69	0.41
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.67	0.41
7:C:55:ARG:HB2	39:C:9109:HOH:O	2.21	0.41
21:R:27:HIS:O	21:R:31:ILE:HG13	2.21	0.41
1:0:1245:C:H5	39:J:3338:HOH:O	2.04	0.41
15:L:72:ASN:HB2	39:L:9389:HOH:O	2.21	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.21	0.41
1:0:2761:A:H2'	39:0:5871:HOH:O	2.21	0.41
28:Y:187:VAL:CG2	28:Y:192:ASP:HB2	2.34	0.40
1:0:2269:C:H2'	1:0:2270:G:H5'	2.03	0.40
17:N:143:ARG:HH12	17:N:173:ASP:CG	2.24	0.40
7:C:27:ARG:HG2	7:C:30:LEU:HD12	2.03	0.40
13:J:39:VAL:CG1	13:J:107:ASN:HB2	2.51	0.40
13:J:6:PHE:O	13:J:8:ALA:N	2.53	0.40
27:X:78:GLU:CG	27:X:79:GLU:N	2.84	0.40
1:0:1202:A:H2'	1:0:1203:G:C5'	2.50	0.40
17:N:69:TYR:CE2	17:N:184:ILE:HD11	2.56	0.40
24:U:6:CYS:C	24:U:8:TYR:N	2.75	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.82	0.40
1:0:2764:C:O2'	1:0:2765:C:H5'	2.21	0.40
23:T:87:VAL:HB	39:T:5545:HOH:O	2.21	0.40
1:0:1471:A:H2'	1:0:1472:C:C6	2.56	0.40
1:0:2079:G:H2'	1:0:2080:G:O4'	2.21	0.40
1:0:1883:U:O2'	1:0:1884:G:H5'	2.21	0.40
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:2869:G:H2'	1:0:2870:C:O4'	2.21	0.40
1:0:536:A:H3'	39:0:5305:HOH:O	2.21	0.40
21:R:39:THR:HB	21:R:42:GLU:OE1	2.21	0.40
6:B:304:PRO:CG	6:B:307:ARG:NH1	2.84	0.40
9:E:11:VAL:CG1	9:E:12:ASP:N	2.82	0.40
15:L:130:ARG:HA	39:L:9363:HOH:O	2.21	0.40
13:J:75:PRO:HD3	13:J:136:SER:OG	2.21	0.40
26:W:35:VAL:CG2	26:W:41:TYR:CD2	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:267:LYS:HA	39:B:9432:HOH:O	2.20	0.40
2:9:3049:G:H2'	2:9:3050:G:O4'	2.22	0.40
6:B:88:GLU:O	6:B:90:THR:HG23	2.21	0.40
8:D:58:VAL:HB	8:D:60:GLU:HG2	2.03	0.40
10:F:100:ASP:O	10:F:101:ALA:O	2.39	0.40
1:0:2765:C:H2'	1:0:2766:A:H8	1.86	0.40
1:0:2832:C:H5	39:0:7392:HOH:O	2.04	0.40
23:T:78:THR:HB	23:T:87:VAL:O	2.22	0.40
12:H:138:CYS:HB2	39:H:9146:HOH:O	2.21	0.40
1:0:707:C:C2	1:0:708:A:C8	3.08	0.40
8:D:35:ALA:C	8:D:37:ALA:N	2.74	0.40
26:W:149:LEU:HG	26:W:153:MET:CE	2.51	0.40
26:W:48:VAL:CG1	26:W:48:VAL:O	2.70	0.40
1:0:2072:G:H3'	1:0:2073:G:C5'	2.51	0.40
1:0:2780:C:H2'	1:0:2781:U:H6	1.86	0.40
26:W:122:ARG:NH2	39:W:5817:HOH:O	2.54	0.40
1:0:110:C:H2'	1:0:111:C:C6	2.56	0.40
21:R:25:PHE:CE2	21:R:29:LYS:CE	3.03	0.40
2:9:3065:A:HO2'	2:9:3066:G:P	2.44	0.40
14:K:13:GLU:OE2	14:K:44:LEU:HB2	2.22	0.40
33:I:71:GLY:O	33:I:72:VAL:C	2.59	0.40
9:E:116:THR:CG2	9:E:151:LEU:HD22	2.51	0.40
1:0:820:G:C5	5:A:171:LYS:HB2	2.57	0.40
26:W:125:HIS:HE1	39:W:3071:HOH:O	2.04	0.40
21:R:72:VAL:HG11	21:R:75:TRP:HB3	2.03	0.40
1:0:2697:A:H2'	1:0:2698:G:O4'	2.22	0.40
1:0:1080:C:H6	1:0:1080:C:O5'	2.04	0.40
9:E:31:ARG:CZ	39:E:5919:HOH:O	2.68	0.40
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.40
15:L:34:GLY:HA3	15:L:38:HIS:CE1	2.56	0.40
1:0:256:C:H2'	1:0:257:G:O4'	2.21	0.40
1:0:156:C:H5''	16:M:171:ARG:CD	2.27	0.40
26:W:5:VAL:HG11	26:W:153:MET:HE3	2.03	0.40
26:W:122:ARG:NH1	26:W:122:ARG:HG2	2.31	0.40
27:X:25:ARG:HG2	39:X:5356:HOH:O	2.22	0.40
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.57	0.40
28:Y:200:THR:HG22	28:Y:201:GLU:CG	2.50	0.40
1:0:396:U:P	32:3:38:ARG:HH11	2.45	0.40
6:B:243:ASN:HA	6:B:244:PRO:C	2.41	0.40
1:0:2011:A:H4'	1:0:2012:U:O5'	2.21	0.40
1:0:2820:A:H2'	1:0:2821:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:15:GLN:OE1	9:E:15:GLN:O	2.39	0.40
1:0:2796:U:H4'	9:E:119:HIS:NE2	2.36	0.40
1:0:538:C:H5''	1:0:539:G:C8	2.56	0.40
1:0:2708:G:H2'	1:0:2709:G:O4'	2.22	0.40
1:0:23:G:C6	1:0:24:G:N1	2.90	0.40
17:N:49:THR:CG2	17:N:56:ASP:HB2	2.50	0.40
1:0:494:C:H2'	1:0:496:G:OP2	2.21	0.40
1:0:812:A:H2'	1:0:813:C:O4'	2.22	0.40
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.21	0.40
6:B:313:PRO:O	6:B:314:ALA:C	2.60	0.40
6:B:217:ARG:CG	6:B:257:THR:HG22	2.49	0.40
25:V:39:ALA:C	25:V:41:GLU:N	2.73	0.40
23:T:1:SER:O	23:T:7:GLN:NE2	2.55	0.40
9:E:145:ALA:O	9:E:148:ILE:HB	2.22	0.40
6:B:146:THR:O	6:B:148:PRO:HD3	2.21	0.40
9:E:107:PHE:CZ	9:E:152:THR:HB	2.56	0.40
19:P:141:ILE:C	19:P:143:ALA:N	2.74	0.40
5:A:76:VAL:CG2	29:Z:63:LYS:HB3	2.51	0.40
14:K:62:PRO:HA	14:K:65:ARG:HH21	1.86	0.40
9:E:15:GLN:NE2	9:E:40:VAL:O	2.54	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
1:0:969:G:H1	1:0:999:C:H42	1.69	0.40
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.40
7:C:221:GLU:HG3	39:C:9149:HOH:O	2.22	0.40
1:0:645:U:OP2	15:L:4:LYS:CE	2.69	0.40
1:0:2290:U:H2'	39:0:7317:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/240 (98%)	205 (87%)	24 (10%)	6 (3%)	7	16
6	B	335/338 (99%)	295 (88%)	33 (10%)	7 (2%)	9	23
7	C	244/246 (99%)	215 (88%)	28 (12%)	1 (0%)	39	69
8	D	134/177 (76%)	94 (70%)	33 (25%)	7 (5%)	2	4
9	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
10	F	117/120 (98%)	104 (89%)	7 (6%)	6 (5%)	2	4
11	G	25/348 (7%)	24 (96%)	0	1 (4%)	4	8
12	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	10	25
13	J	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	9	23
14	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	13	32
15	L	141/165 (86%)	122 (86%)	17 (12%)	2 (1%)	14	35
16	M	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
17	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	16
18	O	113/116 (97%)	109 (96%)	2 (2%)	2 (2%)	11	27
19	P	141/149 (95%)	131 (93%)	7 (5%)	3 (2%)	9	23
20	Q	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
21	R	148/155 (96%)	135 (91%)	11 (7%)	2 (1%)	14	35
22	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
23	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	21	49
24	U	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	9	24
25	V	63/71 (89%)	54 (86%)	7 (11%)	2 (3%)	5	12
26	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	26	55
27	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	7	18
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	55 (78%)	9 (13%)	7 (10%)	1	0
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
32	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	17	42
33	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	3	6
All	All	3705/4430 (84%)	3316 (90%)	321 (9%)	68 (2%)	11	27

