



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:05 PM UTC

PDB ID : 1VQN / pdb_00001vqn
Title : The structure of CC-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 : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

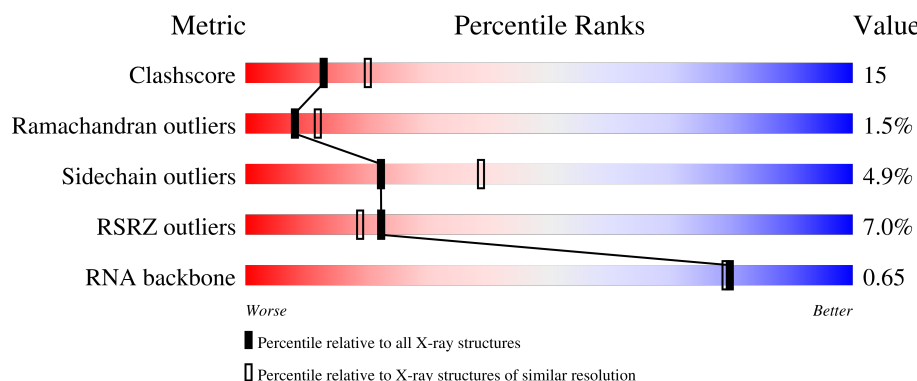
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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

Mol	Chain	Length	Quality of chain
1	0	2922	2% 62% 27% 6%
2	9	122	4% 57% 32% 11%
3	4	4	25% 50% 25%
4	5	6	17% 17% 67% 17%
5	A	240	6% 57% 36% 5%

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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
36	NA	0	9122	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 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*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- 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	S	0	0	0
			93	53	15	22	2	1			

- 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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	9	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	Y	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	9	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	J	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	S	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	A	1	Total 1	Cl 1	0	0
37	B	1	Total 1	Cl 1	0	0
37	J	3	Total 3	Cl 3	0	0
37	L	1	Total 1	Cl 1	0	0
37	M	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	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	9	3	Total 3	Sr 3	0	0
38	A	3	Total 3	Sr 3	0	0
38	B	2	Total 2	Sr 2	0	0
38	F	1	Total 1	Sr 1	0	0
38	H	1	Total 1	Sr 1	0	0
38	L	1	Total 1	Sr 1	0	0
38	R	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	1	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

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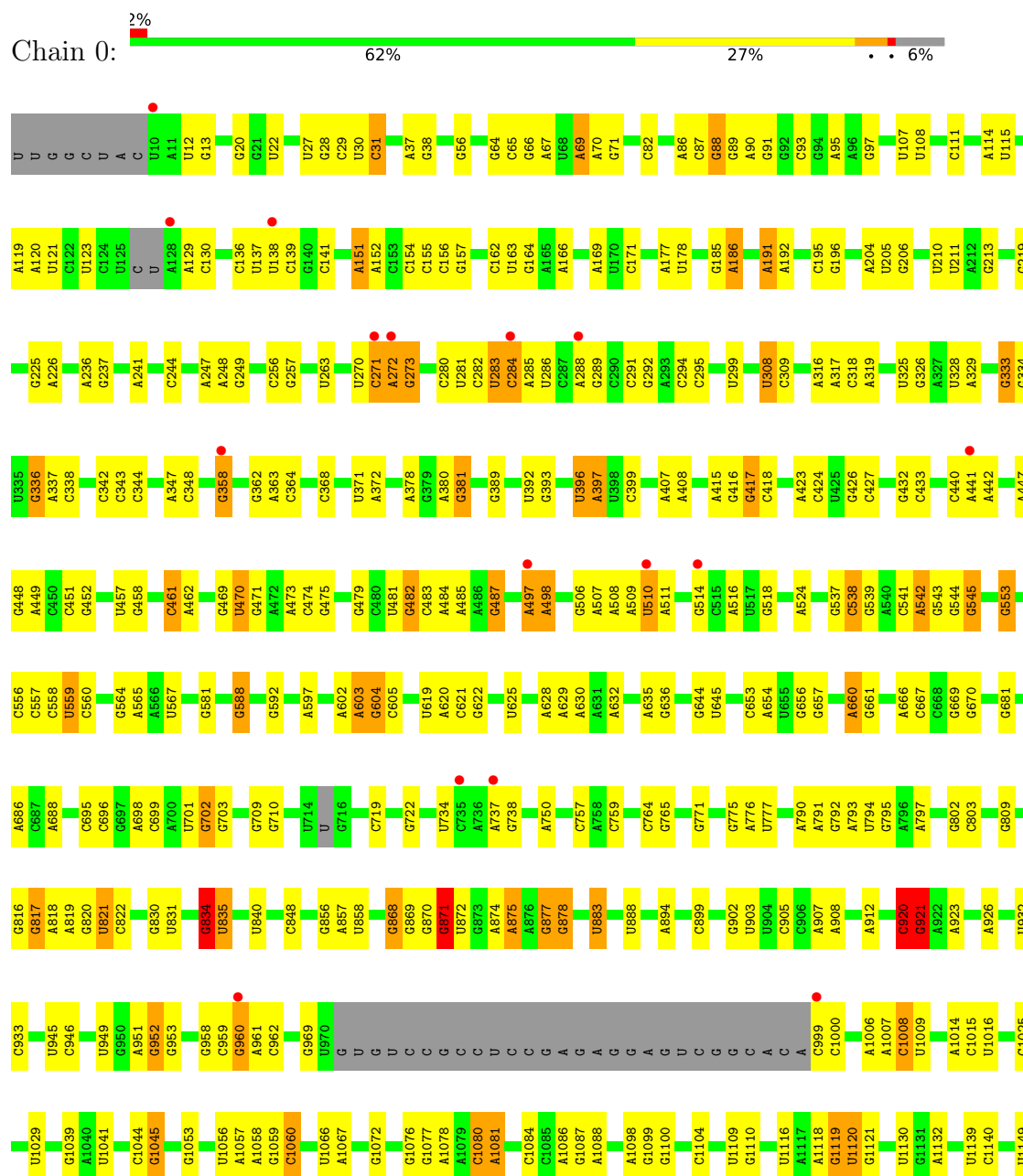
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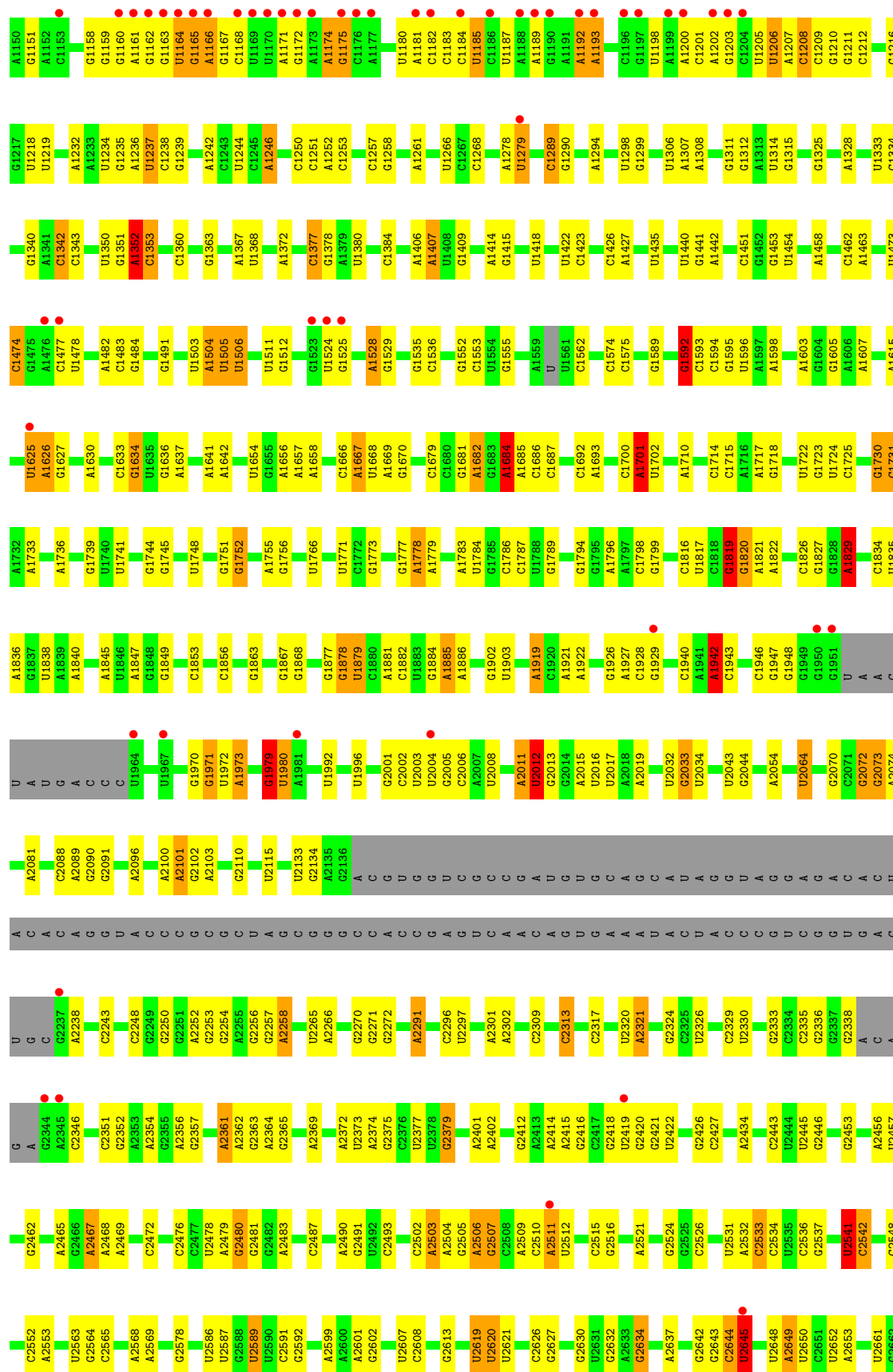
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

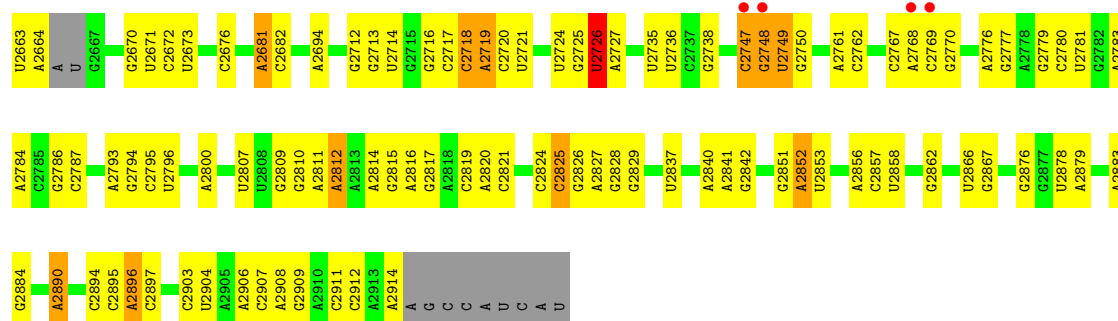
3 Residue-property plots

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

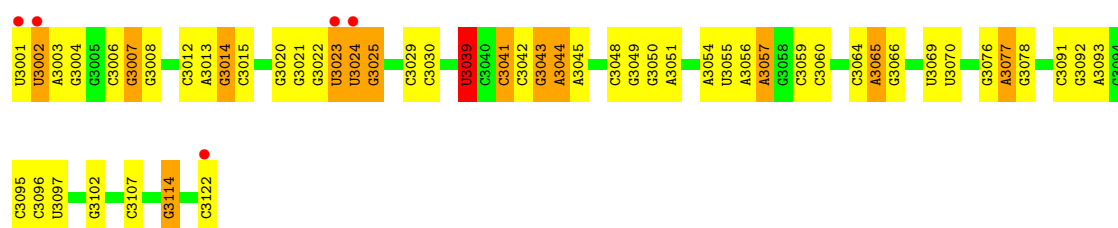
- Molecule 1: 23S ribosomal rna



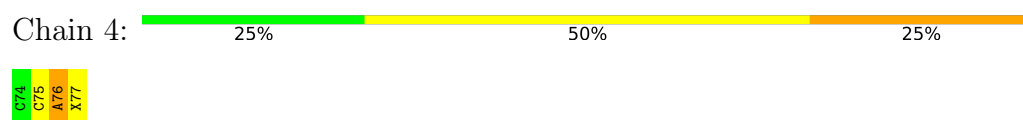




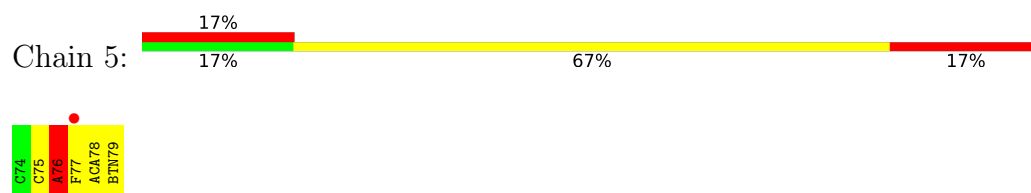
• Molecule 2: 5S ribosomal RNA



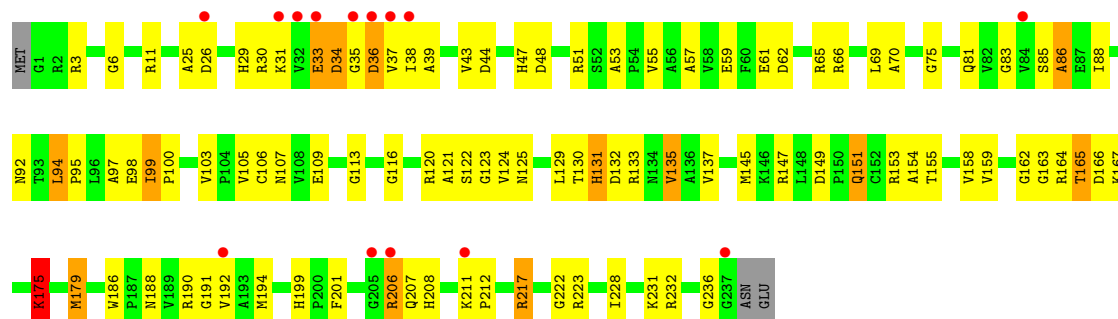
• Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



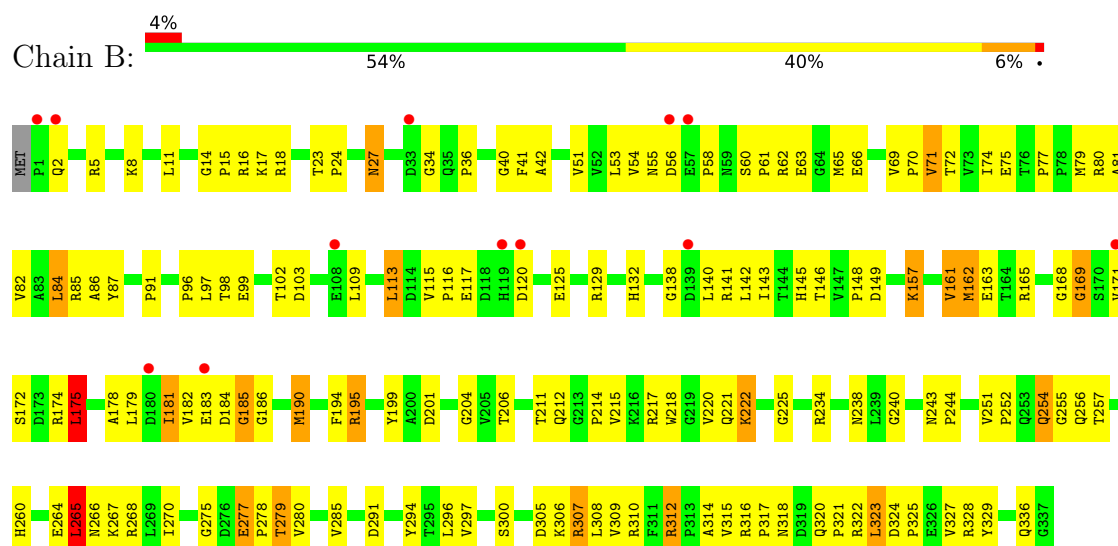
• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'