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
6	B	184	ASP
10	F	101	ALA
12	H	166	SER
12	H	168	ALA
17	N	154	LEU
17	N	164	ASP
17	N	183	ASP
17	N	184	ILE
29	Z	81	ARG
5	A	34	ASP
5	A	36	ASP
5	A	37	VAL
6	B	107	SER
6	B	169	GLY
7	C	8	LEU
13	J	5	GLU
13	J	89	HIS
15	L	80	ASP
18	O	108	GLY
24	U	7	ASP
26	W	49	ASN
27	X	70	ILE
32	3	57	GLY
5	A	119	ALA
8	D	27	ILE
8	D	173	GLU
10	F	61	MET
10	F	104	ALA
11	G	72	ASP
14	K	111	GLY
14	K	126	SER
19	P	116	SER
25	V	43	PRO
29	Z	42	CYS
29	Z	67	GLY
33	I	138	THR
5	A	132	ASP
6	B	2	GLN
8	D	16	PRO
8	D	65	GLU
8	D	171	ASP
10	F	64	PRO

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Mol	Chain	Res	Type
15	L	105	TYR
17	N	68	GLU
19	P	117	SER
19	P	142	ASP
29	Z	41	ASN
29	Z	43	GLY
33	I	81	ASP
5	A	211	LYS
8	D	164	ALA
10	F	44	SER
10	F	100	ASP
12	H	16	ARG
23	T	53	GLY
25	V	40	PRO
27	X	78	GLU
29	Z	20	ARG
29	Z	21	VAL
6	B	34	GLY
13	J	143	LYS
18	O	21	SER
6	B	185	GLY
21	R	114	VAL
8	D	69	ILE
33	I	73	PRO
21	R	81	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/182 (98%)	170 (95%)	9 (5%)	30	60
6	B	282/283 (100%)	267 (95%)	15 (5%)	28	57
7	C	193/193 (100%)	180 (93%)	13 (7%)	20	44
8	D	117/148 (79%)	112 (96%)	5 (4%)	35	66
9	E	152/156 (97%)	147 (97%)	5 (3%)	45	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F	93/94 (99%)	90 (97%)	3 (3%)	46	77
11	G	27/283 (10%)	26 (96%)	1 (4%)	41	72
12	H	132/138 (96%)	126 (96%)	6 (4%)	34	65
13	J	118/121 (98%)	110 (93%)	8 (7%)	20	43
14	K	106/106 (100%)	104 (98%)	2 (2%)	65	88
15	L	113/127 (89%)	110 (97%)	3 (3%)	52	82
16	M	158/158 (100%)	150 (95%)	8 (5%)	29	59
17	N	149/150 (99%)	145 (97%)	4 (3%)	52	82
18	O	93/94 (99%)	91 (98%)	2 (2%)	60	86
19	P	113/117 (97%)	108 (96%)	5 (4%)	35	65
20	Q	79/80 (99%)	74 (94%)	5 (6%)	22	48
21	R	117/122 (96%)	113 (97%)	4 (3%)	44	75
22	S	71/74 (96%)	70 (99%)	1 (1%)	74	92
23	T	105/106 (99%)	98 (93%)	7 (7%)	20	44
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	63	87
26	W	130/130 (100%)	125 (96%)	5 (4%)	40	71
27	X	66/74 (89%)	61 (92%)	5 (8%)	16	37
28	Y	120/196 (61%)	114 (95%)	6 (5%)	30	60
29	Z	60/68 (88%)	60 (100%)	0	100	100
30	1	46/47 (98%)	46 (100%)	0	100	100
31	2	42/46 (91%)	40 (95%)	2 (5%)	31	62
32	3	79/79 (100%)	77 (98%)	2 (2%)	55	84
33	I	58/130 (45%)	57 (98%)	1 (2%)	68	90
All	All	3093/3611 (86%)	2965 (96%)	128 (4%)	37	69

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	33	GLU
5	A	36	ASP
5	A	69	LEU
5	A	78	ASP

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Mol	Chain	Res	Type
5	A	94	LEU
5	A	153	ARG
5	A	179	MET
5	A	217	ARG
6	B	7	ARG
6	B	27	ASN
6	B	49	THR
6	B	63	GLU
6	B	97	LEU
6	B	132	HIS
6	B	162	MET
6	B	192	ASP
6	B	195	ARG
6	B	234	ARG
6	B	254	GLN
6	B	256	GLN
6	B	277	GLU
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	94	THR
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	199	GLU
7	C	214	THR
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	246	ARG
8	D	24	HIS
8	D	61	PHE
8	D	101	THR
8	D	133	ASN
8	D	136	ARG
9	E	15	GLN
9	E	86	VAL
9	E	102	VAL
9	E	126	ILE
9	E	164	ASP

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Mol	Chain	Res	Type
10	F	12	LEU
10	F	99	THR
10	F	105	ASP
11	G	12	ILE
12	H	30	GLN
12	H	84	LYS
12	H	88	ARG
12	H	111	ASP
12	H	132	GLN
12	H	154	TYR
13	J	46	ILE
13	J	52	GLN
13	J	74	ARG
13	J	79	PHE
13	J	107	ASN
13	J	112	ASP
13	J	120	SER
13	J	132	LEU
14	K	10	GLN
14	K	49	LEU
15	L	30	ARG
15	L	35	ARG
15	L	80	ASP
16	M	46	LEU
16	M	68	ARG
16	M	74	LYS
16	M	81	ARG
16	M	93	ARG
16	M	99	ARG
16	M	116	ASN
16	M	164	THR
17	N	17	ARG
17	N	26	LEU
17	N	115	VAL
17	N	152	GLU
18	O	3	THR
18	O	43	VAL
19	P	52	LYS
19	P	73	HIS
19	P	91	LYS
19	P	94	TRP
19	P	98	ILE

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Mol	Chain	Res	Type
20	Q	11	ARG
20	Q	16	ASN
20	Q	30	VAL
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	39	THR
21	R	82	GLU
21	R	132	ARG
22	S	53	ASN
23	T	19	ARG
23	T	23	VAL
23	T	26	THR
23	T	39	ASN
23	T	48	VAL
23	T	96	VAL
23	T	112	LEU
25	V	65	ASP
26	W	35	VAL
26	W	52	VAL
26	W	73	LEU
26	W	122	ARG
26	W	146	ILE
27	X	15	ARG
27	X	27	ASP
27	X	49	ARG
27	X	72	VAL
27	X	79	GLU
28	Y	115	ARG
28	Y	141	THR
28	Y	163	THR
28	Y	189	ASN
28	Y	203	VAL
28	Y	235	GLU
31	2	16	ASN
31	2	18	ASN
32	3	11	CYS
32	3	42	ARG
33	I	86	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	29	HIS
5	A	47	HIS
5	A	92	ASN
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	260	HIS
6	B	320	GLN
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
7	C	163	HIS
8	D	97	GLN
8	D	103	ASN
8	D	133	ASN
9	E	71	ASN
9	E	106	ASN
9	E	143	GLN
11	G	17	GLN
11	G	64	ASN
12	H	31	HIS
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	132	GLN
12	H	145	HIS
12	H	170	ASN
13	J	52	GLN
13	J	107	ASN
14	K	10	GLN
15	L	18	HIS
15	L	41	HIS
15	L	42	ASN
16	M	24	GLN
16	M	58	GLN
16	M	170	ASN
17	N	40	ASN
17	N	107	ASN
17	N	153	GLN
19	P	50	GLN

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Mol	Chain	Res	Type
19	P	66	GLN
19	P	88	GLN
19	P	118	GLN
20	Q	16	ASN
20	Q	40	HIS
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
21	R	123	GLN
22	S	25	GLN
22	S	53	ASN
23	T	39	ASN
23	T	43	ASN
23	T	73	HIS
24	U	39	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	87	HIS
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	23	HIS
28	Y	134	HIS
28	Y	149	GLN
28	Y	189	ASN
30	1	8	GLN
30	1	16	HIS
30	1	28	HIS
31	2	16	ASN
31	2	18	ASN
31	2	41	HIS
31	2	45	ASN
32	3	2	GLN
32	3	30	GLN
32	3	48	ASN
32	3	78	HIS
33	I	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	30 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
3	4	0/3	-	-
4	5	2/6 (33%)	0	0
All	All	2868/3053 (93%)	251 (8%)	31 (1%)

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A

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Mol	Chain	Res	Type
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	705	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G

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Mol	Chain	Res	Type
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1106	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A

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Mol	Chain	Res	Type
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1562	C
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A

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Mol	Chain	Res	Type
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
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	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A

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Mol	Chain	Res	Type
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	2637	A
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G

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Mol	Chain	Res	Type
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1165	G
1	0	1232	A
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1667	A
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U

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Mol	Chain	Res	Type
1	0	2791	U
2	9	3065	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMU	0	2587	1,36	12,22,23	0.97	1 (8%)	19,31,34	3.18	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.03	1 (5%)	21,38,41	2.52	3 (14%)
1	UR3	0	2619	1	12,22,23	0.83	1 (8%)	16,32,35	0.75	0
1	PSU	0	2621	1	13,21,22	1.65	2 (15%)	18,30,33	6.11	3 (16%)
1	1MA	0	628	1,36	14,25,26	0.99	1 (7%)	15,37,40	1.14	1 (6%)
3	5AA	4	76	1,3	16,26,27	0.66	0	15,38,41	1.40	1 (6%)
3	HFA	4	77	3	11,11,12	1.17	1 (9%)	13,13,15	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1,36	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.89	1.48	1.52
1	0	2619	UR3	C6-C5	-2.04	1.33	1.38
1	0	2587	OMU	C4-N3	2.13	1.37	1.33
1	0	2621	PSU	C4-N3	2.70	1.38	1.33
1	0	628	1MA	C6-N6	2.77	1.34	1.29
3	4	77	HFA	OA-CA	2.84	1.49	1.43
1	0	2588	OMG	C6-N1	3.13	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.36	114.71	128.33
1	0	2588	OMG	C5-C6-N1	-8.76	111.61	123.59
1	0	628	1MA	C2-N3-C4	-3.58	110.85	116.40
1	0	2587	OMU	C5-C4-N3	-3.25	114.78	123.12
1	0	2588	OMG	N3-C2-N1	-2.26	124.00	127.44
1	0	2621	PSU	C6-N1-C2	2.53	119.53	115.47
3	4	76	5AA	C2-N1-C6	3.50	118.89	111.43
1	0	2588	OMG	C6-N1-C2	6.57	125.06	115.94
1	0	2587	OMU	C4-N3-C2	13.29	127.31	114.14
1	0	2621	PSU	C4-N3-C2	14.03	127.38	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0
3	4	76	5AA	1	0
3	4	77	HFA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2749/2922 (94%)	-0.30	46 (1%) 73 74	30, 57, 102, 163	0
2	9	122/122 (100%)	-0.16	5 (4%) 41 41	51, 72, 98, 158	0
3	4	1/3 (33%)	0.29	0 100 100	75, 75, 75, 75	0
4	5	4/6 (66%)	0.24	0 100 100	63, 63, 71, 81	0
5	A	237/240 (98%)	0.36	9 (3%) 44 44	37, 61, 97, 120	0
6	B	337/338 (99%)	0.24	9 (2%) 58 58	38, 68, 95, 104	0
7	C	246/246 (100%)	0.00	3 (1%) 81 81	32, 55, 81, 89	0
8	D	140/177 (79%)	2.02	63 (45%) 0 0	67, 111, 136, 143	0
9	E	172/178 (96%)	0.89	23 (13%) 4 3	58, 83, 108, 116	0
10	F	119/120 (99%)	0.93	22 (18%) 2 1	58, 84, 112, 127	0
11	G	29/348 (8%)	2.48	19 (65%) 0 0	78, 96, 110, 112	0
12	H	160/171 (93%)	0.46	11 (6%) 20 18	46, 66, 98, 104	0
13	J	142/145 (97%)	0.08	0 100 100	49, 63, 82, 103	0
14	K	132/132 (100%)	0.23	3 (2%) 64 64	41, 67, 88, 94	0
15	L	145/165 (87%)	0.72	24 (16%) 2 2	34, 77, 120, 133	0
16	M	194/194 (100%)	-0.03	0 100 100	38, 51, 68, 77	0
17	N	186/187 (99%)	0.57	21 (11%) 7 5	47, 72, 120, 126	0
18	O	115/116 (99%)	0.15	0 100 100	47, 66, 83, 96	0
19	P	143/149 (95%)	0.45	7 (4%) 33 32	47, 68, 83, 91	0
20	Q	95/96 (98%)	0.26	3 (3%) 51 51	45, 54, 68, 87	0
21	R	150/155 (96%)	-0.00	2 (1%) 79 79	42, 55, 73, 84	0
22	S	81/85 (95%)	0.26	3 (3%) 45 45	52, 68, 87, 94	0
23	T	119/120 (99%)	0.66	8 (6%) 21 19	48, 67, 99, 115	0
24	U	53/66 (80%)	0.44	4 (7%) 17 15	52, 67, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.57	19 (29%) 1 0	62, 85, 123, 128	0
26	W	154/154 (100%)	0.02	0 100 100	46, 61, 81, 92	0
27	X	82/92 (89%)	0.79	16 (19%) 1 1	53, 69, 89, 106	0
28	Y	142/241 (58%)	0.23	8 (5%) 28 26	35, 56, 79, 97	0
29	Z	73/83 (87%)	0.47	8 (10%) 7 5	54, 72, 84, 105	0
30	1	56/57 (98%)	-0.29	0 100 100	37, 42, 48, 60	0
31	2	46/50 (92%)	1.35	13 (28%) 1 0	42, 71, 124, 132	0
32	3	92/92 (100%)	0.27	3 (3%) 50 50	42, 62, 77, 89	0
33	I	70/162 (43%)	3.70	53 (75%) 0 0	118, 134, 156, 158	0
All	All	6651/7483 (88%)	0.16	405 (6%) 25 23	30, 62, 110, 163	0