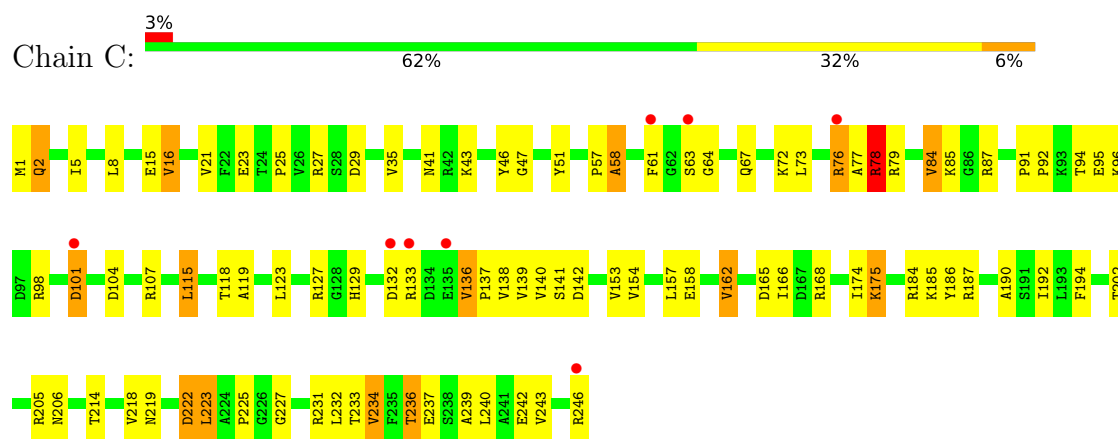
• Molecule 5: 50S ribosomal protein L2P



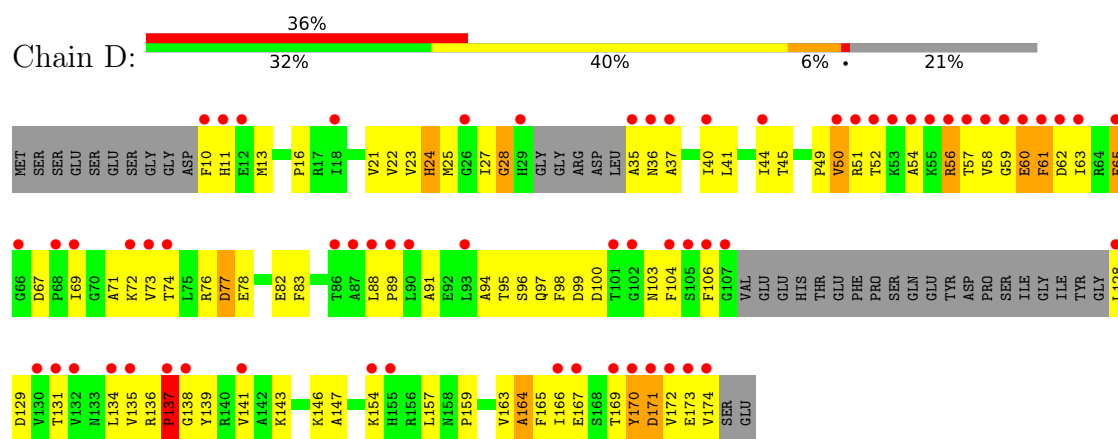
- Molecule 6: 50S ribosomal protein L3P



- Molecule 7: 50S ribosomal protein L4E

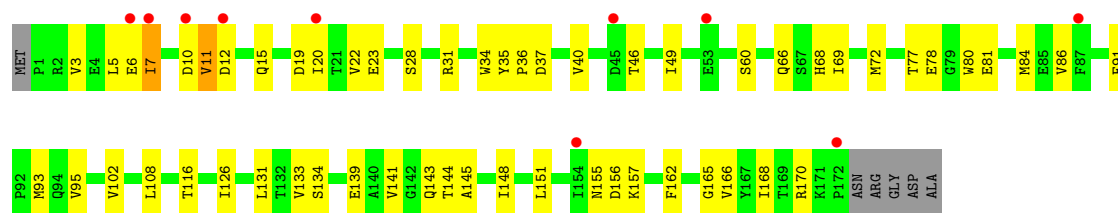


- Molecule 8: 50S ribosomal protein L5P

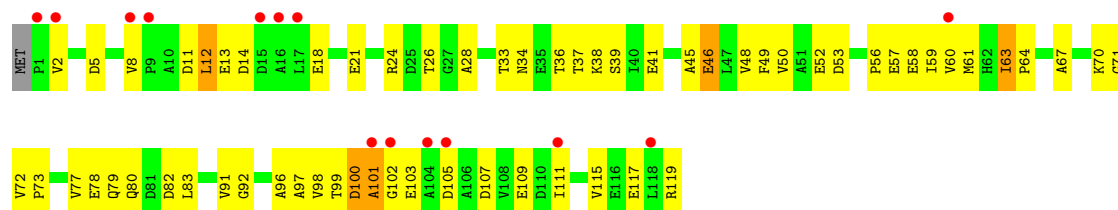


- Molecule 9: 50S ribosomal protein L6P

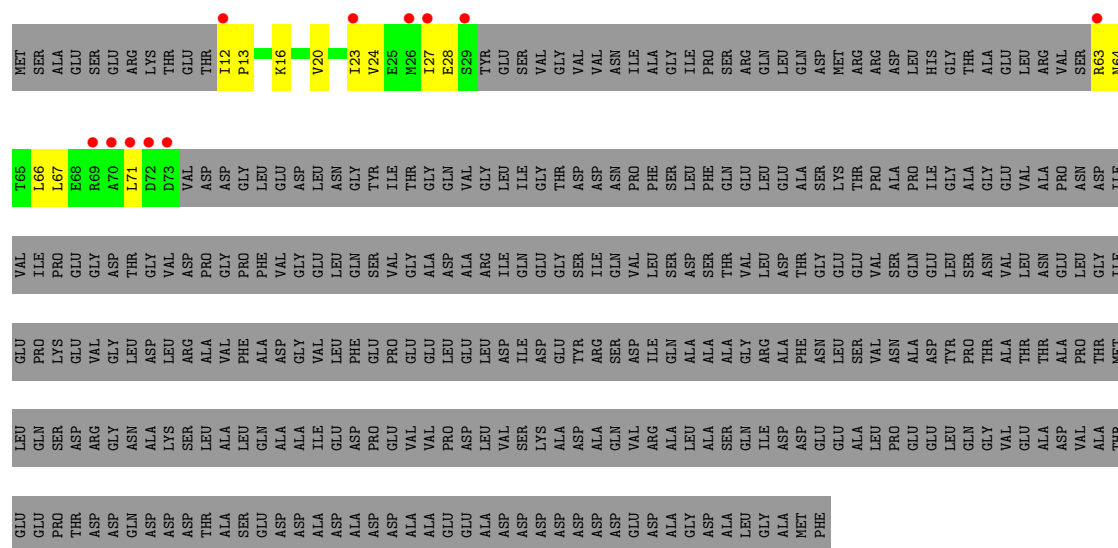




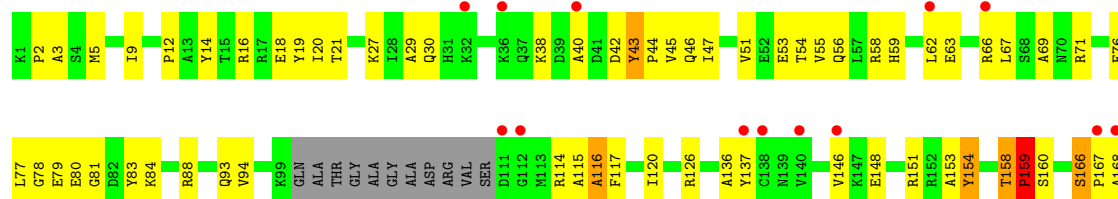
• Molecule 10: 50S ribosomal protein L7AE



• Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

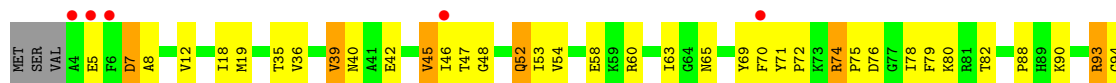


• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

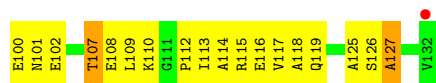
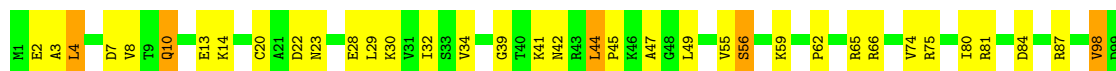




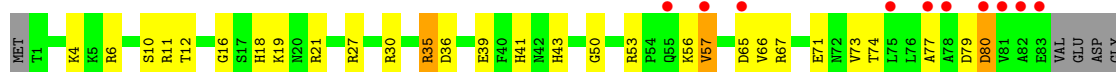
• Molecule 13: 50S ribosomal protein L13P



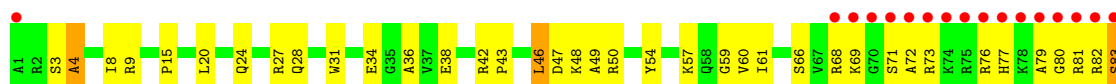
• Molecule 14: 50S ribosomal protein L14P



• Molecule 15: 50S ribosomal protein L15P

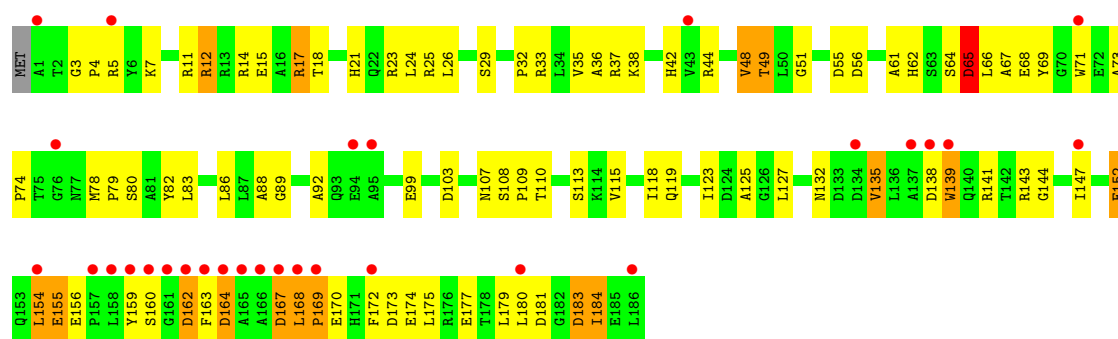


• Molecule 16: 50S Ribosomal Protein L15E

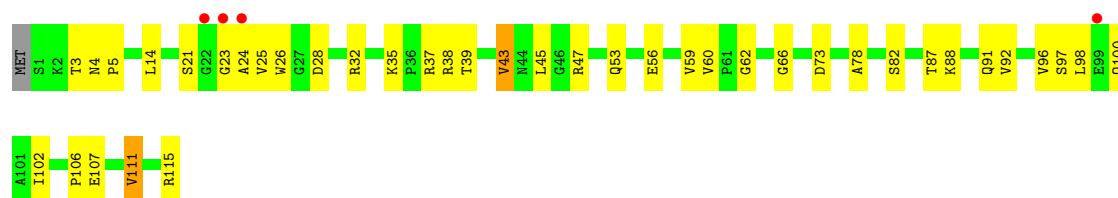


• Molecule 17: 50S ribosomal protein L18P

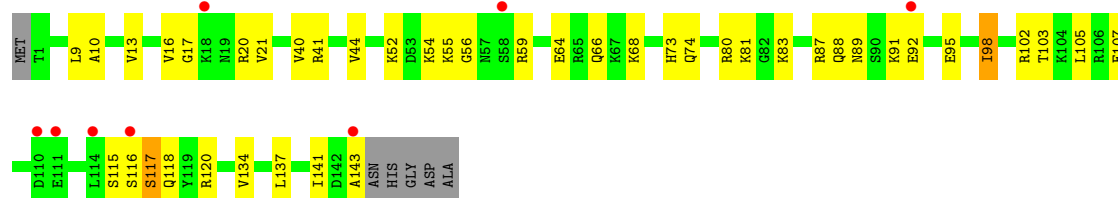




- Molecule 18: 50S ribosomal protein L18e



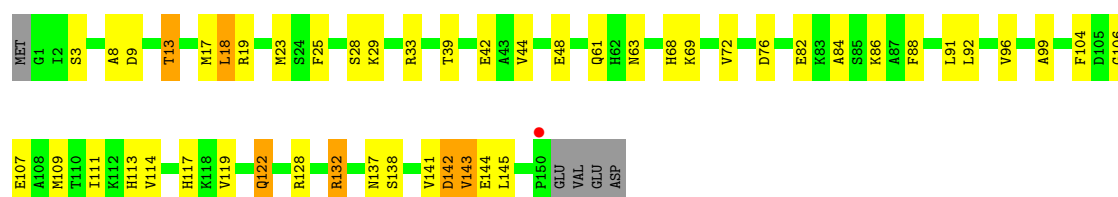
- Molecule 19: 50S ribosomal protein L19E



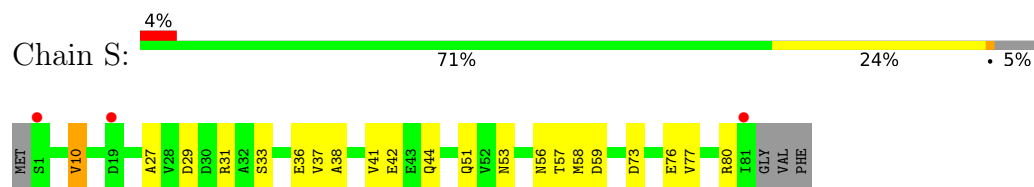
- Molecule 20: 50S ribosomal protein L21e



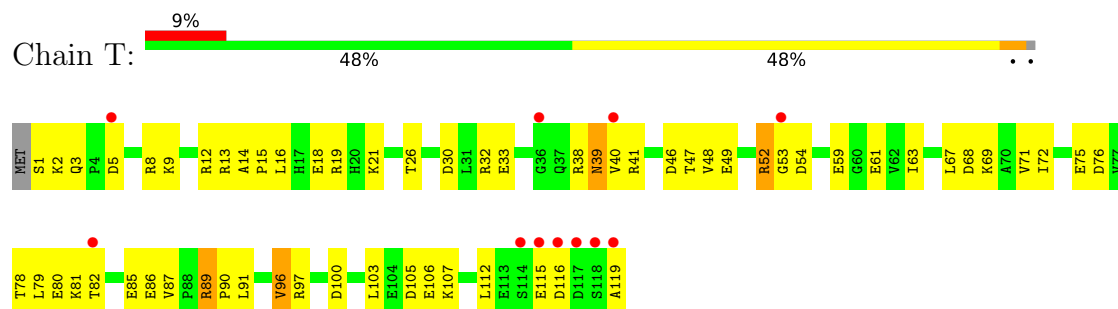
- Molecule 21: 50S ribosomal protein L22P



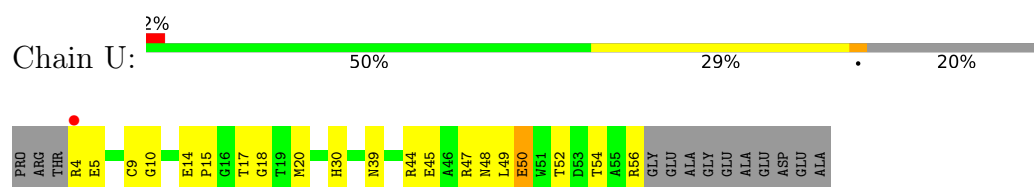
- Molecule 22: 50S ribosomal protein L23P



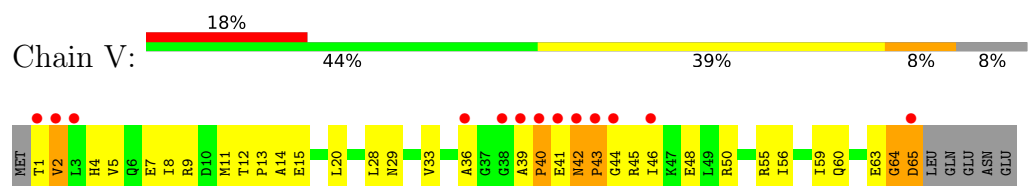
- Molecule 23: 50S ribosomal protein L24P



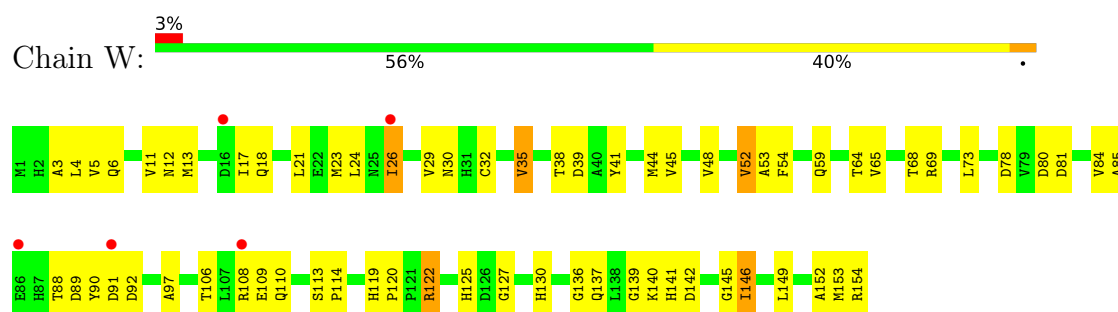
- Molecule 24: 50S ribosomal protein L24E



- Molecule 25: 50S ribosomal protein L29P

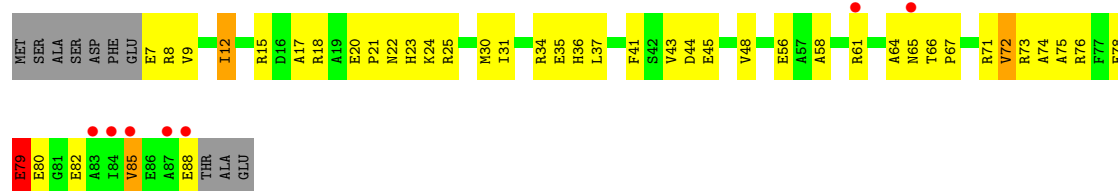


- Molecule 26: 50S ribosomal protein L30P

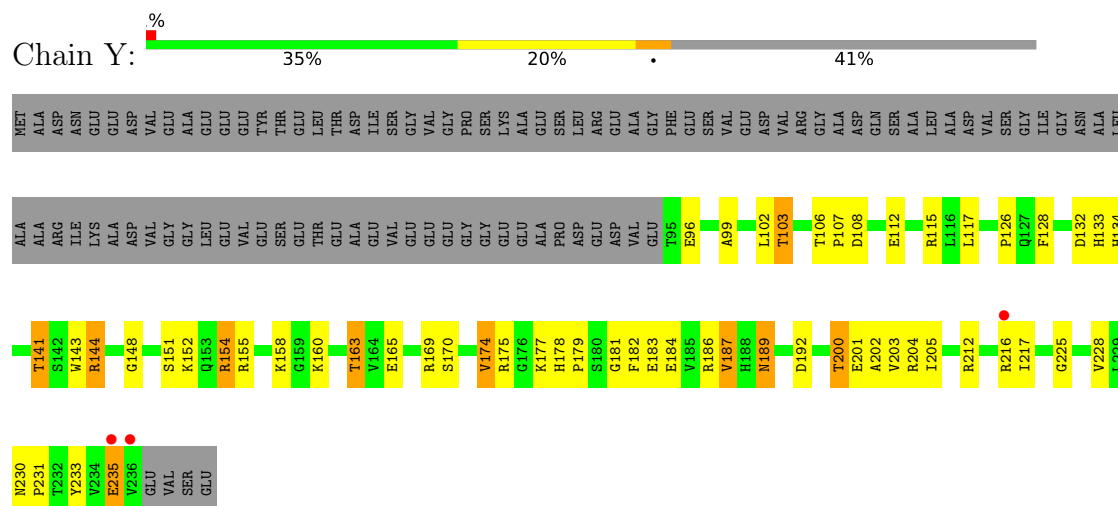


- Molecule 27: 50S ribosomal protein L31e

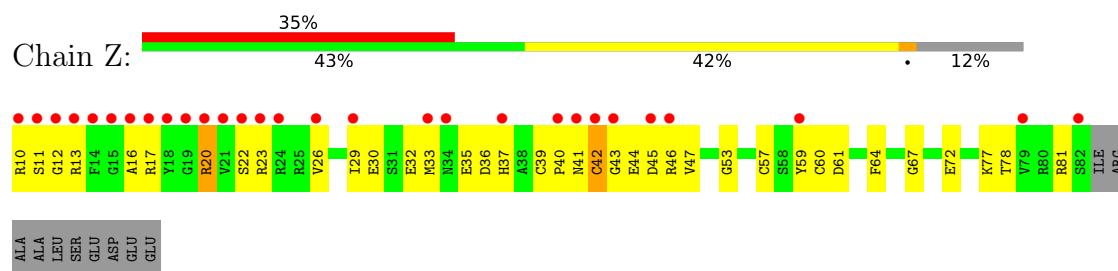




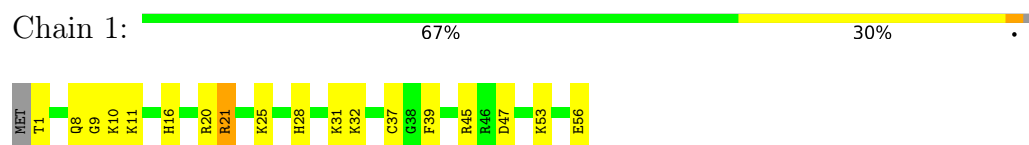
• Molecule 28: 50S ribosomal protein L32E



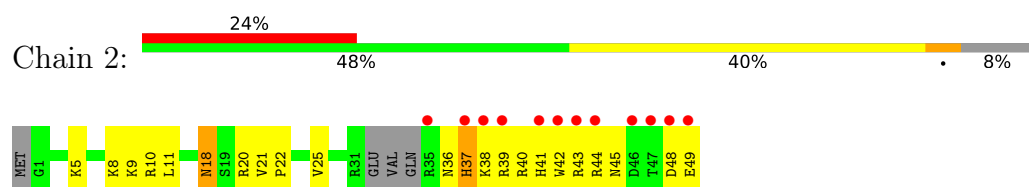
• Molecule 29: 50S ribosomal protein L37Ae



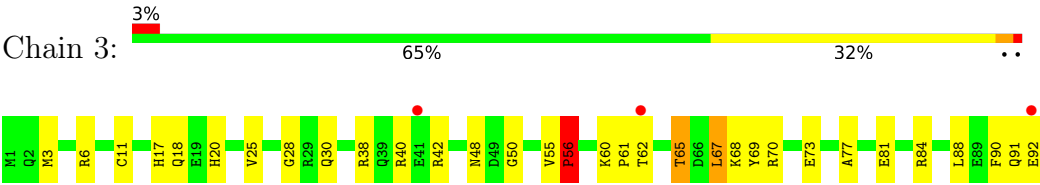
• Molecule 30: 50S ribosomal protein L37e



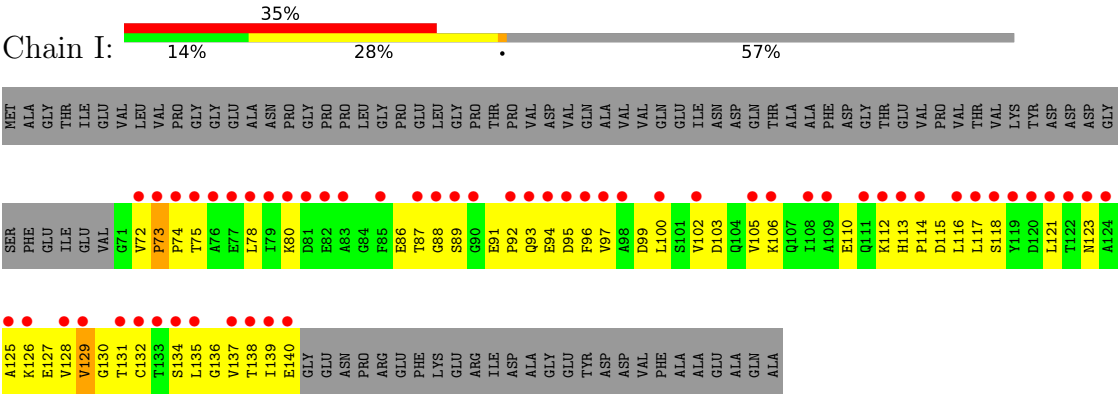
• Molecule 31: 50S ribosomal protein L39e