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	V	1	THR	11.4
33	I	71	GLY	9.4
33	I	93	GLN	9.0
33	I	96	PHE	9.0
33	I	133	THR	8.5
33	I	102	VAL	7.4
11	G	23	ILE	7.3
33	I	117	LEU	7.0
33	I	113	HIS	7.0
33	I	79	ILE	6.9
2	9	3001	U	6.9
8	D	63	ILE	6.8
33	I	75	THR	6.6
8	D	64	ARG	6.6
33	I	109	ALA	6.6
25	V	40	PRO	6.5
8	D	69	ILE	6.4
33	I	116	LEU	6.2
27	X	88	GLU	6.2
33	I	103	ASP	6.2
33	I	118	SER	6.2
11	G	27	ILE	6.1
8	D	10	PHE	6.1
25	V	39	ALA	6.1
31	2	36	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
5	A	37	VAL	6.0
17	N	166	ALA	6.0
33	I	105	VAL	5.9
8	D	57	THR	5.9
2	9	3023	U	5.9
8	D	88	LEU	5.8
2	9	3024	U	5.6
8	D	58	VAL	5.5
15	L	106	VAL	5.4
31	2	45	ASN	5.3
23	T	119	ALA	5.3
8	D	66	GLY	5.3
33	I	137	VAL	5.2
31	2	41	HIS	5.1
8	D	128	LEU	5.0
33	I	76	ALA	5.0
8	D	90	LEU	5.0
8	D	65	GLU	4.9
1	0	1198	U	4.9
33	I	85	PHE	4.8
27	X	74	ALA	4.8
33	I	72	VAL	4.7
1	0	1177	A	4.7
8	D	85	GLN	4.7
31	2	44	ARG	4.6
33	I	77	GLU	4.6
31	2	49	GLU	4.5
1	0	1173	A	4.5
25	V	38	GLY	4.5
8	D	56	ARG	4.5
31	2	38	LYS	4.5
8	D	44	ILE	4.5
15	L	80	ASP	4.4
8	D	68	PRO	4.4
10	F	119	ARG	4.4
8	D	25	MET	4.4
10	F	17	LEU	4.4
33	I	73	PRO	4.3
33	I	74	PRO	4.3
8	D	18	ILE	4.3
11	G	71	LEU	4.3
8	D	27	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
8	D	89	PRO	4.3
8	D	93	LEU	4.3
33	I	111	GLN	4.2
31	2	37	HIS	4.2
31	2	48	ASP	4.2
29	Z	11	SER	4.2
31	2	42	TRP	4.2
27	X	85	VAL	4.1
33	I	114	PRO	4.1
28	Y	235	GLU	4.1
8	D	104	PHE	4.1
31	2	35	ARG	4.1
33	I	126	LYS	4.1
1	0	970	U	4.0
5	A	237	GLY	4.0
15	L	104	ASP	4.0
8	D	62	ASP	4.0
8	D	75	LEU	4.0
29	Z	20	ARG	4.0
25	V	43	PRO	4.0
33	I	78	LEU	4.0
33	I	98	ALA	4.0
8	D	61	PHE	4.0
1	0	2237	G	3.9
33	I	97	VAL	3.9
8	D	71	ALA	3.9
15	L	60	GLU	3.8
8	D	172	VAL	3.8
27	X	71	ARG	3.8
9	E	42	VAL	3.8
1	0	1279	U	3.8
8	D	23	VAL	3.8
33	I	81	ASP	3.8
33	I	88	GLY	3.8
33	I	83	ALA	3.8
8	D	70	GLY	3.7
27	X	73	ARG	3.7
8	D	26	GLY	3.7
24	U	47	ARG	3.7
10	F	49	PHE	3.7
7	C	135	GLU	3.7
1	0	1172	G	3.6

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Mol	Chain	Res	Type	RSRZ
32	3	22	VAL	3.6
8	D	129	ASP	3.6
33	I	139	ILE	3.6
25	V	8	ILE	3.6
1	0	2238	A	3.6
8	D	130	VAL	3.6
8	D	86	THR	3.6
33	I	124	ALA	3.6
15	L	120	LEU	3.6
27	X	10	VAL	3.6
1	0	1199	A	3.6
8	D	170	TYR	3.6
23	T	112	LEU	3.6
17	N	183	ASP	3.6
11	G	24	VAL	3.5
8	D	106	PHE	3.5
32	3	92	GLU	3.5
5	A	36	ASP	3.5
33	I	91	GLU	3.5
33	I	115	ASP	3.5
33	I	135	LEU	3.5
19	P	77	ALA	3.4
8	D	165	PHE	3.4
8	D	51	ARG	3.4
17	N	160	SER	3.4
8	D	134	LEU	3.4
15	L	97	VAL	3.4
8	D	16	PRO	3.4
1	0	282	C	3.4
22	S	81	ILE	3.4
9	E	100	ASP	3.3
17	N	152	GLU	3.3
31	2	43	ARG	3.3
15	L	105	TYR	3.3
17	N	159	TYR	3.3
10	F	106	ALA	3.3
29	Z	21	VAL	3.3
11	G	69	ARG	3.3
24	U	52	THR	3.2
33	I	89	SER	3.2
1	0	960	G	3.2
8	D	59	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
31	2	39	ARG	3.2
8	D	98	PHE	3.2
8	D	87	ALA	3.2
9	E	5	LEU	3.2
33	I	119	TYR	3.1
10	F	45	ALA	3.1
27	X	41	PHE	3.1
8	D	24	HIS	3.1
8	D	84	LEU	3.1
27	X	72	VAL	3.1
33	I	86	GLU	3.1
1	0	1525	G	3.1
33	I	107	GLN	3.1
29	Z	25	ARG	3.1
10	F	16	ALA	3.1
31	2	20	ARG	3.1
15	L	140	VAL	3.1
8	D	67	ASP	3.1
20	Q	64	GLU	3.0
17	N	150	TYR	3.0
25	V	36	ALA	3.0
1	0	497	A	3.0
17	N	68	GLU	3.0
33	I	110	GLU	3.0
12	H	37	GLN	3.0
17	N	149	GLU	3.0
1	0	2637	A	3.0
28	Y	95	THR	3.0
25	V	9	ARG	3.0
33	I	92	PRO	3.0
25	V	3	LEU	2.9
25	V	59	ILE	2.9
9	E	48	VAL	2.9
10	F	98	VAL	2.9
9	E	10	ASP	2.9
23	T	116	ASP	2.9
15	L	91	VAL	2.9
10	F	20	LEU	2.9
24	U	54	THR	2.9
9	E	1	PRO	2.9
33	I	132	CYS	2.9
1	0	735	C	2.9

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Mol	Chain	Res	Type	RSRZ
17	N	158	LEU	2.9
12	H	50	ILE	2.9
33	I	138	THR	2.9
1	0	285	A	2.9
9	E	108	LEU	2.9
12	H	73	LEU	2.9
14	K	132	VAL	2.9
8	D	92	GLU	2.9
1	0	138	U	2.9
9	E	7	ILE	2.8
8	D	41	LEU	2.8
12	H	32	LYS	2.8
9	E	45	ASP	2.8
24	U	55	ALA	2.8
11	G	66	LEU	2.8
11	G	28	GLU	2.8
33	I	106	LYS	2.8
8	D	17	ARG	2.8
25	V	37	GLY	2.8
12	H	146	VAL	2.8
11	G	70	ALA	2.8
28	Y	236	VAL	2.8
33	I	140	GLU	2.8
10	F	19	ALA	2.8
8	D	171	ASP	2.8
11	G	73	ASP	2.8
20	Q	76	VAL	2.8
27	X	76	ARG	2.8
19	P	71	TYR	2.7
5	A	31	LYS	2.7
11	G	22	ALA	2.7
8	D	45	THR	2.7
15	L	123	ASP	2.7
28	Y	108	ASP	2.7
23	T	55	PHE	2.7
29	Z	59	TYR	2.7
25	V	45	ARG	2.7
8	D	73	VAL	2.7
9	E	11	VAL	2.7
1	0	1130	U	2.7
15	L	76	LEU	2.6
17	N	181	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1000	C	2.6
28	Y	97	LEU	2.6
8	D	40	ILE	2.6
17	N	147	ILE	2.6
8	D	157	LEU	2.6
33	I	104	GLN	2.6
1	0	2004	U	2.6
25	V	63	GLU	2.6
15	L	81	VAL	2.6
32	3	1	MET	2.6
1	0	280	C	2.6
9	E	170	ARG	2.6
15	L	130	ARG	2.6
1	0	999	C	2.6
10	F	44	SER	2.6
15	L	96	VAL	2.6
25	V	5	VAL	2.6
14	K	108	GLU	2.5
1	0	1171	A	2.5
11	G	20	VAL	2.5
33	I	136	GLY	2.5
5	A	97	ALA	2.5
17	N	148	ALA	2.5
21	R	6	VAL	2.5
7	C	246	ARG	2.5
33	I	122	THR	2.5
1	0	372	A	2.5
8	D	166	ILE	2.5
2	9	3122	C	2.5
15	L	89	PHE	2.5
1	0	1190	G	2.5
6	B	1	PRO	2.5
9	E	8	PRO	2.5
10	F	28	ALA	2.5
10	F	75	ILE	2.5
9	E	157	LYS	2.5
33	I	121	LEU	2.5
10	F	86	ALA	2.5
10	F	117	GLU	2.5
25	V	46	ILE	2.4
27	X	9	VAL	2.4
9	E	44	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
11	G	26	MET	2.4
9	E	72	MET	2.4
12	H	74	ILE	2.4
6	B	117	GLU	2.4
17	N	165	ALA	2.4
6	B	119	HIS	2.4
11	G	21	ASP	2.4
27	X	7	GLU	2.4
1	0	284	C	2.4
14	K	124	VAL	2.4
1	0	10	U	2.4
10	F	100	ASP	2.4
15	L	75	LEU	2.4
15	L	142	LEU	2.4
1	0	2508	C	2.4
8	D	38	GLU	2.4
20	Q	81	GLU	2.4
28	Y	98	GLN	2.4
12	H	65	SER	2.3
5	A	38	ILE	2.3
5	A	35	GLY	2.3
8	D	94	ALA	2.3
9	E	86	VAL	2.3
9	E	122	THR	2.3
12	H	35	ARG	2.3
15	L	73	VAL	2.3
6	B	181	ILE	2.3
25	V	62	GLU	2.3
33	I	108	ILE	2.3
1	0	370	G	2.3
25	V	52	ALA	2.3
9	E	88	TYR	2.3
19	P	114	LEU	2.3
27	X	77	PHE	2.3
8	D	55	LYS	2.3
8	D	11	HIS	2.3
12	H	162	ARG	2.3
33	I	129	VAL	2.3
9	E	82	TYR	2.3
1	0	2769	C	2.3
6	B	109	LEU	2.3
27	X	75	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
23	T	42	VAL	2.3
10	F	103	GLU	2.2
15	L	101	ASP	2.2
27	X	40	HIS	2.2
12	H	45	VAL	2.2
28	Y	234	VAL	2.2
27	X	11	THR	2.2
1	0	371	U	2.2
28	Y	96	GLU	2.2
17	N	179	LEU	2.2
19	P	9	LEU	2.2
6	B	118	ASP	2.2
10	F	113	ASP	2.2
15	L	125	PHE	2.2
1	0	2345	A	2.2
6	B	128	ILE	2.2
23	T	33	GLU	2.2
1	0	1175	G	2.2
1	0	1197	G	2.2
1	0	1951	G	2.2
10	F	109	GLU	2.2
17	N	155	GLU	2.2
9	E	76	VAL	2.2
2	9	3002	U	2.2
9	E	20	ILE	2.2
33	I	95	ASP	2.2
8	D	83	PHE	2.2
8	D	81	GLU	2.2
12	H	171	ALA	2.2
33	I	128	VAL	2.2
27	X	80	GLU	2.2
1	0	2239	C	2.2
1	0	2664	A	2.2
6	B	134	ALA	2.2
8	D	52	THR	2.2
10	F	26	THR	2.2
11	G	25	GLU	2.2
7	C	61	PHE	2.2
25	V	49	LEU	2.1
5	A	98	GLU	2.1
11	G	72	ASP	2.1
25	V	33	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
29	Z	24	ARG	2.1
22	S	70	GLU	2.1
1	0	1169	U	2.1
1	0	2825	C	2.1
17	N	139	TRP	2.1
22	S	20	PHE	2.1
1	0	1200	A	2.1
1	0	1919	A	2.1
8	D	50	VAL	2.1
17	N	185	GLU	2.1
15	L	62	ALA	2.1
15	L	93	VAL	2.1
29	Z	19	GLY	2.1
11	G	68	GLU	2.1
1	0	130	C	2.1
1	0	969	G	2.1
10	F	18	GLU	2.1
19	P	67	LYS	2.1
8	D	135	VAL	2.1
8	D	29	HIS	2.1
15	L	102	ASP	2.1
17	N	145	ALA	2.1
29	Z	22	SER	2.1
11	G	16	LYS	2.1
23	T	59	GLU	2.1
10	F	12	LEU	2.0
11	G	67	LEU	2.0
9	E	95	VAL	2.0
21	R	55	GLN	2.0
11	G	63	ARG	2.0
17	N	162	ASP	2.0
23	T	35	TYR	2.0
10	F	47	LEU	2.0
17	N	83	LEU	2.0
1	0	1186	C	2.0
9	E	53	GLU	2.0
19	P	16	VAL	2.0
19	P	141	ILE	2.0
17	N	140	GLN	2.0
1	0	281	U	2.0
15	L	90	ARG	2.0
5	A	32	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
6	B	105	PHE	2.0