• 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	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.39	1/65959 (0.0%)	0.62	26/102870 (0.0%)
2	9	0.38	0/2905	0.60	1/4528 (0.0%)
3	4	0.39	0/40	0.83	0/60
4	5	0.45	0/76	1.00	1/112 (0.9%)
5	A	0.42	0/1786	1.00	9/2408 (0.4%)
6	B	0.42	0/2690	0.99	12/3652 (0.3%)
7	C	0.46	0/1884	0.98	6/2551 (0.2%)
8	D	0.34	0/1111	0.85	2/1498 (0.1%)
9	E	0.38	0/1382	0.87	2/1880 (0.1%)
10	F	0.39	0/901	0.86	3/1224 (0.2%)
11	G	0.36	0/241	0.80	0/324
12	H	0.38	0/1287	0.95	6/1725 (0.3%)
13	J	0.41	0/1136	0.97	4/1530 (0.3%)
14	K	0.43	0/1001	1.01	2/1347 (0.1%)
15	L	0.38	0/1130	0.97	2/1509 (0.1%)
16	M	0.42	0/1584	0.89	2/2119 (0.1%)
17	N	0.36	0/1474	1.02	10/1999 (0.5%)
18	O	0.41	0/874	0.91	3/1181 (0.3%)
19	P	0.40	0/1147	0.87	0/1528
20	Q	0.43	0/749	1.00	2/1005 (0.2%)
21	R	0.45	0/1172	0.97	7/1578 (0.4%)
22	S	0.37	0/648	0.87	1/875 (0.1%)
23	T	0.38	0/958	0.95	4/1289 (0.3%)
24	U	0.40	0/417	0.88	1/562 (0.2%)
25	V	0.35	0/502	0.94	3/675 (0.4%)
26	W	0.47	1/1219 (0.1%)	0.96	4/1655 (0.2%)
27	X	0.43	0/664	0.95	4/895 (0.4%)
28	Y	0.46	0/1146	0.99	6/1536 (0.4%)
29	Z	0.35	0/589	0.91	0/787
30	1	0.48	0/438	0.91	1/578 (0.2%)
31	2	0.40	0/401	0.81	0/529
32	3	0.38	0/771	0.85	2/1024 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.35	0/526	0.87	2/716 (0.3%)
All	All	0.39	2/98808 (0.0%)	0.72	128/147749 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	55
2	9	0	1
All	All	0	56

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	35	VAL	CA-CB	5.50	1.58	1.54
1	0	2619	UR3	O3'-P	5.14	1.61	1.56

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	163	PHE	N-CA-C	-10.90	100.11	113.41
6	B	323	LEU	N-CA-C	8.16	120.85	110.24
6	B	175	LEU	N-CA-C	-8.06	102.57	111.36
20	Q	17	LYS	N-CA-C	-8.05	97.67	109.50
1	0	1352	A	C2'-C3'-O3'	7.95	121.43	109.50
21	R	141	VAL	N-CA-C	7.70	118.89	108.11
6	B	157	LYS	N-CA-C	-7.63	104.46	114.31
1	0	1942	A	C5'-C4'-C3'	7.58	127.37	116.00
15	L	57	VAL	N-CA-C	-7.45	105.58	112.43
5	A	70	ALA	N-CA-C	7.41	118.99	109.65
12	H	160	SER	N-CA-C	-7.21	100.82	110.55
22	S	27	ALA	N-CA-C	-7.17	97.56	108.96
1	0	1592	G	N9-C1'-C2'	7.12	122.67	112.00
13	J	107	ASN	CA-C-N	7.02	127.17	119.87
13	J	107	ASN	C-N-CA	7.02	127.17	119.87
5	A	222	GLY	N-CA-C	-6.97	106.12	113.58
6	B	222	LYS	N-CA-C	-6.91	99.71	110.42
7	C	205	ARG	N-CA-C	6.87	119.64	111.33
9	E	11	VAL	N-CA-C	6.85	119.58	108.97
1	0	1819	G	C5'-C4'-C3'	6.83	126.24	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	135	VAL	N-CA-C	-6.79	106.03	113.43
7	C	192	ILE	N-CA-C	6.74	117.78	108.89
1	0	883	U	N1-C1'-C2'	6.71	122.06	112.00
28	Y	143	TRP	N-CA-C	6.67	120.15	110.28
1	0	2726	U	N1-C1'-C2'	6.65	121.97	112.00
21	R	122	GLN	N-CA-C	-6.60	99.15	109.25
16	M	4	ALA	N-CA-C	-6.54	104.23	111.36
13	J	36	VAL	N-CA-C	6.54	118.01	108.53
2	9	3039	U	N1-C1'-C2'	6.49	121.73	112.00
17	N	51	GLY	CA-C-N	6.44	126.20	119.05
17	N	51	GLY	C-N-CA	6.44	126.20	119.05
27	X	12	ILE	N-CA-C	6.43	114.97	107.77
21	R	137	ASN	N-CA-C	6.42	120.37	110.42
1	0	871	G	C5'-C4'-O4'	-6.42	100.17	109.80
1	0	920	C	C2'-C3'-O3'	-6.30	104.24	113.70
17	N	42	HIS	N-CA-C	6.27	119.40	109.81
1	0	1504	A	N9-C1'-C2'	6.23	121.34	112.00
15	L	145	LEU	N-CA-C	-6.21	104.51	111.28
1	0	1120	U	C5'-C4'-C3'	-6.18	106.73	116.00
1	0	2541	U	C2'-C3'-O3'	6.14	122.91	113.70
26	W	35	VAL	N-CA-C	6.10	114.87	107.61
8	D	170	TYR	N-CA-C	6.09	120.27	111.56
5	A	135	VAL	N-CA-C	6.07	116.58	108.27
17	N	169	PRO	N-CA-C	-6.06	106.28	113.86
1	0	2291	A	N9-C1'-C2'	6.06	121.09	112.00
27	X	17	ALA	N-CA-C	-6.05	105.15	112.54
16	M	8	ILE	N-CA-C	-6.00	104.66	110.42
23	T	16	LEU	N-CA-C	5.97	118.27	111.11
27	X	79	GLU	N-CA-C	5.95	117.77	111.28
7	C	78	ARG	N-CA-C	5.95	117.28	108.60
32	3	67	LEU	N-CA-C	5.93	118.72	109.52
1	0	1979	G	C2'-C3'-O3'	5.92	122.58	113.70
7	C	175	LYS	N-CA-C	5.91	118.39	110.35
10	F	63	ILE	CB-CA-C	-5.91	108.08	113.70
6	B	161	VAL	N-CA-C	5.89	116.41	108.17
28	Y	183	GLU	N-CA-C	-5.89	99.65	109.24
5	A	228	ILE	N-CA-C	5.87	116.85	108.93
24	U	50	GLU	N-CA-C	5.86	118.42	111.33
6	B	265	LEU	N-CA-C	5.86	118.46	110.55
18	O	82	SER	N-CA-C	-5.83	102.83	110.53
1	0	2301	A	N9-C1'-C2'	5.77	120.66	112.00
14	K	127	ALA	N-CA-C	-5.74	105.92	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	100	ASP	N-CA-C	-5.73	106.63	113.97
1	0	1701	A	C5'-C4'-C3'	5.72	123.78	115.20
18	O	43	VAL	N-CA-C	5.72	116.82	108.53
1	0	921	G	N9-C1'-C2'	5.71	120.57	112.00
1	0	1261	A	N9-C1'-C2'	5.71	120.57	112.00
14	K	8	VAL	N-CA-C	5.69	116.67	108.48
33	I	91	GLU	CA-C-N	5.67	125.57	119.85
33	I	91	GLU	C-N-CA	5.67	125.57	119.85
23	T	52	ARG	N-CA-C	5.64	122.82	110.80
1	0	1684	A	C2'-C3'-O3'	5.63	117.95	109.50
1	0	206	G	C5'-C4'-C3'	-5.62	107.58	116.00
21	R	3	SER	N-CA-C	-5.61	100.64	109.50
28	Y	230	ASN	CA-C-N	5.59	125.79	120.31
28	Y	230	ASN	C-N-CA	5.59	125.79	120.31
23	T	3	GLN	CA-C-N	5.58	125.69	119.32
23	T	3	GLN	C-N-CA	5.58	125.69	119.32
5	A	188	ASN	N-CA-C	5.57	117.61	108.52
1	0	1615	A	C5'-C4'-C3'	5.55	124.33	116.00
12	H	159	PRO	N-CA-C	5.53	119.71	111.41
1	0	874	A	C4'-C3'-O3'	-5.52	104.73	113.00
27	X	22	ASN	N-CA-C	5.50	117.99	111.33
5	A	133	ARG	N-CA-C	-5.50	106.57	113.72
1	0	834	G	C2'-C3'-O3'	-5.46	105.52	113.70
5	A	25	ALA	N-CA-C	5.38	117.03	108.79
30	1	21	ARG	N-CA-C	5.38	117.97	111.40
25	V	42	ASN	CA-C-N	5.38	126.56	119.84
25	V	42	ASN	C-N-CA	5.38	126.56	119.84
28	Y	202	ALA	N-CA-C	-5.37	101.37	109.85
6	B	23	THR	N-CA-C	-5.35	102.91	109.65
1	0	2012	U	N1-C1'-C2'	5.34	120.01	112.00
1	0	389	G	C5'-C4'-C3'	-5.33	108.00	116.00
4	5	76	A	C2'-C3'-O3'	5.33	117.50	109.50
1	0	2467	A	O4'-C4'-C3'	-5.33	100.78	106.10
6	B	143	ILE	N-CA-C	-5.31	101.88	108.89
32	3	81	GLU	N-CA-C	-5.31	103.48	110.43
5	A	99	ILE	N-CA-C	5.28	113.17	108.63
28	Y	103	THR	N-CA-C	5.28	117.03	111.28
6	B	117	GLU	N-CA-C	-5.23	107.45	113.88
20	Q	49	ASN	N-CA-C	5.22	118.25	110.52
13	J	112	ASP	N-CA-C	-5.20	101.79	110.17
6	B	266	ASN	N-CA-C	5.20	118.50	111.17
12	H	43	TYR	CA-C-N	5.19	124.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	43	TYR	C-N-CA	5.19	124.80	119.56
5	A	175	LYS	N-CA-C	-5.18	105.53	111.07
1	0	2313	C	C5'-C4'-C3'	5.17	123.75	116.00
6	B	120	ASP	CA-C-N	5.16	124.66	119.19
6	B	120	ASP	C-N-CA	5.16	124.66	119.19
17	N	48	VAL	N-CA-C	5.15	116.00	108.53
9	E	37	ASP	N-CA-C	5.13	118.80	112.24
21	R	63	ASN	N-CA-C	5.12	119.49	112.88
7	C	84	VAL	N-CA-C	-5.11	102.28	109.63
21	R	18	LEU	N-CA-C	-5.10	101.83	109.95
26	W	113	SER	CA-C-N	5.10	124.82	119.82
26	W	113	SER	C-N-CA	5.10	124.82	119.82
25	V	64	GLY	N-CA-C	-5.09	107.66	116.01
26	W	52	VAL	N-CA-C	5.09	114.74	108.53
12	H	158	THR	N-CA-C	5.08	121.03	109.81
12	H	116	ALA	N-CA-C	5.07	119.47	113.28
10	F	8	VAL	CA-C-N	5.06	124.97	119.76
10	F	8	VAL	C-N-CA	5.06	124.97	119.76
17	N	3	GLY	CA-C-N	5.06	124.84	119.28
17	N	3	GLY	C-N-CA	5.06	124.84	119.28
18	O	66	GLY	N-CA-C	5.05	125.14	113.18
7	C	41	ASN	N-CA-C	5.04	118.69	112.54
21	R	142	ASP	N-CA-C	-5.01	101.98	109.95
17	N	168	LEU	N-CA-C	5.00	117.98	108.12

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1458	A	Sidechain
1	0	1491	G	Sidechain
1	0	1592	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1885	A	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	2115	U	Sidechain
1	0	22	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2645	U	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain
1	0	2726	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	507	A	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain

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Mol	Chain	Res	Type	Group
2	9	3039	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	769	0
2	9	2600	0	1326	59	0
3	4	72	0	47	1	0
4	5	93	0	63	3	0
5	A	1753	0	1765	117	0
6	B	2625	0	2532	152	0
7	C	1859	0	1816	100	0
8	D	1094	0	1085	100	0
9	E	1357	0	1266	53	0
10	F	890	0	843	58	0
11	G	240	0	231	12	0
12	H	1266	0	1268	66	0
13	J	1120	0	1098	71	0
14	K	992	0	1031	59	0
15	L	1118	0	1076	65	0
16	M	1560	0	1568	76	0
17	N	1445	0	1401	92	0
18	O	865	0	873	42	0
19	P	1136	0	1123	43	0
20	Q	735	0	728	23	0
21	R	1149	0	1122	44	0
22	S	641	0	605	19	0
23	T	950	0	923	54	0
24	U	410	0	364	22	0
25	V	499	0	511	45	0
26	W	1196	0	1137	87	0
27	X	654	0	653	43	0
28	Y	1130	0	1133	61	0
29	Z	578	0	539	37	0
30	1	431	0	426	29	0
31	2	396	0	413	33	0
32	3	755	0	728	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	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	66	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	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	1	0
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	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	4	0
40	K	61	0	0	3	0
40	L	83	0	0	13	0
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	5	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60006	2277	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 15.