1	0	1202	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	5AA	4	76	24/25	0.94	0.21	-	77,82,86,87	0
1	1MA	0	628	23/24	0.99	0.16	-	39,41,42,44	0
3	HFA	4	77	11/12	0.91	0.31	-	86,86,87,88	0
1	UR3	0	2619	21/22	0.98	0.16	-	40,46,49,54	0
1	OMU	0	2587	21/22	0.99	0.15	-	41,43,46,49	0
1	PSU	0	2621	20/21	0.99	0.13	-	34,37,42,43	0
1	OMG	0	2588	24/25	0.98	0.15	-	38,40,45,46	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	CL	0	9315	1/1	0.93	0.60	37.79	89,89,89,89	0
36	NA	0	9174	1/1	0.96	0.49	28.82	74,74,74,74	0
36	NA	0	9178	1/1	0.98	0.53	28.52	75,75,75,75	0
35	K	0	9001	1/1	0.92	0.40	26.75	70,70,70,70	0
36	NA	0	9121	1/1	0.89	0.46	22.92	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9156	1/1	0.98	0.35	22.56	57,57,57,57	0
36	NA	R	9186	1/1	0.76	0.50	20.47	80,80,80,80	0
36	NA	0	9164	1/1	0.91	0.34	17.50	55,55,55,55	0
36	NA	L	9180	1/1	0.92	0.55	16.76	61,61,61,61	0
36	NA	0	9171	1/1	0.75	0.29	14.68	74,74,74,74	0
36	NA	0	9177	1/1	0.85	0.32	12.39	78,78,78,78	0
36	NA	0	9172	1/1	0.81	0.34	11.46	64,64,64,64	0
36	NA	0	9173	1/1	0.97	0.39	10.79	62,62,62,62	0
36	NA	0	9176	1/1	0.94	0.24	9.32	49,49,49,49	0
36	NA	0	9162	1/1	0.99	0.27	8.13	61,61,61,61	0
36	NA	0	9169	1/1	0.87	0.30	7.90	65,65,65,65	0
37	CL	B	9319	1/1	0.98	0.24	7.28	57,57,57,57	0
36	NA	0	9182	1/1	0.89	0.34	6.91	78,78,78,78	0
36	NA	0	9125	1/1	0.98	0.22	6.77	62,62,62,62	0
36	NA	0	9161	1/1	0.90	0.22	6.14	62,62,62,62	0
36	NA	0	9140	1/1	0.93	0.26	6.09	53,53,53,53	0
34	MG	0	8060	1/1	0.98	0.22	6.03	45,45,45,45	0
36	NA	0	9114	1/1	0.95	0.22	5.28	44,44,44,44	0
36	NA	0	9110	1/1	0.87	0.22	4.60	44,44,44,44	0
36	NA	0	9129	1/1	0.69	0.19	4.30	68,68,68,68	0
37	CL	0	9316	1/1	0.98	0.25	4.25	75,75,75,75	0
36	NA	0	9120	1/1	0.98	0.20	4.11	35,35,35,35	0
36	NA	0	9165	1/1	0.95	0.32	3.86	45,45,45,45	0
34	MG	0	8038	1/1	0.98	0.18	2.65	33,33,33,33	0
36	NA	9	9183	1/1	0.93	0.19	2.58	63,63,63,63	0
36	NA	0	9168	1/1	0.88	0.15	2.49	69,69,69,69	0
36	NA	0	9150	1/1	0.90	0.18	2.24	46,46,46,46	0
34	MG	0	8054	1/1	0.96	0.15	1.99	35,35,35,35	0
34	MG	0	8018	1/1	0.96	0.19	1.80	49,49,49,49	0
34	MG	0	8013	1/1	0.95	0.19	1.80	43,43,43,43	0
34	MG	Y	8109	1/1	0.95	0.20	1.49	62,62,62,62	0
36	NA	0	9126	1/1	0.80	0.20	1.20	51,51,51,51	0
34	MG	0	8096	1/1	0.93	0.19	1.07	63,63,63,63	0
36	NA	0	9139	1/1	0.96	0.15	1.04	30,30,30,30	0
34	MG	0	8021	1/1	0.99	0.16	0.89	33,33,33,33	0
34	MG	0	8053	1/1	0.89	0.15	0.79	57,57,57,57	0
34	MG	A	8065	1/1	0.96	0.20	0.41	54,54,54,54	0
34	MG	0	8070	1/1	0.95	0.17	0.27	66,66,66,66	0
36	NA	0	9135	1/1	0.95	0.17	0.26	55,55,55,55	0
37	CL	J	9321	1/1	0.96	0.17	0.05	60,60,60,60	0
36	NA	0	9131	1/1	0.96	0.14	0.01	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	5	8118	1/1	0.91	0.18	0.00	47,47,47,47	0
36	NA	M	9147	1/1	0.97	0.16	-0.23	32,32,32,32	0
36	NA	Q	9148	1/1	0.99	0.19	-0.26	46,46,46,46	0
34	MG	B	8055	1/1	0.96	0.16	-0.33	60,60,60,60	0
34	MG	0	8012	1/1	0.95	0.15	-0.35	43,43,43,43	0
36	NA	0	9153	1/1	0.94	0.14	-0.43	35,35,35,35	0
34	MG	0	8058	1/1	0.99	0.16	-0.48	48,48,48,48	0
36	NA	0	9123	1/1	0.98	0.17	-0.56	47,47,47,47	0
34	MG	0	8064	1/1	0.97	0.13	-0.61	38,38,38,38	0
36	NA	0	9166	1/1	0.84	0.12	-0.63	71,71,71,71	0
34	MG	0	8044	1/1	0.92	0.12	-0.91	52,52,52,52	0
36	NA	0	9133	1/1	0.95	0.13	-0.91	38,38,38,38	0
37	CL	O	9308	1/1	0.97	0.14	-0.92	81,81,81,81	0
34	MG	0	8033	1/1	0.97	0.14	-1.00	44,44,44,44	0
38	CD	Z	9203	1/1	0.99	0.09	-1.03	76,76,76,76	0
37	CL	L	9310	1/1	0.95	0.14	-1.14	72,72,72,72	0
36	NA	0	9117	1/1	0.93	0.12	-1.29	62,62,62,62	0
34	MG	B	8056	1/1	0.98	0.15	-1.36	57,57,57,57	0
37	CL	0	9305	1/1	0.98	0.13	-1.38	62,62,62,62	0
34	MG	0	8057	1/1	0.94	0.14	-1.39	49,49,49,49	0
36	NA	0	9109	1/1	0.99	0.11	-1.41	35,35,35,35	0
34	MG	0	8074	1/1	0.98	0.10	-1.53	38,38,38,38	0
34	MG	0	8086	1/1	0.97	0.06	-1.73	58,58,58,58	0