All (2277) 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.73	1.04
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.39	1.03
13:J:93:ARG:HB3	13:J:93:ARG:HH11	1.21	1.02
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.38	1.02
8:D:25:MET:HE2	8:D:41:LEU:HG	1.40	1.01
1:O:871:G:C8	1:O:871:G:H5'	1.96	0.99
22:S:51:GLN:HE21	22:S:53:ASN:HD21	1.05	0.99
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.46	0.98
7:C:236:THR:HG22	7:C:239:ALA:H	1.24	0.98
1:O:156:C:H5''	16:M:171:ARG:HD3	1.46	0.97
26:W:149:LEU:HG	26:W:153:MET:HE2	1.45	0.97
5:A:211:LYS:HG2	5:A:212:PRO:HD2	1.45	0.96
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.80	0.96
10:F:91:VAL:HG12	10:F:92:GLY:H	1.26	0.96
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.46	0.96
7:C:78:ARG:HH11	7:C:78:ARG:HG3	1.30	0.96
1:O:1771:U:H5'	29:Z:20:ARG:HH21	1.31	0.95
1:O:871:G:H5'	1:O:871:G:H8	1.28	0.95
1:O:870:G:H2'	1:O:871:G:H5''	1.48	0.95
28:Y:235:GLU:CD	28:Y:235:GLU:H	1.75	0.95
1:O:542:A:H5'	1:O:542:A:H8	1.34	0.93
13:J:19:MET:HE3	13:J:132:LEU:HD11	1.50	0.93
14:K:10:GLN:HE21	14:K:10:GLN:H	0.93	0.92
1:O:1242:A:H5'	13:J:82:THR:HG23	1.50	0.92
17:N:11:ARG:HG3	17:N:14:ARG:HH12	1.34	0.92
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.52	0.91
1:O:1372:A:H3'	40:O:7638:HOH:O	1.70	0.91
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.53	0.91
5:A:81:GLN:HB2	5:A:92:ASN:ND2	1.86	0.90
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.53	0.90
1:O:2812:A:H2	1:O:2814:A:H62	1.19	0.90
17:N:144:GLY:O	17:N:147:ILE:HG22	1.70	0.90
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.54	0.90
6:B:238:ASN:HD22	6:B:240:GLY:H	1.18	0.90
31:2:18:ASN:HD21	31:2:40:ARG:H	1.17	0.89
14:K:74:VAL:HG13	14:K:113:ILE:HG23	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:307:ARG:HH11	6:B:307:ARG:HG3	1.36	0.89
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.37	0.89
7:C:1:MET:HG2	7:C:2:GLN:H	1.38	0.89
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.55	0.89
8:D:58:VAL:HB	8:D:62:ASP:HB3	1.54	0.89
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.36	0.88
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.37	0.88
1:O:2717:C:H2'	1:O:2718:C:H5''	1.53	0.88
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.54	0.88
1:O:289:G:H22	1:O:363:A:H2	1.21	0.87
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.73	0.87
19:P:115:SER:H	19:P:118:GLN:HE21	1.20	0.87
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.09	0.87
1:O:541:C:H2'	1:O:542:A:H5''	1.57	0.86
17:N:49:THR:HG22	17:N:56:ASP:HB2	1.55	0.86
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.55	0.86
17:N:113:SER:HB2	40:N:9354:HOH:O	1.75	0.86
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.56	0.85
7:C:5:ILE:HD11	7:C:16:VAL:HG22	1.57	0.85
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.07	0.85
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.57	0.85
1:O:1835:U:H5	1:O:1840:A:N7	1.75	0.85
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.25	0.85
9:E:15:GLN:HG2	9:E:19:ASP:O	1.77	0.85
8:D:172:VAL:HG12	8:D:173:GLU:H	1.40	0.85
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.59	0.84
16:M:99:ARG:HH21	16:M:170:ASN:HD22	1.25	0.84
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.12	0.84
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.58	0.84
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.58	0.84
14:K:10:GLN:HE21	14:K:10:GLN:N	1.74	0.84
15:L:80:ASP:HB2	15:L:90:ARG:O	1.78	0.83
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.94	0.83
19:P:115:SER:OG	19:P:118:GLN:HG3	1.78	0.83
1:O:2506:A:O2'	1:O:2507:G:H8	1.62	0.83
5:A:192:VAL:HG22	40:A:9617:HOH:O	1.78	0.83
26:W:122:ARG:HG2	26:W:122:ARG:HH11	1.43	0.83
1:O:1116:U:HO2'	1:O:1118:A:H2	0.85	0.83
1:O:2717:C:C2'	1:O:2718:C:H5''	2.08	0.83
1:O:1474:C:H6	1:O:1474:C:H5'	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:162:MET:CE	6:B:310:ARG:HD3	2.10	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.82
1:0:2840:A:OP1	6:B:211:THR:HG23	1.77	0.82
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.62	0.82
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.45	0.82
14:K:39:GLY:HA2	40:K:4183:HOH:O	1.80	0.82
27:X:30:MET:HE1	27:X:58:ALA:HB3	1.59	0.82
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.45	0.81
1:0:871:G:H8	1:0:871:G:C5'	1.94	0.81
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.63	0.81
31:2:41:HIS:H	31:2:45:ASN:HD22	1.26	0.81
1:0:288:A:H61	1:0:364:C:H42	1.29	0.80
5:A:191:GLY:HA2	5:A:194:MET:CE	2.11	0.80
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.63	0.80
14:K:107:THR:HG22	14:K:108:GLU:HG3	1.64	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.46	0.80
8:D:136:ARG:HH12	8:D:157:LEU:HA	1.46	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.81	0.79
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.13	0.79
26:W:88:THR:HB	40:W:6679:HOH:O	1.82	0.79
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.79
1:0:2716:G:H5''	6:B:206:THR:HG21	1.65	0.79
14:K:4:LEU:HD22	14:K:116:GLU:HB3	1.63	0.79
11:G:12:ILE:N	11:G:13:PRO:HD3	1.97	0.79
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.64	0.79
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.98	0.79
1:0:1603:A:H5'	1:0:1605:G:O4'	1.83	0.79
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.63	0.79
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.64	0.79
17:N:11:ARG:HA	17:N:14:ARG:NH1	1.97	0.79
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.63	0.79
1:0:2534:C:H1'	40:0:4081:HOH:O	1.80	0.78
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.66	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.11	0.78
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.62	0.78
16:M:107:ARG:HH11	16:M:107:ARG:HG3	1.47	0.78
21:R:99:ALA:HB1	21:R:109:MET:CE	2.12	0.78
1:0:969:G:H1	1:0:999:C:H42	1.32	0.78
26:W:88:THR:HG23	26:W:110:GLN:NE2	1.99	0.78
1:0:2054:A:N3	21:R:128:ARG:NH2	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:H8	1.49	0.77
17:N:12:ARG:HD3	17:N:18:THR:OG1	1.85	0.77
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.67	0.77
1:0:2073:G:H5''	40:0:4400:HOH:O	1.83	0.77
12:H:27:LYS:H	12:H:59:HIS:HD2	1.30	0.77
1:0:1118:A:H8	1:0:1118:A:H3'	1.50	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.66	0.77
5:A:199:HIS:HD2	5:A:201:PHE:H	1.32	0.76
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.68	0.76
13:J:93:ARG:HB3	13:J:93:ARG:NH1	1.99	0.76
40:0:5371:HOH:O	13:J:47:THR:HB	1.83	0.76
10:F:91:VAL:HG12	10:F:92:GLY:N	2.01	0.76
26:W:122:ARG:HH11	26:W:122:ARG:CG	1.97	0.76
26:W:125:HIS:HD2	26:W:127:GLY:H	1.30	0.76
1:0:559:U:H6	1:0:559:U:H5'	1.50	0.76
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.15	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.01	0.76
1:0:1041:U:H5'	40:L:9491:HOH:O	1.85	0.76
8:D:57:THR:HG23	8:D:63:ILE:HA	1.67	0.76
16:M:79:ALA:HB3	16:M:81:ARG:NH1	2.00	0.76
1:0:960:G:H4'	40:0:7866:HOH:O	1.84	0.75
1:0:1667:A:H8	1:0:1667:A:H5'	1.51	0.75
2:9:3014:G:H5'	2:9:3014:G:H8	1.50	0.75
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.67	0.75
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.50	0.75
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.00	0.75
26:W:13:MET:HE2	26:W:18:GLN:HA	1.68	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:2533:C:H5'	1:0:2533:C:H6	1.51	0.75
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.68	0.75
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.75
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.68	0.75
5:A:153:ARG:HB2	5:A:153:ARG:HH11	1.50	0.75
25:V:39:ALA:N	25:V:40:PRO:HD2	2.02	0.75
5:A:33:GLU:H	5:A:33:GLU:CD	1.93	0.75
1:0:1116:U:O2'	1:0:1118:A:H2	1.67	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
5:A:206:ARG:H	5:A:206:ARG:HD3	1.51	0.74
32:3:70:ARG:HG2	32:3:77:ALA:HB2	1.69	0.74
1:0:1244:U:OP1	13:J:18:ILE:HD13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.69	0.74
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.18	0.74
1:0:1118:A:H3'	1:0:1118:A:C8	2.22	0.74
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.68	0.74
1:0:281:U:H2'	1:0:282:C:O4'	1.86	0.74
5:A:35:GLY:O	5:A:36:ASP:HB3	1.88	0.74
17:N:80:SER:HB2	40:N:9333:HOH:O	1.85	0.74
33:I:78:LEU:HD12	33:I:112:LYS:HZ2	1.53	0.74
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.70	0.74
21:R:39:THR:HB	21:R:42:GLU:HG3	1.69	0.74
1:0:1377:C:H5'	1:0:1377:C:H6	1.52	0.73
28:Y:154:ARG:HH12	28:Y:155:ARG:HG3	1.53	0.73
1:0:1751:G:H2'	1:0:1752:G:H5''	1.70	0.73
9:E:36:PRO:HD3	13:J:127:ILE:HD12	1.68	0.73
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.51	0.73
15:L:143:THR:HG22	15:L:144:ASP:H	1.52	0.73
1:0:1206:U:H5'	1:0:1206:U:H6	1.52	0.73
22:S:57:THR:HG22	22:S:59:ASP:H	1.54	0.73
33:I:99:ASP:OD1	33:I:138:THR:HB	1.89	0.73
32:3:65:THR:HG22	32:3:67:LEU:HG	1.69	0.73
9:E:84:MET:HE1	9:E:148:ILE:CD1	2.19	0.73
7:C:236:THR:HG22	7:C:239:ALA:N	2.00	0.73
1:0:111:C:O2'	30:1:20:ARG:HG2	1.88	0.73
1:0:567:U:H5''	40:W:5817:HOH:O	1.88	0.73
25:V:1:THR:HG23	25:V:2:VAL:H	1.54	0.73
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.07	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
23:T:49:GLU:HB3	23:T:59:GLU:HG2	1.71	0.73
16:M:69:LYS:O	16:M:73:ARG:NH2	2.22	0.72
18:O:32:ARG:O	18:O:32:ARG:HD3	1.87	0.72
1:0:506:G:H22	1:0:509:A:H5''	1.53	0.72
1:0:656:G:H5'	18:O:3:THR:HB	1.71	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.18	0.72
1:0:1118:A:H62	1:0:1244:U:H3	1.35	0.72
1:0:2890:A:H1'	24:U:56:ARG:NH2	2.04	0.72
15:L:143:THR:HG22	15:L:144:ASP:N	2.05	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.72
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.05	0.72
26:W:88:THR:HG22	26:W:89:ASP:N	2.03	0.71
1:0:545:G:H5'	1:0:545:G:H8	1.55	0.71
19:P:115:SER:H	19:P:118:GLN:NE2	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1700:C:H5''	1:0:1701:A:OP2	1.90	0.71
10:F:58:GLU:HA	10:F:61:MET:HE2	1.72	0.71
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.19	0.71
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.04	0.71
1:0:2851:G:H2'	1:0:2852:A:H5'	1.72	0.71
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.71	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
8:D:58:VAL:HG12	8:D:60:GLU:HG2	1.72	0.71
33:I:110:GLU:HA	33:I:113:HIS:NE2	2.06	0.71
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.23	0.71
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.71	0.71
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.06	0.71
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.19	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
1:0:1299:G:O6	15:L:6:ARG:HD3	1.91	0.71
28:Y:165:GLU:HB3	40:Y:9390:HOH:O	1.90	0.71
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.70
40:O:7889:HOH:O	6:B:211:THR:HG21	1.91	0.70
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.26	0.70
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.72	0.70
1:0:2364:A:H5''	20:Q:15:LYS:HD3	1.73	0.70
6:B:62:ARG:HA	6:B:65:MET:HE3	1.72	0.70
7:C:236:THR:CG2	7:C:239:ALA:H	2.04	0.70
10:F:58:GLU:CD	16:M:27:ARG:HH22	1.97	0.70
1:0:962:C:H1'	17:N:5:ARG:NH1	2.06	0.70
10:F:77:VAL:HG21	10:F:83:LEU:HD13	1.74	0.70
26:W:80:ASP:O	26:W:84:VAL:HG23	1.90	0.70
10:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.70
12:H:21:THR:O	12:H:120:ILE:HD12	1.92	0.70
19:P:115:SER:N	19:P:118:GLN:HE21	1.89	0.70
27:X:74:ALA:HB2	27:X:85:VAL:HG13	1.72	0.70
16:M:79:ALA:HB3	16:M:81:ARG:HH12	1.57	0.70
7:C:132:ASP:HB3	40:C:9172:HOH:O	1.91	0.70
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.74	0.70
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.04	0.70
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.57	0.70
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.89	0.70
6:B:275:GLY:O	6:B:291:ASP:HA	1.91	0.70
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.72	0.70
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.21	0.70
26:W:13:MET:HE2	26:W:18:GLN:CA	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:52:VAL:HG22	26:W:53:ALA:H	1.57	0.69
33:I:78:LEU:HD12	33:I:112:LYS:NZ	2.07	0.69
1:0:1160:G:H5'	1:0:1161:A:C5'	2.18	0.69
31:2:18:ASN:HD21	31:2:40:ARG:N	1.89	0.69
10:F:37:THR:O	10:F:41:GLU:HG3	1.93	0.69
30:1:28:HIS:CD2	30:1:31:LYS:HG3	2.27	0.69
1:0:1771:U:H5'	29:Z:20:ARG:NH2	2.07	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.22	0.69
1:0:481:U:H5''	40:0:6167:HOH:O	1.92	0.69
6:B:125:GLU:O	6:B:129:ARG:HG3	1.93	0.69
1:0:2491:G:H1'	40:0:7335:HOH:O	1.93	0.69
5:A:51:ARG:HB2	40:A:9591:HOH:O	1.93	0.69
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.74	0.69
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.90	0.69
22:S:77:VAL:O	22:S:80:ARG:HG2	1.92	0.69
26:W:88:THR:HG22	26:W:89:ASP:H	1.57	0.69
28:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.92	0.69
1:0:380:A:OP2	16:M:9:ARG:HD2	1.93	0.69
8:D:172:VAL:HG12	8:D:173:GLU:N	2.07	0.69
1:0:1474:C:H5'	1:0:1474:C:C6	2.26	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.74	0.69
18:O:32:ARG:NE	18:O:35:LYS:HD2	2.08	0.69
1:0:2749:U:H5'	40:0:8429:HOH:O	1.92	0.68
26:W:122:ARG:NH2	26:W:154:ARG:HG2	2.07	0.68
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.57	0.68
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.68
26:W:130:HIS:O	26:W:136:GLY:HA3	1.93	0.68
16:M:107:ARG:HG3	16:M:107:ARG:NH1	2.05	0.68
6:B:238:ASN:HD22	6:B:240:GLY:N	1.92	0.68
14:K:23:ASN:HD21	14:K:107:THR:HB	1.58	0.68
15:L:67:ARG:O	15:L:71:GLU:HG3	1.93	0.68
33:I:134:SER:O	33:I:135:LEU:HD23	1.93	0.68
17:N:164:ASP:CG	17:N:167:ASP:HA	2.18	0.68
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.23	0.68
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.94	0.68
26:W:137:GLN:NE2	26:W:141:HIS:HE1	1.90	0.68
7:C:2:GLN:HB3	40:C:9195:HOH:O	1.94	0.68
9:E:6:GLU:HA	9:E:46:THR:HG22	1.74	0.68
13:J:131:THR:HG22	13:J:134:GLU:H	1.56	0.68
1:0:1201:C:H2'	1:0:1202:A:H5'	1.74	0.68
12:H:56:GLN:NE2	12:H:93:GLN:HG2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.08	0.68
19:P:91:LYS:O	19:P:95:GLU:HG3	1.93	0.68
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.67
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.60	0.67
17:N:62:HIS:HB3	17:N:65:ASP:OD1	1.95	0.67
1:0:1182:C:H1'	1:0:1192:A:H8	1.58	0.67
6:B:62:ARG:HA	6:B:65:MET:CE	2.24	0.67
12:H:30:GLN:H	12:H:66:ARG:NH1	1.93	0.67
12:H:59:HIS:HA	12:H:62:LEU:HD23	1.76	0.67
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.24	0.67
18:O:96:VAL:HG13	18:O:100:GLN:HB2	1.75	0.67
1:0:2908:A:H2'	1:0:2909:G:O4'	1.95	0.67
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.67
8:D:159:PRO:O	8:D:163:VAL:HG23	1.94	0.67
27:X:71:ARG:HD3	40:X:2171:HOH:O	1.95	0.67
1:0:1184:C:H1'	40:0:7899:HOH:O	1.93	0.67
1:0:2676:C:H4'	13:J:70:PHE:CE1	2.30	0.67
1:0:2676:C:H4'	13:J:70:PHE:CD1	2.30	0.67
23:T:115:GLU:HG3	23:T:116:ASP:N	2.09	0.67
24:U:5:GLU:HG2	24:U:10:GLY:O	1.95	0.67
1:0:883:U:H2'	1:0:883:U:O2	1.95	0.67
1:0:2468:A:H61	32:3:48:ASN:HD21	1.43	0.67
5:A:199:HIS:CD2	5:A:201:PHE:H	2.11	0.67
1:0:797:A:C4'	29:Z:10:ARG:N	2.57	0.67
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.75	0.67
12:H:27:LYS:N	12:H:59:HIS:HD2	1.92	0.67
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.19	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
1:0:1183:C:H2'	40:0:6739:HOH:O	1.94	0.66
10:F:13:GLU:OE2	10:F:78:GLU:HG2	1.95	0.66
27:X:71:ARG:HB3	27:X:88:GLU:OE1	1.95	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:2073:G:OP2	1:0:2490:A:H5'	1.94	0.66
5:A:153:ARG:HB2	5:A:153:ARG:NH1	2.10	0.66
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.42	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.76	0.66
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.78	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:140:LEU:HA	40:B:9575:HOH:O	1.95	0.66
28:Y:144:ARG:HH11	28:Y:144:ARG:CG	2.09	0.66
1:O:2505:G:O2'	1:O:2506:A:H5'	1.96	0.66
29:Z:22:SER:O	29:Z:26:VAL:HG23	1.94	0.66
6:B:51:VAL:HG23	6:B:329:TYR:O	1.96	0.66
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.78	0.66
1:O:1116:U:H3	1:O:1246:A:H62	1.44	0.65
1:O:1159:G:H21	1:O:1189:A:H8	1.44	0.65
6:B:254:GLN:HG2	6:B:255:GLY:N	2.10	0.65
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.78	0.65
6:B:53:LEU:HD11	6:B:327:VAL:HG22	1.77	0.65
13:J:45:VAL:HG11	13:J:121:LEU:HD22	1.79	0.65
18:O:32:ARG:HH21	18:O:35:LYS:NZ	1.94	0.65
19:P:9:LEU:O	19:P:13:VAL:HG12	1.97	0.65
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.59	0.65
1:O:1687:C:O2	30:1:9:GLY:HA2	1.97	0.65
6:B:16:ARG:NH1	40:B:9612:HOH:O	2.28	0.65
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.77	0.65
15:L:73:VAL:HG23	15:L:74:THR:H	1.62	0.65
21:R:23:MET:HE3	21:R:28:SER:OG	1.97	0.65
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.95	0.65
28:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
33:I:92:PRO:C	33:I:94:GLU:H	2.05	0.65
18:O:32:ARG:HH21	18:O:35:LYS:HZ1	1.44	0.65
23:T:32:ARG:NH1	23:T:38:ARG:HH12	1.94	0.65
1:O:1162:G:H1'	33:I:117:LEU:HD11	1.79	0.65
5:A:48:ASP:HB3	40:A:9591:HOH:O	1.95	0.65
12:H:166:SER:HB3	12:H:167:PRO:HD3	1.78	0.65
1:O:2521:A:OP2	12:H:3:ALA:HB3	1.96	0.65
1:O:2661:U:H3	1:O:2812:A:H62	1.43	0.65
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.79	0.65
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.27	0.65
28:Y:144:ARG:HH11	28:Y:144:ARG:HG3	1.60	0.65
1:O:1175:G:H1'	1:O:1193:A:H2'	1.78	0.65
6:B:307:ARG:HG3	6:B:307:ARG:NH1	2.05	0.65
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.64
1:O:1119:G:H22	1:O:1246:A:H2	1.41	0.64
1:O:1730:G:H5'	1:O:1731:C:C5	2.31	0.64
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.26	0.64
1:O:2896:A:H5''	40:O:6599:HOH:O	1.96	0.64
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.97	0.64
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.96	0.64
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.33	0.64
26:W:48:VAL:O	26:W:48:VAL:HG12	1.97	0.64
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.61	0.64
1:0:272:A:H5'	1:0:273:G:OP2	1.97	0.64
1:0:1209:C:H2'	1:0:1210:G:H8	1.61	0.64
16:M:68:ARG:NH2	16:M:73:ARG:HD3	2.13	0.64
18:O:21:SER:OG	18:O:106:PRO:HB2	1.98	0.64
23:T:112:LEU:HD23	23:T:119:ALA:HB3	1.79	0.64
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.70	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.78	0.64
25:V:39:ALA:C	25:V:41:GLU:H	2.06	0.64
1:0:381:G:H5''	40:M:9373:HOH:O	1.97	0.64
1:0:1878:G:H1'	40:0:6620:HOH:O	1.97	0.64
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.80	0.64
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.78	0.64
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.79	0.64
24:U:45:GLU:HB2	24:U:48:ASN:ND2	2.12	0.64
14:K:49:LEU:HD12	14:K:80:ILE:HG21	1.80	0.64
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.28	0.64
20:Q:75:ILE:HD13	20:Q:84:ILE:HD11	1.78	0.64
31:2:18:ASN:ND2	31:2:40:ARG:H	1.93	0.64
1:0:709:G:O2'	18:O:25:VAL:HG12	1.97	0.64
23:T:9:LYS:HE3	23:T:13:ARG:HH12	1.58	0.64
26:W:108:ARG:HG3	26:W:114:PRO:HG3	1.80	0.64
33:I:125:ALA:O	33:I:129:VAL:HG23	1.97	0.64
1:0:2064:U:H5'	1:0:2652:U:H4'	1.80	0.64
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.26	0.64
14:K:75:ARG:HD3	14:K:112:PRO:O	1.98	0.64
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.28	0.64
7:C:157:LEU:HD13	7:C:166:ILE:HD11	1.81	0.63
12:H:166:SER:CB	12:H:167:PRO:CD	2.75	0.63
33:I:110:GLU:HA	33:I:113:HIS:CE1	2.33	0.63
2:9:3039:U:HO2'	2:9:3042:C:H5	1.44	0.63
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.63
7:C:77:ALA:O	7:C:78:ARG:HG3	1.97	0.63
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.33	0.63
1:0:263:U:O4'	10:F:59:ILE:HD13	1.99	0.63
1:0:1427:A:H61	1:0:1440:U:H1'	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.98	0.63
1:0:447:A:P	23:T:1:SER:HB2	2.38	0.63
5:A:36:ASP:C	5:A:38:ILE:H	2.06	0.63
16:M:80:GLY:O	16:M:81:ARG:HD2	1.99	0.63
33:I:113:HIS:N	33:I:114:PRO:HD2	2.14	0.63
1:0:88:G:H2'	1:0:89:G:C8	2.34	0.63
1:0:2587:OMU:H5	40:0:7918:HOH:O	1.97	0.63
25:V:20:LEU:HD22	25:V:60:GLN:HE22	1.63	0.63
1:0:2541:U:H4'	1:0:2542:C:OP1	1.97	0.63
40:0:9739:HOH:O	16:M:82:ARG:HD2	1.98	0.63
14:K:55:VAL:HG12	14:K:56:SER:N	2.13	0.63
2:9:3014:G:H5'	2:9:3014:G:C8	2.33	0.63
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.80	0.63
1:0:2533:C:H5'	1:0:2533:C:C6	2.32	0.62
13:J:90:LYS:HB2	37:J:9302:CL:CL	2.35	0.62
30:1:25:LYS:HD2	31:2:49:GLU:H	1.64	0.62
32:3:38:ARG:HB3	32:3:42:ARG:HH12	1.64	0.62
1:0:2896:A:N3	1:0:2896:A:H2'	2.15	0.62
30:1:45:ARG:NH2	40:1:9488:HOH:O	2.31	0.62
1:0:1206:U:H2'	1:0:1207:A:O4'	2.00	0.62
1:0:1528:A:H2'	1:0:1529:G:O4'	1.98	0.62
12:H:27:LYS:H	12:H:59:HIS:CD2	2.17	0.62
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.34	0.62
16:M:164:THR:HG22	16:M:166:ALA:N	2.14	0.62
26:W:4:LEU:HD11	26:W:45:VAL:HG12	1.81	0.62
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.29	0.62
1:0:524:A:H5''	21:R:29:LYS:HD3	1.82	0.62
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.64	0.62
2:9:3029:C:O3'	8:D:138:GLY:HA2	2.00	0.62
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.80	0.62
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.65	0.62
17:N:154:LEU:HG	17:N:155:GLU:H	1.63	0.62
21:R:18:LEU:HB2	21:R:143:VAL:HG13	1.82	0.62
21:R:44:VAL:O	21:R:48:GLU:HG3	2.00	0.62
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.80	0.62
27:X:25:ARG:HD3	27:X:64:ALA:O	1.99	0.62
30:1:10:LYS:HG3	40:1:9492:HOH:O	1.98	0.62
1:0:1183:C:N4	1:0:1184:C:H41	1.98	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
2:9:3051:A:H5'	17:N:160:SER:HB3	1.82	0.62
40:9:4707:HOH:O	17:N:147:ILE:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.30	0.62
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.62
1:0:1328:A:OP1	28:Y:169:ARG:HD2	2.00	0.62
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.15	0.62
12:H:20:ILE:HG23	12:H:120:ILE:HD11	1.81	0.62
13:J:19:MET:HE2	13:J:79:PHE:HA	1.80	0.62
16:M:164:THR:HG22	16:M:167:GLY:H	1.65	0.62
1:0:470:U:O2'	30:1:16:HIS:HD2	1.83	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.81	0.62
11:G:12:ILE:N	11:G:13:PRO:CD	2.63	0.62
19:P:64:GLU:HG2	40:P:165:HOH:O	2.00	0.62
21:R:104:PHE:HB3	21:R:109:MET:HE2	1.80	0.62
23:T:71:VAL:HG12	23:T:72:ILE:N	2.15	0.62
29:Z:72:GLU:OE1	29:Z:77:LYS:HE2	1.99	0.62
6:B:141:ARG:HD2	6:B:163:GLU:OE2	1.99	0.61
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.81	0.61
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.81	0.61
30:1:8:GLN:HE22	30:1:11:LYS:NZ	1.97	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
6:B:225:GLY:HA3	40:B:9562:HOH:O	2.00	0.61
24:U:14:GLU:O	24:U:17:THR:HB	2.01	0.61
28:Y:187:VAL:HG12	28:Y:205:ILE:HA	1.81	0.61
1:0:485:A:N3	1:0:487:G:H5''	2.14	0.61
1:0:2807:U:P	6:B:27:ASN:HD21	2.24	0.61
17:N:11:ARG:CG	17:N:14:ARG:HH12	2.09	0.61
24:U:52:THR:HG22	24:U:54:THR:N	2.16	0.61
30:1:25:LYS:HD2	31:2:49:GLU:N	2.15	0.61
33:I:128:VAL:C	33:I:130:GLY:H	2.08	0.61
1:0:289:G:N2	1:0:363:A:H2	1.94	0.61
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.64	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.15	0.61
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.61
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.00	0.61
6:B:175:LEU:O	6:B:175:LEU:HD23	2.00	0.61
8:D:59:GLY:O	8:D:61:PHE:N	2.33	0.61
25:V:56:ILE:HG22	25:V:60:GLN:HE21	1.66	0.61
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.80	0.61
16:M:60:VAL:C	16:M:61:ILE:HD12	2.25	0.61
27:X:43:VAL:HG12	27:X:44:ASP:N	2.16	0.61
1:0:282:C:H1'	1:0:368:C:N4	2.15	0.61
1:0:553:G:P	28:Y:204:ARG:HH22	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:136:ARG:NH1	8:D:157:LEU:HA	2.15	0.61
9:E:35:TYR:HA	13:J:127:ILE:HD12	1.82	0.61
18:O:25:VAL:HG23	18:O:26:TRP:N	2.16	0.61
1:O:280:C:H2'	1:O:281:U:O4'	2.01	0.61
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.35	0.61
17:N:164:ASP:OD1	17:N:167:ASP:HA	2.01	0.61
20:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.00	0.61
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.83	0.61
1:O:263:U:O2	16:M:42:ARG:HD2	2.01	0.61
5:A:69:LEU:HD23	5:A:107:ASN:HB2	1.81	0.61
1:O:2563:U:H2'	1:O:2565:C:O5'	2.00	0.61
6:B:102:THR:CG2	6:B:182:VAL:HG12	2.31	0.61
8:D:13:MET:HA	8:D:137:PRO:HG2	1.83	0.61
17:N:132:ASN:O	17:N:135:VAL:HG12	2.00	0.61
32:3:65:THR:HG23	32:3:88:LEU:HD22	1.83	0.61
1:O:475:G:OP1	7:C:73:LEU:HD22	2.01	0.60
5:A:81:GLN:HB2	5:A:92:ASN:HD21	1.62	0.60
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.36	0.60
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.30	0.60
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.83	0.60
1:O:902:G:N7	15:L:18:HIS:HD2	1.99	0.60
1:O:2769:C:C2'	1:O:2770:G:H5'	2.32	0.60
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.83	0.60
7:C:136:VAL:HG22	7:C:137:PRO:HA	1.83	0.60
9:E:68:HIS:O	9:E:72:MET:HG3	2.00	0.60
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.31	0.60
7:C:139:VAL:HG13	40:C:9254:HOH:O	2.00	0.60
16:M:71:SER:HB2	16:M:92:THR:HG22	1.83	0.60
33:I:129:VAL:O	33:I:129:VAL:HG12	2.01	0.60
1:O:338:C:H4'	7:C:174:ILE:CD1	2.32	0.60
1:O:2291:A:C8	1:O:2309:C:H5'	2.36	0.60
1:O:2426:G:H1'	40:O:6592:HOH:O	2.00	0.60
16:M:183:THR:HG22	16:M:194:ALA:HB1	1.82	0.60
25:V:39:ALA:N	25:V:40:PRO:CD	2.64	0.60
28:Y:187:VAL:HB	28:Y:203:VAL:HG22	1.83	0.60
1:O:848:C:H5'	40:O:7714:HOH:O	2.02	0.60
1:O:2365:G:H5''	40:Q:6597:HOH:O	2.01	0.60
5:A:65:ARG:C	5:A:66:ARG:HG3	2.26	0.60
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.83	0.60
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.02	0.60
8:D:94:ALA:HA	8:D:174:VAL:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:112:GLU:HA	28:Y:112:GLU:OE1	2.00	0.60
1:O:156:C:H5''	16:M:171:ARG:CD	2.28	0.60
1:O:1201:C:H5''	40:O:6728:HOH:O	2.01	0.60
1:O:1943:C:H4'	5:A:211:LYS:O	2.02	0.60
2:9:3013:A:O2'	2:9:3014:G:H5''	2.01	0.60
1:O:2346:C:O2'	8:D:52:THR:HG21	2.00	0.60
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.60
22:S:57:THR:HG22	22:S:59:ASP:N	2.16	0.60
1:O:2427:C:OP2	32:3:84:ARG:HD2	2.00	0.60
2:9:3004:G:H21	17:N:44:ARG:NH1	2.00	0.60
26:W:21:LEU:HB3	26:W:26:ILE:HG12	1.83	0.60
1:O:2507:G:H2'	1:O:2510:C:H42	1.66	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.83	0.60
8:D:135:VAL:HG22	8:D:136:ARG:N	2.17	0.60
10:F:46:GLU:O	10:F:73:PRO:HD2	2.02	0.60
26:W:125:HIS:CD2	26:W:127:GLY:H	2.16	0.60
1:O:236:A:H8	1:O:236:A:OP1	1.84	0.60
1:O:1164:U:OP1	33:I:74:PRO:HA	2.01	0.60
14:K:113:ILE:HG22	14:K:114:ALA:N	2.16	0.60
33:I:113:HIS:CE1	33:I:121:LEU:HD22	2.36	0.60
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.82	0.59
13:J:75:PRO:HD3	13:J:136:SER:OG	2.01	0.59
19:P:16:VAL:HG12	19:P:17:GLY:N	2.17	0.59
6:B:71:VAL:HG11	6:B:296:LEU:HD22	1.83	0.59
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.84	0.59
12:H:170:ASN:HD22	12:H:170:ASN:N	2.00	0.59
25:V:56:ILE:O	25:V:60:GLN:HG3	2.02	0.59
1:O:396:U:O2'	1:O:418:C:H4'	2.02	0.59
40:O:4936:HOH:O	16:M:83:SER:HB3	2.01	0.59
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.83	0.59
25:V:11:MET:HB3	25:V:15:GLU:HB2	1.84	0.59
28:Y:154:ARG:NH1	28:Y:155:ARG:HG3	2.16	0.59
5:A:153:ARG:HH11	5:A:153:ARG:CB	2.15	0.59
17:N:162:ASP:HA	40:N:9328:HOH:O	2.03	0.59
24:U:20:MET:HE2	24:U:30:HIS:NE2	2.18	0.59
26:W:119:HIS:HD2	26:W:120:PRO:O	1.86	0.59
33:I:106:LYS:O	33:I:110:GLU:HG3	2.02	0.59
1:O:462:A:N3	31:2:37:HIS:HB3	2.18	0.59
1:O:1555:G:H4'	1:O:1630:A:H2	1.68	0.59
1:O:1878:G:O2'	1:O:1879:U:C6	2.55	0.59
8:D:25:MET:HE2	8:D:41:LEU:CG	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:91:VAL:CG1	10:F:92:GLY:H	2.10	0.59
23:T:38:ARG:NH1	40:T:6217:HOH:O	2.35	0.59
33:I:105:VAL:HG11	33:I:129:VAL:HG22	1.84	0.59
31:2:36:ASN:HB3	31:2:39:ARG:NE	2.17	0.59
7:C:236:THR:H	7:C:239:ALA:HB3	1.68	0.59
1:0:1946:C:H2'	1:0:1971:G:C8	2.37	0.59
5:A:33:GLU:O	5:A:34:ASP:HB2	2.02	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.17	0.59
17:N:23:ARG:HG2	17:N:23:ARG:HH11	1.67	0.59
21:R:106:GLY:HA2	21:R:109:MET:HE3	1.83	0.59
30:1:8:GLN:HE22	30:1:11:LYS:HZ1	1.51	0.59
1:0:316:A:H5'	23:T:54:ASP:OD2	2.02	0.58
1:0:1187:U:HO2'	1:0:1189:A:H2	1.51	0.58
1:0:1418:U:OP1	31:2:42:TRP:HB3	2.02	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:2649:A:H5'	1:0:2649:A:H8	1.67	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.58
1:0:797:A:H4'	29:Z:10:ARG:N	2.18	0.58
6:B:265:LEU:HD21	6:B:316:ARG:HD3	1.85	0.58
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.51	0.58
14:K:62:PRO:HG3	14:K:65:ARG:HH21	1.66	0.58
25:V:12:THR:HG22	25:V:15:GLU:CG	2.21	0.58
1:0:343:C:O2'	1:0:344:C:H5'	2.02	0.58
6:B:254:GLN:HG2	6:B:255:GLY:H	1.68	0.58
28:Y:189:ASN:C	28:Y:189:ASN:HD22	2.11	0.58
16:M:24:GLN:NE2	16:M:27:ARG:HH11	2.02	0.58
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.28	0.58
32:3:55:VAL:HG22	40:3:9444:HOH:O	2.02	0.58
1:0:1163:G:H5'	33:I:115:ASP:O	2.04	0.58
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
6:B:41:PHE:HB3	6:B:190:MET:HE1	1.86	0.58
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.85	0.58
14:K:109:LEU:CD1	14:K:113:ILE:HD11	2.32	0.58
15:L:148:GLU:HB2	40:L:9486:HOH:O	2.03	0.58
16:M:164:THR:HG22	16:M:166:ALA:H	1.68	0.58
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.85	0.58
17:N:143:ARG:HH21	17:N:169:PRO:HB2	1.68	0.58
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58
6:B:87:TYR:O	6:B:138:GLY:N	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.86	0.58
1:0:2081:A:H4'	13:J:69:TYR:CE1	2.39	0.58
8:D:50:VAL:O	8:D:71:ALA:HA	2.04	0.58
15:L:133:VAL:HA	40:L:9470:HOH:O	2.04	0.58
24:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
7:C:168:ARG:NH2	7:C:190:ALA:O	2.36	0.58
12:H:58:ARG:HH11	12:H:58:ARG:HG3	1.68	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.58
1:0:969:G:H1	1:0:999:C:N4	2.01	0.58
6:B:85:ARG:NH1	40:B:9629:HOH:O	2.37	0.58
13:J:47:THR:HG22	13:J:48:GLY:N	2.17	0.58
26:W:38:THR:HG22	26:W:39:ASP:N	2.19	0.58
7:C:242:GLU:HB2	40:C:9192:HOH:O	2.04	0.58
17:N:115:VAL:HG22	40:N:9354:HOH:O	2.04	0.58
1:0:474:C:O3'	7:C:73:LEU:HD21	2.03	0.57
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.57
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.86	0.57
8:D:25:MET:CE	8:D:37:ALA:HB1	2.33	0.57
9:E:81:GLU:HG2	9:E:134:SER:CB	2.33	0.57
10:F:60:VAL:O	10:F:60:VAL:HG12	2.04	0.57
12:H:30:GLN:H	12:H:66:ARG:HH11	1.51	0.57
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.04	0.57
6:B:5:ARG:HH11	6:B:8:LYS:HE2	1.69	0.57
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.86	0.57
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.63	0.57
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.85	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.57
17:N:110:THR:HB	17:N:113:SER:OG	2.04	0.57
26:W:13:MET:HE3	26:W:17:ILE:HG22	1.85	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.57
11:G:24:VAL:O	11:G:28:GLU:HB2	2.04	0.57
18:O:25:VAL:HG23	18:O:26:TRP:H	1.69	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.03	0.57
5:A:88:ILE:O	5:A:88:ILE:HG22	2.03	0.57
5:A:179:MET:HG2	5:A:186:TRP:CB	2.35	0.57
8:D:138:GLY:N	40:D:7597:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1878:G:HO2'	1:0:1879:U:H6	1.49	0.57
1:0:2541:U:H3'	1:0:2541:U:H6	1.70	0.57
6:B:321:PRO:HA	40:B:9650:HOH:O	2.03	0.57
13:J:74:ARG:O	13:J:78:ILE:HG12	2.03	0.57
1:0:1666:C:O2'	1:0:1667:A:H5''	2.04	0.57
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.86	0.57
25:V:55:ARG:O	25:V:59:ILE:HG12	2.04	0.57
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.25	0.57
6:B:17:LYS:O	6:B:260:HIS:HD2	1.87	0.57
8:D:170:TYR:O	8:D:171:ASP:HB3	2.03	0.57
26:W:139:GLY:O	26:W:141:HIS:HD2	1.87	0.57
29:Z:30:GLU:HA	29:Z:33:MET:HE3	1.86	0.57
5:A:165:THR:HG22	40:A:9604:HOH:O	2.05	0.57
6:B:162:MET:HE3	6:B:310:ARG:HD3	1.84	0.57
1:0:462:A:C2	31:2:37:HIS:HB3	2.39	0.57
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.57
1:0:1625:U:H4'	40:0:5209:HOH:O	2.05	0.57
1:0:1919:A:H4'	40:0:5385:HOH:O	2.05	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.57
2:9:3008:G:O6	17:N:11:ARG:NH1	2.33	0.57
16:M:77:HIS:HD2	16:M:79:ALA:O	1.88	0.57
18:O:78:ALA:C	18:O:98:LEU:HD13	2.30	0.57
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
5:A:179:MET:HA	5:A:179:MET:HE3	1.86	0.56
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.35	0.56
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.56
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.86	0.56