36	NA	0	9102	1/1	0.95	0.13	-1.77	54,54,54,54	0
38	CD	U	9201	1/1	0.99	0.07	-1.77	78,78,78,78	0
36	NA	J	9146	1/1	0.91	0.12	-1.84	41,41,41,41	0
34	MG	0	8032	1/1	0.97	0.13	-1.85	47,47,47,47	0
34	MG	0	8091	1/1	0.95	0.12	-1.86	74,74,74,74	0
34	MG	0	8108	1/1	0.97	0.12	-1.91	58,58,58,58	0
34	MG	0	8015	1/1	0.97	0.09	-2.01	37,37,37,37	0
38	CD	3	9204	1/1	0.98	0.06	-2.02	64,64,64,64	0
36	NA	R	9138	1/1	0.96	0.10	-2.07	67,67,67,67	0
36	NA	0	9127	1/1	0.93	0.13	-2.16	46,46,46,46	0
37	CL	K	9312	1/1	0.99	0.10	-2.20	60,60,60,60	0
36	NA	0	9144	1/1	0.98	0.10	-2.20	37,37,37,37	0
37	CL	M	9318	1/1	0.97	0.11	-2.25	45,45,45,45	0
34	MG	T	8073	1/1	0.82	0.06	-2.68	68,68,68,68	0
36	NA	0	9105	1/1	0.97	0.12	-2.72	45,45,45,45	0
37	CL	3	9304	1/1	0.93	0.12	-2.82	67,67,67,67	0
34	MG	0	8080	1/1	0.95	0.11	-2.86	43,43,43,43	0
34	MG	0	8107	1/1	0.98	0.08	-3.00	49,49,49,49	0
34	MG	3	8078	1/1	0.95	0.07	-3.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9132	1/1	0.92	0.08	-3.26	34,34,34,34	0
34	MG	0	8028	1/1	0.99	0.12	-3.31	43,43,43,43	0
36	NA	0	9167	1/1	0.96	0.08	-3.41	56,56,56,56	0
34	MG	0	8003	1/1	0.99	0.13	-3.46	36,36,36,36	0
38	CD	1	9202	1/1	1.00	0.05	-3.51	65,65,65,65	0
36	NA	A	9145	1/1	0.97	0.09	-3.52	41,41,41,41	0
34	MG	0	8007	1/1	0.97	0.10	-3.52	25,25,25,25	0
34	MG	0	8022	1/1	0.99	0.09	-3.98	39,39,39,39	0
36	NA	0	9143	1/1	0.97	0.09	-4.03	38,38,38,38	0
34	MG	0	8112	1/1	0.97	0.09	-4.10	43,43,43,43	0
34	MG	0	8084	1/1	0.95	0.10	-4.25	47,47,47,47	0
35	K	0	9002	1/1	0.98	0.10	-4.28	47,47,47,47	0
34	MG	0	8019	1/1	0.96	0.08	-4.81	35,35,35,35	0
34	MG	0	8017	1/1	0.98	0.07	-4.82	31,31,31,31	0
34	MG	0	8020	1/1	0.98	0.09	-5.13	33,33,33,33	0
34	MG	0	8002	1/1	0.94	0.10	-5.32	48,48,48,48	0
34	MG	0	8008	1/1	0.99	0.09	-5.41	31,31,31,31	0
34	MG	0	8035	1/1	0.98	0.10	-5.47	49,49,49,49	0
34	MG	0	8006	1/1	0.98	0.09	-5.61	43,43,43,43	0
36	NA	0	9103	1/1	0.99	0.08	-5.98	48,48,48,48	0
34	MG	0	8052	1/1	0.97	0.08	-6.01	51,51,51,51	0
34	MG	0	8010	1/1	0.97	0.10	-6.06	42,42,42,42	0
34	MG	0	8004	1/1	0.97	0.06	-6.35	38,38,38,38	0
34	MG	0	8067	1/1	0.94	0.09	-7.91	52,52,52,52	0
34	MG	0	8001	1/1	0.99	0.06	-7.95	37,37,37,37	0
34	MG	0	8077	1/1	0.99	0.07	-10.08	28,28,28,28	0
34	MG	0	8110	1/1	0.99	0.07	-12.28	36,36,36,36	0
36	NA	0	9152	1/1	0.80	0.73	-	76,76,76,76	0
34	MG	0	8047	1/1	0.95	0.18	-	85,85,85,85	0
34	MG	0	8098	1/1	0.97	0.12	-	46,46,46,46	0
34	MG	0	8111	1/1	0.98	0.11	-	59,59,59,59	0
34	MG	0	8115	1/1	0.97	0.20	-	54,54,54,54	0
34	MG	0	8034	1/1	0.98	0.12	-	38,38,38,38	0
37	CL	0	9314	1/1	0.98	0.13	-	57,57,57,57	0
34	MG	0	8093	1/1	0.97	0.16	-	65,65,65,65	0
34	MG	0	8083	1/1	0.97	0.13	-	45,45,45,45	0
36	NA	9	9151	1/1	0.81	0.13	-	80,80,80,80	0
36	NA	0	9141	1/1	0.91	0.12	-	52,52,52,52	0
36	NA	0	9108	1/1	0.78	0.15	-	57,57,57,57	0
36	NA	0	9158	1/1	0.95	0.38	-	122,122,122,122	0
34	MG	0	8041	1/1	0.93	0.36	-	87,87,87,87	0
36	NA	0	9116	1/1	0.96	0.16	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8045	1/1	0.86	0.30	-	87,87,87,87	0
34	MG	0	8046	1/1	0.81	0.14	-	68,68,68,68	0
36	NA	R	9137	1/1	0.92	0.07	-	47,47,47,47	0
34	MG	0	8104	1/1	0.93	0.24	-	59,59,59,59	0
36	NA	0	9154	1/1	0.98	0.16	-	38,38,38,38	0
36	NA	0	9115	1/1	0.96	0.15	-	41,41,41,41	0
34	MG	0	8099	1/1	0.94	0.11	-	55,55,55,55	0
34	MG	0	8043	1/1	0.89	0.10	-	55,55,55,55	0
36	NA	0	9107	1/1	0.80	0.29	-	55,55,55,55	0
37	CL	R	9306	1/1	0.92	0.19	-	67,67,67,67	0
36	NA	0	9175	1/1	0.79	0.81	-	61,61,61,61	0
36	NA	0	9160	1/1	0.96	0.51	-	48,48,48,48	0
36	NA	0	9130	1/1	0.98	0.22	-	49,49,49,49	0
34	MG	0	8100	1/1	0.96	0.22	-	79,79,79,79	0
36	NA	0	9119	1/1	0.95	0.13	-	45,45,45,45	0
36	NA	0	9181	1/1	0.90	0.17	-	69,69,69,69	0
34	MG	0	8072	1/1	0.96	0.27	-	56,56,56,56	0
34	MG	K	8069	1/1	0.95	0.12	-	48,48,48,48	0
37	CL	Y	9320	1/1	0.95	0.14	-	55,55,55,55	0