26:W:88:THR:CG2	26:W:89:ASP:H	2.18	0.56
1:0:1684:A:H1'	31:2:43:ARG:HH22	1.70	0.56
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.05	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.69	0.56
1:0:2815:G:N7	13:J:80:LYS:NZ	2.53	0.56
1:0:2824:C:H5''	1:0:2825:C:H5'	1.86	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.56
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.04	0.56
13:J:19:MET:HE1	13:J:78:ILE:HG22	1.87	0.56
13:J:99:GLU:HA	40:J:7377:HOH:O	2.05	0.56
14:K:114:ALA:HB3	14:K:117:VAL:HG23	1.86	0.56
21:R:9:ASP:O	21:R:13:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:17:THR:CG2	24:U:18:GLY:N	2.67	0.56
26:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.56
1:0:1426:C:H2'	40:0:3203:HOH:O	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
8:D:49:PRO:HA	8:D:73:VAL:HG22	1.87	0.56
24:U:17:THR:HG22	24:U:18:GLY:N	2.19	0.56
26:W:4:LEU:O	26:W:32:CYS:HA	2.05	0.56
28:Y:187:VAL:HB	28:Y:203:VAL:CG2	2.35	0.56
1:0:757:C:OP1	15:L:27:ARG:HD2	2.05	0.56
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.56
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.87	0.56
17:N:169:PRO:O	17:N:172:PHE:HB3	2.06	0.56
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.35	0.56
26:W:122:ARG:CG	26:W:122:ARG:NH1	2.64	0.56
29:Z:29:ILE:O	29:Z:33:MET:HB2	2.06	0.56
1:0:93:C:H5''	25:V:1:THR:HB	1.88	0.56
1:0:2346:C:H6	1:0:2346:C:O5'	1.87	0.56
40:0:9699:HOH:O	6:B:214:PRO:HD2	2.04	0.56
13:J:19:MET:CE	13:J:132:LEU:HD11	2.29	0.56
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.87	0.56
19:P:40:VAL:O	19:P:44:VAL:HG23	2.05	0.56
21:R:99:ALA:CB	21:R:109:MET:HE1	2.25	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
1:0:538:C:OP2	28:Y:134:HIS:HE1	1.89	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.87	0.56
40:0:3149:HOH:O	19:P:81:LYS:HG2	2.06	0.56
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.35	0.56
1:0:244:C:OP2	10:F:38:LYS:HE3	2.05	0.56
1:0:920:C:H4'	1:0:921:G:C2	2.40	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.56
40:0:8433:HOH:O	12:H:154:TYR:HB2	2.06	0.56
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.69	0.56
8:D:103:ASN:ND2	8:D:134:LEU:H	2.03	0.56
15:L:136:ALA:HB3	40:L:9470:HOH:O	2.06	0.56
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.06	0.56
1:0:2421:G:H1'	40:0:4280:HOH:O	2.06	0.56
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.88	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:949:U:H4'	20:Q:95:GLU:HA	1.86	0.56
8:D:76:ARG:O	8:D:77:ASP:HB2	2.06	0.56
8:D:135:VAL:HG21	8:D:139:TYR:CG	2.41	0.56
1:0:120:A:H5'	30:1:20:ARG:HH21	1.71	0.55
1:0:1352:A:O2'	1:0:1353:C:OP1	2.22	0.55
1:0:2032:U:H2'	1:0:2033:G:H5''	1.88	0.55
6:B:297:VAL:HB	40:B:9600:HOH:O	2.05	0.55
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.86	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
8:D:135:VAL:HG22	8:D:136:ARG:H	1.71	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:621:C:H5'	28:Y:132:ASP:OD2	2.07	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
2:9:3024:U:H3'	2:9:3025:G:H5'	1.88	0.55
8:D:24:HIS:HB2	8:D:72:LYS:CB	2.35	0.55
1:0:1748:U:H4'	40:0:7953:HOH:O	2.04	0.55
1:0:2481:G:H5''	40:0:5094:HOH:O	2.05	0.55
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.88	0.55
6:B:305:ASP:O	6:B:306:LYS:HB2	2.07	0.55
25:V:1:THR:HG23	25:V:2:VAL:N	2.20	0.55
1:0:164:G:H4'	15:L:30:ARG:HD3	1.89	0.55
1:0:1180:U:O2'	33:I:92:PRO:HD2	2.05	0.55
1:0:2416:G:O2'	17:N:25:ARG:HG2	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.37	0.55
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.88	0.55
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.52	0.55
1:0:407:A:H2'	1:0:408:A:C8	2.41	0.55
1:0:1205:U:H2'	1:0:1206:U:H5'	1.89	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.55
12:H:166:SER:HB3	12:H:167:PRO:CD	2.35	0.55
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.55
16:M:57:LYS:HE2	16:M:140:ALA:O	2.06	0.55
1:0:2851:G:O2'	1:0:2852:A:H5'	2.05	0.55
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.42	0.55
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.89	0.55
1:0:121:U:OP2	31:2:10:ARG:NH2	2.35	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.42	0.55
1:0:1168:C:H5''	33:I:87:THR:CG2	2.37	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:120:VAL:HG11	16:M:130:GLU:HG3	1.88	0.55
29:Z:37:HIS:O	29:Z:45:ASP:HA	2.07	0.55
1:0:2591:C:H2'	1:0:2592:G:O4'	2.06	0.55
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.22	0.55
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.07	0.55
13:J:76:ASP:HA	40:J:5907:HOH:O	2.06	0.55
13:J:130:VAL:HG12	13:J:131:THR:N	2.22	0.55
15:L:10:SER:O	15:L:11:ARG:HB3	2.06	0.55
23:T:63:ILE:HD11	23:T:75:GLU:HB2	1.89	0.55
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.07	0.55
27:X:78:GLU:HG2	27:X:79:GLU:OE2	2.07	0.55
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.54
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.72	0.54
2:9:3056:A:C6	8:D:13:MET:HE3	2.43	0.54
6:B:40:GLY:HA3	40:B:9641:HOH:O	2.06	0.54
6:B:58:PRO:HA	6:B:63:GLU:CD	2.32	0.54
14:K:30:LYS:O	14:K:55:VAL:HG13	2.06	0.54
17:N:32:PRO:HD2	17:N:99:GLU:O	2.06	0.54
28:Y:108:ASP:OD1	28:Y:108:ASP:N	2.36	0.54
28:Y:154:ARG:HH12	28:Y:155:ARG:CG	2.20	0.54
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.55	0.54
29:Z:53:GLY:HA2	29:Z:67:GLY:O	2.06	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
8:D:24:HIS:HB2	8:D:72:LYS:HB3	1.89	0.54
14:K:4:LEU:CD2	14:K:116:GLU:HB3	2.36	0.54
28:Y:133:HIS:HD2	40:Y:9381:HOH:O	1.90	0.54
1:0:1202:A:H2'	1:0:1203:G:O4'	2.08	0.54
1:0:1451:C:H5'	1:0:1505:U:C5	2.43	0.54
1:0:2414:A:H2'	1:0:2415:A:C8	2.43	0.54
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.72	0.54
5:A:192:VAL:HB	40:A:9580:HOH:O	2.06	0.54
6:B:321:PRO:HG3	40:B:9595:HOH:O	2.06	0.54
7:C:1:MET:HG2	7:C:2:GLN:N	2.16	0.54
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
1:0:1189:A:O2'	1:0:1208:C:H2'	2.07	0.54
1:0:1853:C:OP1	5:A:231:LYS:HG3	2.08	0.54
2:9:3107:C:H5	40:9:3167:HOH:O	1.90	0.54
9:E:144:THR:O	9:E:148:ILE:HG13	2.08	0.54
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.36	0.54
14:K:125:ALA:C	14:K:127:ALA:H	2.14	0.54
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:164:THR:CG2	16:M:165:GLY:N	2.70	0.54
1:0:291:C:H2'	1:0:292:G:O4'	2.08	0.54
9:E:145:ALA:HB1	9:E:168:ILE:HD11	1.88	0.54
1:0:95:A:H5''	1:0:97:G:O4'	2.08	0.54
1:0:1773:G:C8	29:Z:16:ALA:HA	2.43	0.54
1:0:2748:G:H2'	40:0:7972:HOH:O	2.07	0.54
40:0:7978:HOH:O	16:M:91:ILE:HG12	2.07	0.54
18:O:47:ARG:HH11	18:O:47:ARG:HG3	1.73	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
1:0:441:A:H1'	1:0:442:A:N7	2.22	0.54
1:0:482:G:H4'	1:0:508:A:N1	2.23	0.54
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.73	0.54
9:E:93:MET:HE1	9:E:165:GLY:N	2.23	0.54
17:N:152:GLU:C	17:N:154:LEU:H	2.16	0.54
18:O:97:SER:H	18:O:100:GLN:NE2	2.05	0.54
1:0:69:A:H5'	1:0:69:A:H8	1.73	0.54
1:0:328:U:O4'	7:C:202:THR:HG22	2.08	0.54
1:0:603:A:H5''	1:0:604:G:OP1	2.08	0.54
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.54
8:D:154:LYS:H	8:D:154:LYS:HD2	1.73	0.54
16:M:187:LEU:HD23	16:M:194:ALA:HB3	1.89	0.54
23:T:32:ARG:NH1	23:T:38:ARG:NH1	2.54	0.54
33:I:113:HIS:HE1	33:I:121:LEU:HD22	1.70	0.54
1:0:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
1:0:2837:U:H2'	40:0:7305:HOH:O	2.09	0.53
5:A:105:VAL:HG12	5:A:106:CYS:N	2.24	0.53
16:M:61:ILE:HD12	16:M:61:ILE:N	2.23	0.53
28:Y:170:SER:OG	28:Y:175:ARG:HG3	2.08	0.53
1:0:1477:C:O2'	1:0:1478:U:H5'	2.08	0.53
1:0:1730:G:C5'	1:0:1731:C:C6	2.91	0.53
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.20	0.53
16:M:182:LYS:O	16:M:194:ALA:HB2	2.07	0.53
1:0:475:G:H5'	7:C:73:LEU:HD23	1.90	0.53
1:0:1172:G:H1'	40:0:5505:HOH:O	2.09	0.53
1:0:1184:C:H4'	33:I:126:LYS:HB3	1.89	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.08	0.53
19:P:103:THR:O	19:P:107:GLU:HG3	2.08	0.53
33:I:93:GLN:HA	33:I:96:PHE:HE2	1.73	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:653:C:H2'	1:0:654:A:C8	2.43	0.53
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:62:ARG:CA	6:B:65:MET:HE3	2.39	0.53
6:B:102:THR:HG21	6:B:182:VAL:O	2.07	0.53
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.73	0.53
8:D:36:ASN:HA	40:D:7500:HOH:O	2.07	0.53
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.08	0.53
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.38	0.53
18:O:53:GLN:HG2	18:O:56:GLU:OE1	2.08	0.53
31:2:36:ASN:HB3	31:2:39:ARG:HG3	1.90	0.53
32:3:56:PRO:HA	40:3:9486:HOH:O	2.09	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.44	0.53
1:0:1838:U:H1'	1:0:2644:C:H5'	1.91	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.89	0.53
7:C:25:PRO:HG2	40:C:9126:HOH:O	2.09	0.53
15:L:119:THR:HG23	15:L:139:SER:OG	2.08	0.53
23:T:47:THR:HB	23:T:100:ASP:HB3	1.90	0.53
30:1:25:LYS:HD2	31:2:48:ASP:CA	2.38	0.53
1:0:1077:G:H2'	1:0:1080:C:H42	1.73	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.53
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.44	0.53
1:0:2883:A:H2'	1:0:2884:G:O4'	2.09	0.53
6:B:146:THR:C	6:B:148:PRO:HD3	2.34	0.53
9:E:3:VAL:CG2	9:E:49:ILE:HB	2.38	0.53
1:0:151:A:H2'	1:0:152:A:O4'	2.08	0.53
1:0:516:A:H5'	40:0:6167:HOH:O	2.09	0.53
1:0:775:G:OP1	30:1:16:HIS:HE1	1.91	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.70	0.53
10:F:117:GLU:C	10:F:119:ARG:H	2.17	0.53
1:0:447:A:OP2	23:T:1:SER:HB2	2.08	0.53
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.53
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.72	0.53
1:0:545:G:H5'	1:0:545:G:C8	2.42	0.53
1:0:1786:C:OP1	19:P:74:GLN:HG2	2.09	0.53
5:A:121:ALA:O	5:A:124:VAL:HG22	2.09	0.53
13:J:39:VAL:HG11	13:J:107:ASN:CG	2.34	0.53
14:K:49:LEU:HD12	14:K:80:ILE:HD13	1.90	0.53
18:O:97:SER:OG	18:O:100:GLN:HG3	2.09	0.53
1:0:1552:G:N2	1:0:1634:G:H1'	2.24	0.53
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
1:0:1741:U:H3'	40:0:3363:HOH:O	2.09	0.53
40:0:4793:HOH:O	31:2:38:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:84:MET:HE2	9:E:133:VAL:CG2	2.39	0.53
12:H:116:ALA:O	12:H:117:PHE:C	2.52	0.53
19:P:16:VAL:HG13	19:P:20:ARG:NH1	2.24	0.53
30:1:1:THR:HA	40:1:9468:HOH:O	2.08	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:362:G:H2'	1:0:363:A:C8	2.44	0.52
1:0:1252:A:H2'	1:0:1253:C:O4'	2.09	0.52
1:0:1836:A:H1'	30:1:1:THR:O	2.09	0.52
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.91	0.52
8:D:62:ASP:HA	40:D:4233:HOH:O	2.08	0.52
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.39	0.52
32:3:30:GLN:HG3	40:3:9452:HOH:O	2.09	0.52
33:I:113:HIS:N	33:I:114:PRO:CD	2.72	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
1:0:2817:G:P	40:0:8435:HOH:O	2.67	0.52
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.24	0.52
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.43	0.52
22:S:73:ASP:OD1	22:S:76:GLU:HG3	2.09	0.52
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.24	0.52
33:I:138:THR:HG22	33:I:139:ILE:N	2.24	0.52
40:0:5237:HOH:O	29:Z:13:ARG:HD3	2.09	0.52
6:B:36:PRO:HB3	6:B:174:ARG:CB	2.40	0.52
9:E:10:ASP:HA	40:E:3707:HOH:O	2.08	0.52
17:N:86:LEU:HD21	17:N:180:LEU:CD1	2.40	0.52
21:R:114:VAL:HA	21:R:144:GLU:O	2.09	0.52
26:W:88:THR:CG2	26:W:89:ASP:N	2.69	0.52
4:5:77:PHE:CE1	4:5:79:BTN:H62	2.43	0.52
7:C:236:THR:HG22	7:C:239:ALA:CB	2.40	0.52
15:L:134:GLU:HG3	40:L:9452:HOH:O	2.09	0.52
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.52
26:W:29:VAL:O	26:W:30:ASN:HB2	2.10	0.52
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.90	0.52
7:C:246:ARG:NH1	40:C:9180:HOH:O	2.43	0.52
12:H:63:GLU:HA	40:H:9546:HOH:O	2.08	0.52
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.25	0.52
1:0:1562:C:H42	1:0:2738:G:H1	1.58	0.52
1:0:2326:U:H4'	1:0:2412:G:C4'	2.40	0.52
1:0:2644:C:O2'	1:0:2645:U:H5'	2.08	0.52
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.90	0.52
25:V:12:THR:HG23	25:V:14:ALA:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:52:VAL:HG22	26:W:53:ALA:N	2.23	0.52
30:1:28:HIS:HD2	30:1:31:LYS:H	1.57	0.52
1:0:2502:C:H2'	1:0:2503:A:H5'	1.91	0.52
17:N:24:LEU:HD22	40:Q:2847:HOH:O	2.10	0.52
32:3:70:ARG:HB3	40:3:9508:HOH:O	2.09	0.52
1:0:1462:C:H2'	1:0:1463:A:C8	2.45	0.52
5:A:109:GLU:HG2	5:A:116:GLY:N	2.25	0.52
23:T:40:VAL:HG22	23:T:41:ARG:N	2.25	0.52
1:0:497:A:H2'	1:0:498:A:C5'	2.40	0.52
8:D:136:ARG:HB3	8:D:137:PRO:HD2	1.91	0.52
12:H:38:LYS:HE2	12:H:42:ASP:HB2	1.92	0.52
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.39	0.52
16:M:31:TRP:CA	16:M:34:GLU:HG3	2.40	0.52
33:I:112:LYS:C	33:I:114:PRO:HD2	2.35	0.52
33:I:139:ILE:C	33:I:140:GLU:HG3	2.34	0.52
1:0:2419:U:H5''	1:0:2420:G:H5'	1.91	0.52
2:9:3069:U:OP1	17:N:4:PRO:HG3	2.10	0.52
12:H:76:GLU:O	12:H:77:LEU:HD23	2.09	0.52
16:M:107:ARG:NH1	40:M:9378:HOH:O	2.43	0.52
17:N:167:ASP:C	17:N:168:LEU:HG	2.35	0.52
19:P:141:ILE:C	19:P:143:ALA:H	2.17	0.52
23:T:19:ARG:HD3	23:T:67:LEU:O	2.10	0.52
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.43	0.52
1:0:1119:G:H2'	13:J:52:GLN:HE22	1.73	0.51
6:B:41:PHE:HB3	6:B:190:MET:CE	2.40	0.51
6:B:254:GLN:HG3	40:B:9531:HOH:O	2.10	0.51
8:D:65:GLU:HA	40:D:6752:HOH:O	2.08	0.51
13:J:130:VAL:HG12	13:J:131:THR:H	1.74	0.51
15:L:36:ASP:HB2	40:L:9431:HOH:O	2.09	0.51
17:N:64:SER:C	17:N:66:LEU:H	2.18	0.51
28:Y:187:VAL:HG23	40:Y:9369:HOH:O	2.10	0.51
1:0:497:A:H2'	1:0:498:A:H5'	1.91	0.51
1:0:899:C:H5'	40:0:3792:HOH:O	2.09	0.51
1:0:2320:U:H4'	1:0:2321:A:O4'	2.10	0.51
1:0:2645:U:C6	1:0:2645:U:OP2	2.63	0.51
2:9:3051:A:H5'	17:N:160:SER:CB	2.40	0.51
6:B:58:PRO:HA	6:B:63:GLU:OE2	2.11	0.51
6:B:162:MET:HE1	6:B:308:LEU:HD21	1.92	0.51
11:G:64:ASN:HD22	11:G:64:ASN:N	2.07	0.51
12:H:63:GLU:O	12:H:67:LEU:HB2	2.09	0.51
13:J:71:TYR:CD1	13:J:72:PRO:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:49:GLU:CB	23:T:59:GLU:HG2	2.39	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.51
1:0:2415:A:H2'	1:0:2416:G:H5'	1.91	0.51
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.10	0.51
6:B:75:GLU:C	6:B:77:PRO:HD3	2.35	0.51
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.40	0.51
7:C:127:ARG:CZ	7:C:225:PRO:HG2	2.40	0.51
7:C:236:THR:HA	40:C:9257:HOH:O	2.10	0.51
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.51	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.57	0.51
5:A:36:ASP:O	5:A:38:ILE:N	2.44	0.51
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.91	0.51
6:B:41:PHE:CG	6:B:79:MET:HE2	2.46	0.51
24:U:9:CYS:O	24:U:52:THR:HG23	2.10	0.51
27:X:76:ARG:HG3	27:X:76:ARG:NH1	2.24	0.51
33:I:89:SER:HB3	33:I:97:VAL:CG2	2.40	0.51
1:0:1234:U:N3	6:B:244:PRO:HB3	2.25	0.51
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.94	0.51
8:D:49:PRO:HB3	40:D:5828:HOH:O	2.10	0.51
9:E:34:TRP:O	13:J:127:ILE:HD11	2.11	0.51
16:M:99:ARG:NH2	16:M:170:ASN:HD22	2.00	0.51
17:N:67:ALA:HA	17:N:71:TRP:HB3	1.93	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.09	0.51
1:0:1384:C:H5'	27:X:30:MET:HG2	1.92	0.51
6:B:199:TYR:CE2	6:B:268:ARG:HB2	2.46	0.51
1:0:317:A:H5''	23:T:52:ARG:HD2	1.92	0.51
1:0:1189:A:H3'	40:0:8193:HOH:O	2.10	0.51
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.51
40:0:5933:HOH:O	5:A:164:ARG:CZ	2.59	0.51
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.10	0.51
23:T:112:LEU:CD2	23:T:119:ALA:HB3	2.39	0.51
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.51
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.11	0.51
5:A:211:LYS:CG	5:A:212:PRO:HD2	2.30	0.51
10:F:36:THR:HG23	10:F:97:ALA:HB2	1.93	0.51
18:O:73:ASP:HA	18:O:92:VAL:O	2.11	0.51
21:R:39:THR:HG22	21:R:107:GLU:O	2.10	0.51
33:I:78:LEU:CD1	33:I:112:LYS:HZ2	2.24	0.51
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.51
1:0:1484:G:H2'	40:0:9725:HOH:O	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1886:A:O2'	29:Z:20:ARG:HB2	2.11	0.51
6:B:14:GLY:HA2	6:B:15:PRO:C	2.36	0.51
11:G:67:LEU:O	11:G:71:LEU:HG	2.11	0.51
15:L:35:ARG:HB2	15:L:35:ARG:NH1	2.25	0.51
1:0:308:U:H5'	23:T:97:ARG:NH2	2.26	0.51
1:0:475:G:C5'	7:C:73:LEU:HD23	2.40	0.51
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.51
40:0:7340:HOH:O	16:M:178:LYS:HB2	2.11	0.51
7:C:236:THR:O	7:C:237:GLU:C	2.53	0.51
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.51
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.56	0.51
17:N:66:LEU:HD11	17:N:175:LEU:HD21	1.92	0.51
1:0:1077:G:H2'	1:0:1080:C:N4	2.25	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:1306:U:OP1	7:C:184:ARG:HD2	2.11	0.50
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.92	0.50
1:0:2421:G:H2'	40:0:4646:HOH:O	2.10	0.50
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.50
2:9:3054:A:H2	40:9:3535:HOH:O	1.93	0.50
2:9:3054:A:O2'	2:9:3055:U:H5'	2.11	0.50
6:B:42:ALA:H	6:B:79:MET:HE2	1.76	0.50
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.92	0.50
6:B:72:THR:HB	40:B:9600:HOH:O	2.11	0.50
13:J:45:VAL:HG11	13:J:121:LEU:CD2	2.40	0.50
14:K:115:ARG:HG3	14:K:116:GLU:N	2.27	0.50
15:L:145:LEU:HD23	15:L:145:LEU:O	2.11	0.50
22:S:29:ASP:OD1	22:S:31:ARG:NH1	2.44	0.50
1:0:299:U:H5'	40:0:7775:HOH:O	2.11	0.50
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.50
1:0:2016:U:H2'	1:0:2017:U:O4'	2.10	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
6:B:265:LEU:CD2	6:B:316:ARG:HD3	2.41	0.50
7:C:236:THR:HG21	40:C:9184:HOH:O	2.10	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.46	0.50
20:Q:75:ILE:HD13	20:Q:84:ILE:CD1	2.41	0.50
26:W:21:LEU:HD22	26:W:26:ILE:HD13	1.92	0.50
33:I:87:THR:HG22	33:I:88:GLY:N	2.25	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.50
1:0:2296:C:H2'	1:0:2297:U:H6	1.77	0.50
40:0:6777:HOH:O	28:Y:158:LYS:HD3	2.12	0.50
40:0:7989:HOH:O	32:3:61:PRO:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:69:ILE:HA	9:E:72:MET:HE3	1.92	0.50
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.94	0.50
19:P:115:SER:HG	19:P:118:GLN:HG3	1.76	0.50
25:V:8:ILE:HA	25:V:11:MET:HE3	1.93	0.50
31:2:20:ARG:HG3	31:2:39:ARG:HH21	1.76	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.47	0.50
1:0:2906:A:H5'	1:0:2907:C:O4'	2.12	0.50
9:E:133:VAL:HG12	9:E:141:VAL:HG13	1.94	0.50
21:R:92:LEU:HD23	21:R:145:LEU:HD21	1.94	0.50
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.94	0.50
1:0:2816:A:H2'	40:0:8435:HOH:O	2.12	0.50
5:A:163:GLY:HA2	5:A:166:ASP:OD2	2.12	0.50
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.25	0.50
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.41	0.50
26:W:122:ARG:CZ	40:W:5817:HOH:O	2.58	0.50
1:0:1992:U:OP2	14:K:66:ARG:HD2	2.11	0.50
2:9:3059:C:H2'	2:9:3060:C:C6	2.46	0.50
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.92	0.50
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.42	0.50
12:H:158:THR:HB	12:H:159:PRO:HD3	1.94	0.50
13:J:74:ARG:NH1	13:J:105:LEU:HD11	2.27	0.50
16:M:82:ARG:O	16:M:84:LYS:N	2.44	0.50
21:R:69:LYS:HB2	21:R:72:VAL:HG23	1.92	0.50
1:0:155:C:OP2	16:M:188:ARG:HD3	2.11	0.50
1:0:1714:C:O2'	1:0:1715:C:H5'	2.11	0.50
1:0:2338:G:OP1	8:D:97:GLN:HG2	2.11	0.50
9:E:93:MET:HE1	9:E:165:GLY:H	1.76	0.50
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.94	0.50
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.93	0.50
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.27	0.50
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.46	0.50
1:0:123:U:H5'	40:0:7132:HOH:O	2.12	0.50
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.50
7:C:154:VAL:O	7:C:158:GLU:HG3	2.12	0.50
15:L:77:ALA:C	15:L:79:ASP:H	2.20	0.50
29:Z:10:ARG:HA	40:Z:9215:HOH:O	2.11	0.50
1:0:247:A:H2'	40:0:4495:HOH:O	2.11	0.50
1:0:962:C:H1'	17:N:5:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.50
1:0:2827:A:H2'	1:0:2828:G:O4'	2.12	0.50
2:9:3007:G:H4'	17:N:55:ASP:OD2	2.12	0.50
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.50
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.35	0.50
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.47	0.50
1:0:1745:G:H22	1:0:2033:G:H5'	1.77	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.49
7:C:57:PRO:HG2	7:C:73:LEU:HD13	1.93	0.49
8:D:25:MET:SD	8:D:40:ILE:HD11	2.51	0.49
10:F:13:GLU:OE1	10:F:77:VAL:HG13	2.12	0.49
15:L:101:ASP:C	15:L:103:ALA:H	2.20	0.49
18:O:96:VAL:CG1	18:O:100:GLN:HB2	2.40	0.49
19:P:13:VAL:HG11	19:P:40:VAL:CG1	2.42	0.49
1:0:204:A:H2'	1:0:205:U:H5'	1.93	0.49
1:0:926:A:O2'	15:L:41:HIS:HD2	1.95	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
1:0:2748:G:H1'	40:0:8408:HOH:O	2.11	0.49
6:B:51:VAL:HG23	6:B:327:VAL:HG13	1.94	0.49
6:B:310:ARG:HD2	40:B:9586:HOH:O	2.10	0.49
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.47	0.49
8:D:167:GLU:C	8:D:169:THR:H	2.20	0.49
25:V:59:ILE:O	25:V:63:GLU:HG2	2.11	0.49
33:I:131:THR:O	33:I:135:LEU:HG	2.12	0.49
1:0:820:G:H5'	1:0:821:U:H5'	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
7:C:127:ARG:HD3	7:C:129:HIS:HE1	1.76	0.49
13:J:88:PRO:O	13:J:94:GLY:HA3	2.12	0.49
15:L:143:THR:CG2	15:L:144:ASP:N	2.75	0.49
17:N:89:GLY:O	17:N:92:ALA:HB3	2.12	0.49
17:N:119:GLN:O	17:N:123:ILE:HG13	2.12	0.49
28:Y:177:LYS:HD3	28:Y:181:GLY:O	2.12	0.49
1:0:1506:U:H6	1:0:1506:U:H5'	1.78	0.49
2:9:3095:C:O2'	2:9:3096:C:H5'	2.12	0.49
11:G:20:VAL:O	11:G:24:VAL:HG23	2.13	0.49
13:J:12:VAL:HG21	13:J:116:LEU:HD11	1.94	0.49
14:K:22:ASP:O	14:K:110:LYS:HE3	2.12	0.49
14:K:55:VAL:CG1	14:K:56:SER:N	2.74	0.49
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.77	0.49
23:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.49
27:X:61:ARG:HH11	27:X:61:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:21:ARG:HD2	30:1:39:PHE:HB2	1.95	0.49
32:3:3:MET:O	32:3:90:PHE:HA	2.12	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.27	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.11	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:2333:G:P	8:D:56:ARG:HH22	2.36	0.49
6:B:84:LEU:HD13	6:B:84:LEU:O	2.13	0.49
8:D:10:PHE:CE1	8:D:11:HIS:HB3	2.47	0.49
8:D:56:ARG:N	40:D:6752:HOH:O	2.46	0.49
9:E:81:GLU:HA	9:E:133:VAL:O	2.12	0.49
10:F:38:LYS:NZ	16:M:3:SER:HA	2.27	0.49
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.94	0.49
1:0:288:A:H2'	1:0:289:G:C8	2.47	0.49
1:0:333:G:O2'	1:0:334:G:H5'	2.13	0.49
1:0:1755:A:H2'	1:0:1756:G:O4'	2.12	0.49
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.42	0.49
6:B:175:LEU:HD23	6:B:175:LEU:C	2.37	0.49
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.10	0.49
25:V:1:THR:CG2	25:V:2:VAL:H	2.19	0.49
1:0:793:A:H5''	19:P:83:LYS:HG2	1.95	0.49
1:0:830:G:O2'	1:0:831:U:H5'	2.13	0.49
1:0:960:G:N3	1:0:960:G:H2'	2.28	0.49
1:0:1119:G:H8	13:J:52:GLN:NE2	2.10	0.49
1:0:1878:G:O2'	1:0:1879:U:OP2	2.30	0.49
1:0:2453:G:H5''	40:L:9438:HOH:O	2.12	0.49
1:0:2531:U:O2'	1:0:2532:A:H5'	2.12	0.49
1:0:2735:U:H2'	1:0:2736:U:C6	2.47	0.49
2:9:3078:G:N2	2:9:3102:G:H2'	2.28	0.49
3:4:75:C:N4	3:4:76:PPU:H102	2.28	0.49
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.43	0.49
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.43	0.49
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.93	0.49
19:P:16:VAL:HG13	19:P:20:ARG:CZ	2.43	0.49
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.94	0.49
25:V:1:THR:HG22	25:V:48:GLU:OE1	2.13	0.49
25:V:12:THR:HG23	25:V:14:ALA:N	2.27	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
1:0:2032:U:C2'	1:0:2033:G:H5''	2.42	0.49
1:0:2781:U:H1'	9:E:139:GLU:OE2	2.12	0.49
5:A:94:LEU:HD23	5:A:94:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:29:ALA:C	12:H:30:GLN:HG3	2.38	0.49
12:H:148:GLU:OE1	12:H:148:GLU:HA	2.11	0.49
23:T:41:ARG:HG2	23:T:41:ARG:NH1	2.27	0.49
23:T:69:LYS:O	23:T:71:VAL:HG23	2.13	0.49
1:O:1979:G:O2'	1:O:1980:U:OP1	2.30	0.49
1:O:2252:A:H2'	1:O:2253:G:O4'	2.13	0.49
5:A:129:LEU:CD1	5:A:145:MET:HE1	2.43	0.49
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.46	0.49
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.48	0.49
8:D:37:ALA:O	8:D:40:ILE:HG12	2.12	0.49
8:D:172:VAL:CG1	8:D:173:GLU:H	2.18	0.49
9:E:11:VAL:HG12	9:E:12:ASP:N	2.26	0.49
9:E:80:TRP:O	9:E:134:SER:HA	2.13	0.49
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.13	0.49
21:R:84:ALA:O	21:R:88:PHE:HD1	1.96	0.49
26:W:122:ARG:HG3	26:W:152:ALA:O	2.13	0.49
33:I:132:CYS:C	33:I:134:SER:H	2.21	0.49
1:O:65:C:O2'	1:O:66:G:H5'	2.12	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
8:D:51:ARG:HD3	40:D:7636:HOH:O	2.13	0.49
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.94	0.49
17:N:155:GLU:O	17:N:156:GLU:HG3	2.12	0.49
17:N:164:ASP:OD2	17:N:167:ASP:HA	2.12	0.49
18:O:97:SER:H	18:O:100:GLN:HE21	1.59	0.49
28:Y:186:ARG:HG2	28:Y:186:ARG:HH11	1.76	0.49
1:O:1730:G:H5'	1:O:1731:C:H5	1.77	0.48
1:O:2265:U:H2'	1:O:2266:A:C8	2.48	0.48
5:A:36:ASP:C	5:A:38:ILE:N	2.71	0.48
8:D:60:GLU:O	8:D:61:PHE:C	2.55	0.48
16:M:82:ARG:O	16:M:83:SER:C	2.56	0.48
30:1:25:LYS:HG3	31:2:49:GLU:H	1.77	0.48
1:O:750:A:O3'	7:C:101:ASP:HB2	2.12	0.48
1:O:2784:A:H1'	9:E:60:SER:OG	2.13	0.48
5:A:167:LYS:HB2	29:Z:29:ILE:HD13	1.95	0.48
14:K:28:GLU:HB3	14:K:59:LYS:HB2	1.94	0.48
16:M:49:ALA:C	16:M:54:TYR:HB3	2.39	0.48
16:M:99:ARG:HH21	16:M:170:ASN:ND2	2.02	0.48
31:2:41:HIS:HD2	31:2:44:ARG:H	1.61	0.48
33:I:138:THR:HG22	33:I:139:ILE:H	1.78	0.48
1:O:2809:G:H2'	1:O:2810:G:O4'	2.13	0.48
2:9:3024:U:H3'	2:9:3025:G:C5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:129:LEU:HD13	5:A:145:MET:HE1	1.94	0.48
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.14	0.48
8:D:99:ASP:HB3	8:D:103:ASN:H	1.77	0.48
15:L:97:VAL:HG12	15:L:98:GLU:O	2.13	0.48
1:O:399:C:H5'	16:M:179:GLY:O	2.13	0.48
1:O:426:G:H2'	1:O:427:C:O4'	2.13	0.48
1:O:1242:A:C5'	13:J:82:THR:HG23	2.34	0.48
1:O:1654:U:H2'	5:A:47:HIS:HD2	1.77	0.48
1:O:2064:U:H5'	1:O:2652:U:O3'	2.13	0.48
40:O:5270:HOH:O	17:N:21:HIS:HD2	1.94	0.48
40:O:6232:HOH:O	14:K:87:ARG:CZ	2.60	0.48
8:D:103:ASN:HD21	8:D:134:LEU:H	1.60	0.48
16:M:36:ALA:HB1	40:M:9352:HOH:O	2.13	0.48
20:Q:40:HIS:CD2	20:Q:60:THR:HG23	2.49	0.48
20:Q:75:ILE:CD1	20:Q:84:ILE:HD11	2.42	0.48
21:R:17:MET:HE1	21:R:19:ARG:NH2	2.28	0.48
22:S:44:GLN:HE21	25:V:28:LEU:CD2	2.27	0.48
26:W:65:VAL:HA	26:W:68:THR:HG22	1.95	0.48
28:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.46	0.48
1:O:2541:U:H3'	1:O:2541:U:C6	2.47	0.48
8:D:134:LEU:CD1	8:D:166:ILE:HD11	2.41	0.48
12:H:169:GLY:C	12:H:170:ASN:HD22	2.20	0.48
15:L:145:LEU:HD23	15:L:145:LEU:C	2.38	0.48
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.96	0.48
1:O:1171:A:H2'	1:O:1172:G:H5'	1.94	0.48
1:O:2456:A:H2'	1:O:2457:U:C6	2.48	0.48
1:O:2779:G:H21	9:E:143:GLN:NE2	2.12	0.48
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.96	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
25:V:7:GLU:O	25:V:11:MET:HG3	2.13	0.48
27:X:61:ARG:HB2	27:X:65:ASN:O	2.14	0.48
1:O:31:C:OP2	23:T:8:ARG:NH1	2.44	0.48
1:O:1736:A:H1'	40:O:8069:HOH:O	2.13	0.48
6:B:243:ASN:HA	6:B:244:PRO:C	2.37	0.48
13:J:19:MET:CE	13:J:132:LEU:HD21	2.44	0.48
15:L:130:ARG:O	15:L:131:GLU:C	2.57	0.48
17:N:154:LEU:O	17:N:155:GLU:HB3	2.14	0.48
26:W:5:VAL:HG11	26:W:153:MET:HE1	1.96	0.48
27:X:61:ARG:HD2	27:X:65:ASN:O	2.14	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
32:3:42:ARG:HH11	32:3:42:ARG:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.48
12:H:58:ARG:O	12:H:62:LEU:HD22	2.14	0.48
23:T:61:GLU:HG3	40:T:3851:HOH:O	2.14	0.48
25:V:39:ALA:O	25:V:41:GLU:N	2.47	0.48
26:W:41:TYR:HA	26:W:44:MET:HE3	1.95	0.48
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.48
1:0:656:G:OP2	18:O:37:ARG:HD2	2.13	0.48
1:0:776:A:OP1	30:1:28:HIS:HE1	1.97	0.48
1:0:1044:C:H3'	1:0:1045:G:H5''	1.96	0.48
1:0:1730:G:C5'	1:0:1731:C:H6	2.26	0.48
1:0:2480:G:H3'	40:0:4750:HOH:O	2.14	0.48
40:0:7242:HOH:O	17:N:4:PRO:HD2	2.12	0.48
6:B:277:GLU:N	6:B:278:PRO:HD2	2.29	0.48
9:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.48
12:H:83:TYR:CD1	12:H:83:TYR:C	2.92	0.48
13:J:47:THR:CG2	13:J:48:GLY:N	2.77	0.48
16:M:134:ILE:O	16:M:136:PRO:HD3	2.13	0.48
26:W:88:THR:HG22	26:W:90:TYR:CD1	2.49	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
1:0:1236:A:C8	13:J:63:ILE:HD11	2.49	0.48
4:5:75:C:H2'	4:5:76:A:O4'	2.14	0.48
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.96	0.48
22:S:57:THR:HG22	22:S:58:MET:N	2.28	0.48
27:X:9:VAL:HG13	27:X:88:GLU:OE1	2.14	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
1:0:1098:A:H2'	1:0:1099:G:O4'	2.14	0.47
1:0:1189:A:H1'	1:0:1209:C:C1'	2.44	0.47
1:0:2504:A:H4'	12:H:71:ARG:HH11	1.80	0.47
1:0:2862:G:H4'	6:B:336:GLN:O	2.14	0.47
6:B:91:PRO:O	13:J:144:THR:HG21	2.14	0.47
10:F:49:PHE:HE1	10:F:98:VAL:HG23	1.79	0.47
14:K:10:GLN:NE2	14:K:10:GLN:N	2.48	0.47
15:L:145:LEU:O	15:L:148:GLU:HG3	2.13	0.47
24:U:4:ARG:HG2	24:U:4:ARG:HH11	1.79	0.47
33:I:132:CYS:C	33:I:134:SER:N	2.71	0.47
1:0:2253:G:O2'	1:0:2254:G:H5'	2.15	0.47
1:0:2719:A:C2	6:B:70:PRO:HG3	2.49	0.47
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.11	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:96:VAL:CG1	23:T:97:ARG:N	2.78	0.47
1:0:308:U:C4	1:0:342:C:H1'	2.49	0.47
1:0:392:U:C5'	16:M:193:LYS:HB3	2.45	0.47
7:C:133:ARG:NH1	40:C:9220:HOH:O	2.47	0.47
12:H:38:LYS:HE2	12:H:42:ASP:CB	2.45	0.47
13:J:54:VAL:O	13:J:58:GLU:HG3	2.14	0.47
21:R:82:GLU:O	21:R:86:LYS:HG3	2.14	0.47
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.77	0.47
30:1:25:LYS:CD	31:2:49:GLU:H	2.27	0.47
1:0:210:U:H2'	1:0:211:U:C6	2.49	0.47
1:0:347:A:H2'	1:0:348:C:O4'	2.14	0.47
1:0:1058:A:H2'	1:0:1060:C:H5''	1.96	0.47
1:0:1149:U:H5''	1:0:1151:G:O4'	2.14	0.47
1:0:2626:C:H2'	1:0:2627:G:C8	2.50	0.47
2:9:3076:G:H3'	2:9:3077:A:C5'	2.26	0.47
6:B:254:GLN:NE2	40:B:9587:HOH:O	2.44	0.47
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.31	0.47
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.96	0.47
12:H:77:LEU:HD12	12:H:83:TYR:CD2	2.49	0.47
18:O:39:THR:O	18:O:115:ARG:NH2	2.47	0.47
21:R:119:VAL:O	21:R:119:VAL:HG12	2.13	0.47
22:S:57:THR:CG2	22:S:58:MET:N	2.77	0.47
32:3:11:CYS:HB2	32:3:20:HIS:CE1	2.49	0.47
1:0:912:A:C4	1:0:1294:A:C2	3.02	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
5:A:123:GLY:HA3	5:A:162:GLY:CA	2.44	0.47
6:B:178:ALA:O	6:B:182:VAL:HG23	2.15	0.47
7:C:157:LEU:CD1	7:C:166:ILE:HD11	2.44	0.47
17:N:15:GLU:HB3	17:N:17:ARG:HD2	1.97	0.47
26:W:64:THR:O	26:W:68:THR:HG22	2.15	0.47
32:3:17:HIS:O	32:3:18:GLN:HG3	2.15	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.15	0.47
1:0:1167:G:H4'	33:I:135:LEU:HD22	1.96	0.47
2:9:3003:A:H2'	40:9:2430:HOH:O	2.15	0.47
12:H:154:TYR:CD1	12:H:154:TYR:C	2.92	0.47
17:N:154:LEU:O	17:N:155:GLU:CB	2.63	0.47
1:0:635:A:H2'	1:0:636:G:H5''	1.96	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
1:0:999:C:H2'	1:0:1000:C:O4'	2.15	0.47
1:0:1667:A:H5'	1:0:1667:A:C8	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.30	0.47
1:0:2434:A:O3'	32:3:28:GLY:HA3	2.15	0.47
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.79	0.47
7:C:140:VAL:HB	40:C:9257:HOH:O	2.14	0.47
7:C:142:ASP:CG	7:C:237:GLU:HB3	2.39	0.47
8:D:173:GLU:HG3	8:D:174:VAL:N	2.30	0.47
10:F:14:ASP:O	10:F:18:GLU:HG3	2.14	0.47
10:F:60:VAL:O	10:F:60:VAL:CG1	2.62	0.47
13:J:142:ASN:O	13:J:144:THR:N	2.48	0.47
14:K:113:ILE:CG2	14:K:114:ALA:N	2.77	0.47
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.80	0.47
16:M:86:GLN:O	16:M:88:VAL:HG23	2.15	0.47
16:M:165:GLY:O	16:M:169:ARG:HG3	2.15	0.47
17:N:7:LYS:HE3	20:Q:21:ARG:O	2.13	0.47
21:R:132:ARG:NH2	40:R:9489:HOH:O	2.46	0.47
22:S:38:ALA:O	22:S:42:GLU:HG3	2.15	0.47
24:U:49:LEU:HG	40:U:3805:HOH:O	2.14	0.47
25:V:64:GLY:O	25:V:65:ASP:CB	2.62	0.47
27:X:7:GLU:HA	27:X:74:ALA:O	2.15	0.47
32:3:20:HIS:HA	32:3:70:ARG:O	2.15	0.47
32:3:91:GLN:O	32:3:92:GLU:HB2	2.15	0.47
1:0:171:C:OP2	16:M:84:LYS:HG3	2.14	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.15	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.47
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.14	0.47
1:0:1921:A:O2'	1:0:1922:A:H5'	2.15	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:B:215:VAL:HA	6:B:220:VAL:HG22	1.97	0.47
6:B:294:TYR:HE2	40:B:9643:HOH:O	1.97	0.47
17:N:17:ARG:HB3	17:N:17:ARG:NH1	2.27	0.47
33:I:75:THR:HA	33:I:112:LYS:NZ	2.29	0.47
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.97	0.47
40:0:5212:HOH:O	6:B:300:SER:HB3	2.15	0.47
5:A:69:LEU:HD23	5:A:107:ASN:CB	2.45	0.47
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.95	0.47
9:E:77:THR:OG1	9:E:78:GLU:N	2.47	0.47
14:K:7:ASP:OD2	14:K:81:ARG:NH2	2.48	0.47