38	CD	O	9205	1/1	0.82	0.07	-	146,146,146,146	0
36	NA	0	9149	1/1	0.97	0.13	-	43,43,43,43	0
36	NA	0	9184	1/1	0.54	0.79	-	103,103,103,103	0
34	MG	0	8101	1/1	0.95	0.15	-	74,74,74,74	0
34	MG	0	8027	1/1	0.99	0.14	-	48,48,48,48	0
34	MG	0	8117	1/1	0.96	0.06	-	34,34,34,34	0
34	MG	0	8014	1/1	0.95	0.12	-	50,50,50,50	0
36	NA	H	9122	1/1	0.82	0.23	-	75,75,75,75	0
34	MG	0	8030	1/1	0.98	0.15	-	36,36,36,36	0
37	CL	Y	9317	1/1	0.95	0.13	-	72,72,72,72	0
34	MG	0	8106	1/1	0.88	0.11	-	57,57,57,57	0
34	MG	0	8082	1/1	0.86	0.23	-	72,72,72,72	0
36	NA	0	9179	1/1	0.97	0.18	-	72,72,72,72	0
34	MG	0	8031	1/1	0.99	0.08	-	29,29,29,29	0
34	MG	0	8076	1/1	0.89	0.10	-	68,68,68,68	0
36	NA	0	9170	1/1	0.95	0.70	-	85,85,85,85	0
36	NA	0	9134	1/1	0.98	0.07	-	46,46,46,46	0
34	MG	0	8049	1/1	0.88	0.29	-	93,93,93,93	0
34	MG	0	8089	1/1	0.91	0.07	-	65,65,65,65	0
34	MG	0	8103	1/1	0.95	0.12	-	66,66,66,66	0
36	NA	0	9111	1/1	0.92	0.18	-	71,71,71,71	0
34	MG	A	8066	1/1	0.97	0.07	-	67,67,67,67	0
34	MG	0	8009	1/1	0.99	0.13	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9113	1/1	0.96	0.19	-	71,71,71,71	0
34	MG	0	8071	1/1	0.98	0.10	-	62,62,62,62	0
34	MG	0	8092	1/1	0.88	0.55	-	102,102,102,102	0
34	MG	0	8029	1/1	0.98	0.17	-	39,39,39,39	0
34	MG	0	8039	1/1	0.97	0.12	-	50,50,50,50	0
34	MG	0	8023	1/1	0.99	0.22	-	53,53,53,53	0
34	MG	0	8040	1/1	0.96	0.15	-	55,55,55,55	0
34	MG	0	8036	1/1	0.99	0.16	-	32,32,32,32	0
34	MG	0	8081	1/1	0.98	0.15	-	59,59,59,59	0
37	CL	A	9309	1/1	0.97	0.23	-	72,72,72,72	0
34	MG	0	8094	1/1	0.95	0.14	-	80,80,80,80	0
34	MG	0	8116	1/1	0.96	0.30	-	67,67,67,67	0
34	MG	0	8051	1/1	0.94	0.18	-	87,87,87,87	0
34	MG	0	8048	1/1	0.99	0.13	-	63,63,63,63	0
37	CL	0	9313	1/1	0.98	0.14	-	64,64,64,64	0
34	MG	0	8068	1/1	0.95	0.04	-	75,75,75,75	0
34	MG	0	8062	1/1	0.94	0.16	-	64,64,64,64	0
37	CL	J	9302	1/1	0.90	0.16	-	86,86,86,86	0
34	MG	0	8024	1/1	0.82	0.14	-	61,61,61,61	0
34	MG	0	8113	1/1	0.75	0.21	-	56,56,56,56	0
34	MG	0	8102	1/1	0.91	0.09	-	64,64,64,64	0
36	NA	0	9128	1/1	0.94	0.12	-	43,43,43,43	0
36	NA	0	9163	1/1	0.86	0.34	-	75,75,75,75	0
34	MG	0	8061	1/1	0.99	0.12	-	36,36,36,36	0
36	NA	0	9155	1/1	0.84	0.51	-	80,80,80,80	0
36	NA	0	9106	1/1	0.95	0.75	-	49,49,49,49	0
36	NA	0	9118	1/1	0.98	0.17	-	54,54,54,54	0
34	MG	0	8085	1/1	0.83	0.14	-	68,68,68,68	0
36	NA	C	9104	1/1	0.91	0.09	-	43,43,43,43	0
34	MG	0	8025	1/1	0.99	0.12	-	45,45,45,45	0
34	MG	0	8016	1/1	0.94	0.19	-	40,40,40,40	0
34	MG	0	8079	1/1	0.99	0.15	-	34,34,34,34	0
36	NA	0	9185	1/1	0.81	0.55	-	61,61,61,61	0
36	NA	0	9159	1/1	0.92	0.36	-	62,62,62,62	0
36	NA	0	9124	1/1	0.94	0.16	-	69,69,69,69	0
34	MG	0	8026	1/1	0.98	0.14	-	31,31,31,31	0
34	MG	0	8090	1/1	0.84	0.41	-	77,77,77,77	0
34	MG	0	8087	1/1	0.82	0.13	-	53,53,53,53	0
36	NA	S	9112	1/1	0.77	0.36	-	74,74,74,74	0
34	MG	0	8042	1/1	0.96	0.10	-	47,47,47,47	0
34	MG	0	8063	1/1	0.95	0.08	-	68,68,68,68	0
34	MG	0	8075	1/1	0.96	0.10	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	CL	J	9301	1/1	0.93	0.20	-	69,69,69,69	0
36	NA	0	9101	1/1	0.94	0.15	-	47,47,47,47	0
34	MG	0	8011	1/1	1.00	0.16	-	29,29,29,29	0
34	MG	0	8114	1/1	0.74	0.24	-	62,62,62,62	0
34	MG	0	8088	1/1	0.90	0.05	-	41,41,41,41	0
36	NA	0	9157	1/1	0.96	0.05	-	75,75,75,75	0
34	MG	0	8059	1/1	0.98	0.08	-	52,52,52,52	0
34	MG	0	8050	1/1	0.91	0.09	-	86,86,86,86	0
34	MG	0	8037	1/1	0.98	0.08	-	47,47,47,47	0
34	MG	0	8097	1/1	0.93	0.12	-	46,46,46,46	0
36	NA	0	9136	1/1	0.91	0.10	-	68,68,68,68	0
36	NA	0	9142	1/1	0.91	0.21	-	45,45,45,45	0
37	CL	0	9322	1/1	0.93	0.76	-	90,90,90,90	0
34	MG	9	8095	1/1	0.96	0.09	-	73,73,73,73	0
37	CL	0	9303	1/1	0.95	0.19	-	63,63,63,63	0
37	CL	0	9311	1/1	0.97	0.14	-	58,58,58,58	0
34	MG	0	8005	1/1	0.99	0.10	-	38,38,38,38	0
37	CL	N	9307	1/1	0.90	0.23	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.