15:L:21:ARG:N	40:L:9425:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:97:VAL:HB	15:L:100:ALA:HB2	1.97	0.47
24:U:52:THR:HG22	24:U:54:THR:H	1.79	0.47
27:X:80:GLU:O	27:X:80:GLU:HG2	2.15	0.47
1:O:1268:C:O2'	28:Y:169:ARG:HB2	2.15	0.47
1:O:1299:G:N7	15:L:6:ARG:NH1	2.63	0.47
1:O:1634:G:H3'	40:O:4467:HOH:O	2.14	0.47
1:O:1641:A:C2'	1:O:1642:A:H5'	2.43	0.47
1:O:1783:A:O2'	1:O:1784:U:H5'	2.15	0.47
1:O:2506:A:O2'	1:O:2507:G:O5'	2.33	0.47
9:E:157:LYS:HD2	9:E:162:PHE:CZ	2.50	0.47
10:F:58:GLU:HA	10:F:61:MET:HG3	1.97	0.47
13:J:52:GLN:HG3	13:J:53:ILE:N	2.30	0.47
16:M:47:ASP:CG	16:M:48:LYS:N	2.73	0.47
22:S:53:ASN:ND2	40:S:9479:HOH:O	2.49	0.47
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.45	0.47
1:O:451:C:O2'	1:O:452:G:H5'	2.15	0.46
1:O:657:G:OP1	7:C:27:ARG:NH2	2.30	0.46
1:O:894:A:N1	7:C:87:ARG:NH2	2.63	0.46
1:O:1192:A:H3'	1:O:1193:A:H5'	1.96	0.46
1:O:1794:G:N2	1:O:1796:A:H3'	2.30	0.46
1:O:2374:A:H2'	1:O:2375:G:C8	2.51	0.46
7:C:153:VAL:O	7:C:157:LEU:HG	2.15	0.46
8:D:65:GLU:HG3	40:D:6752:HOH:O	2.14	0.46
8:D:154:LYS:HD2	8:D:154:LYS:N	2.30	0.46
17:N:38:LYS:HD3	17:N:107:ASN:ND2	2.29	0.46
28:Y:155:ARG:NH1	40:Y:9355:HOH:O	2.49	0.46
33:I:100:LEU:O	33:I:139:ILE:HG23	2.15	0.46
1:O:56:G:H5''	25:V:50:ARG:NH1	2.31	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.14	0.46
1:O:449:A:N7	7:C:43:LYS:HG2	2.31	0.46
1:O:603:A:H1'	1:O:605:C:C2	2.50	0.46
1:O:1180:U:H1'	40:I:1549:HOH:O	2.14	0.46
1:O:1406:A:H5'	1:O:1407:A:C8	2.51	0.46
1:O:2256:G:H2'	1:O:2257:G:C5'	2.46	0.46
1:O:2270:G:H4'	5:A:223:ARG:NH1	2.30	0.46
40:O:5814:HOH:O	26:W:122:ARG:NH2	2.47	0.46
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.96	0.46
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.97	0.46
8:D:166:ILE:HB	40:D:6326:HOH:O	2.14	0.46
10:F:102:GLY:O	10:F:103:GLU:HB2	2.15	0.46
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:75:GLU:O	23:T:76:ASP:HB2	2.16	0.46
32:3:65:THR:HG22	32:3:67:LEU:CG	2.42	0.46
1:0:397:A:O2'	1:0:417:G:N3	2.45	0.46
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.46
1:0:1679:C:H5'	40:0:9938:HOH:O	2.16	0.46
5:A:65:ARG:HG2	5:A:65:ARG:HH11	1.80	0.46
7:C:21:VAL:C	7:C:23:GLU:H	2.23	0.46
8:D:60:GLU:O	8:D:60:GLU:HG3	2.15	0.46
10:F:56:PRO:HB2	10:F:58:GLU:OE1	2.16	0.46
10:F:105:ASP:O	10:F:109:GLU:HB2	2.16	0.46
15:L:57:VAL:HG12	15:L:57:VAL:O	2.15	0.46
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.97	0.46
1:0:1799:G:H21	19:P:88:GLN:NE2	2.14	0.46
1:0:2453:G:H5'	40:0:5233:HOH:O	2.16	0.46
40:0:3854:HOH:O	6:B:222:LYS:HE2	2.16	0.46
5:A:36:ASP:O	5:A:36:ASP:CG	2.59	0.46
7:C:218:VAL:HG12	40:C:9232:HOH:O	2.16	0.46
8:D:172:VAL:CG1	8:D:173:GLU:N	2.78	0.46
10:F:70:LYS:C	10:F:72:VAL:H	2.22	0.46
13:J:131:THR:HG22	13:J:133:GLY:N	2.30	0.46
25:V:4:HIS:O	25:V:8:ILE:HG13	2.15	0.46
25:V:29:ASN:O	25:V:33:VAL:HG23	2.16	0.46
33:I:74:PRO:C	33:I:112:LYS:HZ1	2.23	0.46
1:0:1435:U:H5'	40:0:3203:HOH:O	2.15	0.46
1:0:2072:G:H3'	1:0:2073:G:C5'	2.45	0.46
6:B:41:PHE:HA	6:B:79:MET:CE	2.45	0.46
8:D:58:VAL:N	8:D:62:ASP:O	2.45	0.46
8:D:173:GLU:O	8:D:174:VAL:C	2.59	0.46
10:F:57:GLU:O	10:F:61:MET:HG3	2.15	0.46
24:U:45:GLU:HB2	24:U:48:ASN:HD22	1.78	0.46
27:X:72:VAL:CG2	27:X:85:VAL:HG12	2.42	0.46
28:Y:102:LEU:HD11	28:Y:225:GLY:HA2	1.97	0.46
1:0:702:G:O2'	1:0:703:G:H5'	2.16	0.46
1:0:1014:A:H2'	1:0:1015:C:H5'	1.97	0.46
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.16	0.46
13:J:107:ASN:C	13:J:107:ASN:HD22	2.24	0.46
18:O:26:TRP:N	40:O:3062:HOH:O	2.49	0.46
26:W:4:LEU:CD2	26:W:52:VAL:HG21	2.39	0.46
30:1:56:GLU:HG2	30:1:56:GLU:OXT	2.16	0.46
1:0:319:A:H4'	1:0:338:C:C5	2.49	0.46
1:0:1636:G:O2'	1:0:1637:A:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1789:G:O6	19:P:73:HIS:HE1	1.99	0.46
1:0:2511:A:H2'	1:0:2512:U:O4'	2.15	0.46
6:B:215:VAL:HB	6:B:234:ARG:HH12	1.81	0.46
8:D:10:PHE:CG	8:D:11:HIS:N	2.84	0.46
12:H:45:VAL:HA	12:H:167:PRO:O	2.15	0.46
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.30	0.46
15:L:145:LEU:C	15:L:147:GLU:H	2.23	0.46
21:R:39:THR:CG2	21:R:107:GLU:O	2.63	0.46
23:T:71:VAL:HG13	23:T:91:LEU:O	2.16	0.46
25:V:39:ALA:C	25:V:41:GLU:N	2.73	0.46
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.51	0.46
29:Z:17:ARG:HD3	40:Z:9220:HOH:O	2.15	0.46
29:Z:39:CYS:SG	29:Z:41:ASN:HB3	2.55	0.46
33:I:103:ASP:HA	33:I:106:LYS:HD2	1.97	0.46
1:0:894:A:C2	7:C:87:ARG:NH2	2.83	0.46
1:0:1778:A:H2'	1:0:1779:A:H5'	1.97	0.46
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.46
2:9:3057:A:H8	8:D:141:VAL:HG21	1.80	0.46
6:B:87:TYR:HD1	40:B:9575:HOH:O	1.99	0.46
6:B:294:TYR:CD1	6:B:294:TYR:C	2.93	0.46
7:C:236:THR:O	7:C:239:ALA:N	2.49	0.46
13:J:71:TYR:CG	13:J:72:PRO:HD2	2.51	0.46
14:K:2:GLU:O	14:K:3:ALA:C	2.58	0.46
15:L:79:ASP:HB3	40:L:9453:HOH:O	2.15	0.46
17:N:183:ASP:O	17:N:184:ILE:O	2.34	0.46
21:R:114:VAL:HG13	21:R:114:VAL:O	2.15	0.46
26:W:142:ASP:HB2	40:W:6373:HOH:O	2.15	0.46
27:X:34:ARG:NH1	27:X:48:VAL:O	2.48	0.46
27:X:43:VAL:CG1	27:X:44:ASP:N	2.79	0.46
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.51	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.16	0.46
1:0:2487:C:H5	40:0:5422:HOH:O	1.98	0.46
6:B:51:VAL:HG21	6:B:327:VAL:HG13	1.94	0.46
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.97	0.46
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.97	0.46
14:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.46
15:L:35:ARG:C	15:L:35:ARG:HD3	2.41	0.46
15:L:91:VAL:CG1	15:L:120:LEU:HD23	2.46	0.46
27:X:20:GLU:HG3	27:X:21:PRO:HD2	1.98	0.46
1:0:802:G:H2'	1:0:803:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
1:0:1200:A:H3'	40:0:6272:HOH:O	2.15	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.51	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.46
1:0:1799:G:H21	19:P:88:GLN:HE22	1.64	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.46
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.31	0.46
2:9:3064:C:H2'	2:9:3065:A:H5'	1.97	0.46
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.46
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.46	0.46
7:C:107:ARG:NE	40:C:9266:HOH:O	2.32	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
25:V:45:ARG:HA	25:V:48:GLU:HB2	1.98	0.46
28:Y:152:LYS:HB3	28:Y:160:LYS:HG3	1.98	0.46
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.45
1:0:1878:G:O2'	1:0:1879:U:C5	2.61	0.45
1:0:2346:C:H4'	8:D:52:THR:CG2	2.47	0.45
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.16	0.45
5:A:217:ARG:CG	5:A:217:ARG:NH1	2.78	0.45
5:A:232:ARG:NH2	5:A:236:GLY:O	2.45	0.45
12:H:54:THR:O	12:H:55:VAL:HG13	2.16	0.45
14:K:101:ASN:O	14:K:102:GLU:HB2	2.17	0.45
14:K:118:ALA:O	14:K:119:GLN:C	2.59	0.45
26:W:3:ALA:O	26:W:54:PHE:HA	2.16	0.45
26:W:13:MET:HE3	26:W:17:ILE:CG2	2.45	0.45
26:W:21:LEU:HD13	26:W:26:ILE:HD11	1.99	0.45
32:3:6:ARG:HA	32:3:20:HIS:O	2.16	0.45
1:0:1067:A:H5'	40:0:4906:HOH:O	2.15	0.45
1:0:2338:G:H2'	8:D:129:ASP:OD1	2.16	0.45
6:B:86:ALA:HA	40:B:9575:HOH:O	2.15	0.45
7:C:5:ILE:HG13	7:C:15:GLU:HA	1.99	0.45
7:C:78:ARG:NH1	7:C:78:ARG:CG	2.76	0.45
13:J:8:ALA:HA	13:J:35:THR:HG22	1.98	0.45
26:W:11:VAL:O	26:W:12:ASN:HB2	2.15	0.45
26:W:59:GLN:NE2	26:W:97:ALA:HB3	2.32	0.45
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	1.98	0.45
33:I:92:PRO:C	33:I:94:GLU:N	2.72	0.45
1:0:1942:A:H3'	40:0:7785:HOH:O	2.16	0.45
1:0:1980:U:H5'	1:0:2626:C:H1'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
5:A:130:THR:HB	5:A:137:VAL:HB	1.97	0.45
12:H:43:TYR:HA	12:H:44:PRO:HD3	1.77	0.45
12:H:114:ARG:O	12:H:115:ALA:C	2.60	0.45
12:H:170:ASN:N	12:H:170:ASN:ND2	2.61	0.45
18:O:60:VAL:C	18:O:62:GLY:H	2.24	0.45
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.98	0.45
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.45
1:0:1205:U:H2'	1:0:1206:U:H5''	1.99	0.45
1:0:1441:G:H1'	40:0:8275:HOH:O	2.16	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.80	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
6:B:168:GLY:O	6:B:169:GLY:O	2.35	0.45
9:E:7:ILE:HD11	9:E:11:VAL:C	2.41	0.45
16:M:66:SER:HB3	16:M:128:TRP:CD1	2.51	0.45
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.51	0.45
33:I:116:LEU:HD22	33:I:127:GLU:OE1	2.17	0.45
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45
1:0:447:A:OP1	23:T:2:LYS:HG2	2.16	0.45
1:0:2101:A:H2'	7:C:63:SER:OG	2.16	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.45
1:0:2747:C:H4'	40:0:8429:HOH:O	2.16	0.45
6:B:97:LEU:HD21	40:B:9637:HOH:O	2.17	0.45
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.32	0.45
16:M:68:ARG:O	16:M:68:ARG:HD3	2.17	0.45
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.46	0.45
17:N:154:LEU:CG	17:N:155:GLU:H	2.25	0.45
23:T:107:LYS:NZ	40:T:4056:HOH:O	2.49	0.45
25:V:1:THR:O	25:V:2:VAL:C	2.59	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.45
2:9:3045:A:H4'	8:D:143:LYS:O	2.16	0.45
5:A:81:GLN:H	5:A:92:ASN:CG	2.24	0.45
5:A:85:SER:O	5:A:86:ALA:C	2.60	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.35	0.45
9:E:69:ILE:HA	9:E:72:MET:CE	2.47	0.45
9:E:95:VAL:HG11	9:E:131:LEU:HD11	1.97	0.45
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:131:THR:HB	13:J:134:GLU:OE1	2.16	0.45
15:L:143:THR:CG2	15:L:144:ASP:H	2.23	0.45
17:N:103:ASP:C	17:N:103:ASP:OD1	2.60	0.45
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.45	0.45
23:T:78:THR:HB	23:T:87:VAL:O	2.17	0.45
25:V:8:ILE:HG21	25:V:59:ILE:HG13	1.98	0.45
27:X:30:MET:HE1	27:X:58:ALA:CB	2.39	0.45
33:I:89:SER:HB2	33:I:95:ASP:HB2	1.99	0.45
1:O:1163:G:H2'	1:O:1164:U:C5	2.52	0.45
40:O:6180:HOH:O	23:T:68:ASP:HB2	2.16	0.45
5:A:223:ARG:CZ	40:A:9562:HOH:O	2.64	0.45
20:Q:30:VAL:HG12	20:Q:30:VAL:O	2.17	0.45
24:U:14:GLU:OE1	24:U:15:PRO:HD2	2.17	0.45
26:W:85:ALA:HB2	26:W:91:ASP:O	2.17	0.45
26:W:88:THR:CG2	26:W:90:TYR:HD1	2.29	0.45
26:W:108:ARG:CG	26:W:114:PRO:HG3	2.44	0.45
33:I:75:THR:OG1	33:I:112:LYS:HE2	2.17	0.45
1:O:962:C:H5'	40:O:7430:HOH:O	2.16	0.45
1:O:1167:G:H2'	1:O:1168:C:O4'	2.17	0.45
1:O:1201:C:C2'	1:O:1202:A:H5'	2.43	0.45
1:O:1574:C:H2'	1:O:1575:C:C6	2.52	0.45
1:O:2256:G:H2'	1:O:2257:G:H5'	1.99	0.45
5:A:131:HIS:O	5:A:132:ASP:HB2	2.17	0.45
7:C:119:ALA:HA	7:C:137:PRO:HD3	1.99	0.45
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.30	0.45
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.99	0.45
20:Q:53:HIS:CE1	20:Q:55:ARG:HB2	2.52	0.45
23:T:71:VAL:HG12	23:T:72:ILE:H	1.82	0.45
1:O:790:A:H1'	1:O:1710:A:H2'	1.99	0.45
1:O:1168:C:H5''	33:I:87:THR:HG23	1.99	0.45
1:O:1477:C:H5'	1:O:1868:G:C5'	2.47	0.45
1:O:2250:G:OP1	5:A:31:LYS:HD3	2.17	0.45
14:K:80:ILE:O	14:K:87:ARG:HA	2.16	0.45
16:M:46:LEU:HD22	16:M:50:ARG:HG3	1.98	0.45
17:N:67:ALA:C	17:N:69:TYR:N	2.74	0.45
20:Q:40:HIS:HD2	20:Q:60:THR:HG23	1.82	0.45
21:R:119:VAL:O	21:R:119:VAL:CG1	2.64	0.45
28:Y:187:VAL:HG23	28:Y:192:ASP:HB3	1.98	0.45
1:O:622:G:P	28:Y:148:GLY:HA3	2.57	0.45
1:O:816:G:H5'	1:O:1598:A:H4'	1.97	0.45
1:O:907:A:H2'	1:O:908:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.45
1:0:1180:U:H2'	1:0:1181:A:O4'	2.17	0.45
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.45
1:0:2541:U:C6	1:0:2541:U:C3'	3.00	0.45
5:A:167:LYS:HE3	29:Z:26:VAL:HG13	1.99	0.45
5:A:206:ARG:HD3	5:A:206:ARG:N	2.27	0.45
12:H:146:VAL:HG22	40:H:9543:HOH:O	2.17	0.45
16:M:120:VAL:CG1	16:M:130:GLU:HG3	2.46	0.45
16:M:158:ARG:HB2	16:M:163:LEU:HB2	1.97	0.45
18:O:23:GLY:C	40:O:3062:HOH:O	2.59	0.45
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.32	0.45
19:P:16:VAL:HG12	19:P:17:GLY:H	1.80	0.45
24:U:4:ARG:HG2	24:U:4:ARG:NH1	2.32	0.45
28:Y:144:ARG:CG	28:Y:144:ARG:NH1	2.71	0.45
1:0:1350:U:H2'	1:0:1351:G:O4'	2.17	0.44
1:0:2365:G:H4'	20:Q:45:PRO:O	2.17	0.44
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.44
1:0:2769:C:H2'	1:0:2770:G:O4'	2.17	0.44
4:5:76:A:OP1	4:5:76:A:H4'	2.17	0.44
5:A:105:VAL:HG12	5:A:106:CYS:H	1.82	0.44
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.67	0.44
10:F:33:THR:HG21	10:F:59:ILE:O	2.17	0.44
15:L:89:PHE:CD1	15:L:89:PHE:N	2.85	0.44
17:N:49:THR:HG22	17:N:56:ASP:CB	2.39	0.44
18:O:24:ALA:O	18:O:28:ASP:HB2	2.17	0.44
23:T:85:GLU:CG	23:T:86:GLU:N	2.79	0.44
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.98	0.44
28:Y:163:THR:HB	40:Y:9397:HOH:O	2.16	0.44
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.44
1:0:1163:G:H1	1:0:1184:C:N4	2.15	0.44
1:0:1593:C:OP1	19:P:117:SER:HB3	2.17	0.44
1:0:2443:C:H5'	15:L:57:VAL:HG21	1.99	0.44
2:9:3001:U:H5''	2:9:3003:A:OP1	2.17	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.44
2:9:3056:A:C3'	2:9:3057:A:H5''	2.47	0.44
6:B:175:LEU:C	6:B:175:LEU:CD2	2.91	0.44
9:E:31:ARG:NH1	40:E:5919:HOH:O	2.49	0.44
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.44
12:H:58:ARG:HG3	40:H:9520:HOH:O	2.18	0.44
14:K:115:ARG:O	14:K:118:ALA:HB3	2.16	0.44
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:149:ARG:O	15:L:150:GLN:HB2	2.16	0.44
25:V:42:ASN:O	25:V:44:GLY:N	2.50	0.44
1:0:656:G:H1'	40:C:9267:HOH:O	2.17	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.34	0.44
6:B:8:LYS:HG3	6:B:220:VAL:HG12	1.99	0.44
6:B:113:LEU:HD21	6:B:161:VAL:HG21	1.98	0.44
6:B:185:GLY:HA2	40:B:9628:HOH:O	2.16	0.44
7:C:107:ARG:NH1	40:C:9238:HOH:O	2.50	0.44
7:C:115:LEU:O	7:C:118:THR:HB	2.17	0.44
8:D:164:ALA:O	8:D:165:PHE:C	2.60	0.44
9:E:22:VAL:O	9:E:28:SER:HA	2.17	0.44
13:J:39:VAL:CG1	13:J:40:ASN:N	2.81	0.44
27:X:41:PHE:O	27:X:43:VAL:HG23	2.16	0.44
27:X:73:ARG:HB2	27:X:88:GLU:OE2	2.17	0.44
33:I:97:VAL:N	33:I:136:GLY:O	2.51	0.44
1:0:154:C:P	16:M:188:ARG:HH12	2.40	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
1:0:2453:G:H4'	15:L:50:GLY:C	2.42	0.44
5:A:179:MET:HG2	5:A:186:TRP:CG	2.52	0.44
8:D:78:GLU:O	8:D:82:GLU:HG3	2.18	0.44
10:F:5:ASP:O	10:F:119:ARG:NH1	2.50	0.44
13:J:42:GLU:O	13:J:131:THR:HG23	2.18	0.44
15:L:35:ARG:HB2	15:L:35:ARG:HH11	1.82	0.44
19:P:143:ALA:HA	40:P:164:HOH:O	2.17	0.44
1:0:82:C:OP1	23:T:67:LEU:HB2	2.18	0.44
1:0:407:A:H5'	40:0:6529:HOH:O	2.18	0.44
1:0:2100:A:H4'	7:C:64:GLY:O	2.16	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.44
2:9:3114:G:O6	17:N:11:ARG:HD3	2.17	0.44
12:H:78:GLY:C	12:H:80:GLU:H	2.25	0.44
21:R:119:VAL:HG21	21:R:142:ASP:CG	2.43	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.44
1:0:1104:C:H4'	13:J:88:PRO:HD3	1.99	0.44
1:0:1185:U:H5'	40:0:7899:HOH:O	2.18	0.44
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.82	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.52	0.44
1:0:2019:A:H5'	40:0:5087:HOH:O	2.17	0.44
40:0:3165:HOH:O	26:W:119:HIS:HE1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:53:LEU:CD1	6:B:327:VAL:HG22	2.46	0.44
6:B:85:ARG:HB2	6:B:99:GLU:HG2	1.99	0.44
18:O:60:VAL:HG12	18:O:62:GLY:H	1.81	0.44
23:T:71:VAL:CG1	23:T:72:ILE:N	2.80	0.44
25:V:56:ILE:HG22	25:V:60:GLN:NE2	2.32	0.44
33:I:92:PRO:O	33:I:94:GLU:N	2.50	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
1:0:645:U:OP2	15:L:4:LYS:HE2	2.18	0.44
1:0:1162:G:H1'	33:I:117:LEU:CD1	2.47	0.44
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.44
1:0:2296:C:H2'	1:0:2297:U:C6	2.52	0.44
1:0:2533:C:H6	1:0:2533:C:C5'	2.25	0.44
1:0:2748:G:H4'	1:0:2749:U:C5'	2.47	0.44
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.44
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.18	0.44
6:B:96:PRO:HG3	40:B:9629:HOH:O	2.17	0.44
6:B:217:ARG:HD3	6:B:218:TRP:NE1	2.33	0.44
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.33	0.44
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.44
17:N:183:ASP:O	17:N:184:ILE:C	2.61	0.44
25:V:5:VAL:HG23	40:V:2271:HOH:O	2.18	0.44
26:W:122:ARG:NE	40:W:5817:HOH:O	2.50	0.44
27:X:9:VAL:HG13	27:X:88:GLU:OE2	2.17	0.44
27:X:18:ARG:NH1	40:X:4132:HOH:O	2.50	0.44
28:Y:189:ASN:C	28:Y:189:ASN:ND2	2.76	0.44
28:Y:203:VAL:CG1	28:Y:228:VAL:HG22	2.48	0.44
31:2:5:LYS:O	31:2:9:LYS:HG3	2.17	0.44
33:I:139:ILE:HG22	33:I:140:GLU:N	2.32	0.44
1:0:29:C:O2'	1:0:30:U:H5'	2.18	0.44
1:0:656:G:H4'	40:C:9167:HOH:O	2.18	0.44
1:0:1044:C:H5''	40:0:9648:HOH:O	2.18	0.44
1:0:1119:G:H8	13:J:52:GLN:HE22	1.66	0.44
1:0:1350:U:H1'	40:0:3273:HOH:O	2.17	0.44
1:0:1771:U:C4'	29:Z:20:ARG:HE	2.30	0.44
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.44
1:0:2712:G:H5'	40:K:4183:HOH:O	2.17	0.44
1:0:2895:C:H4'	40:X:4132:HOH:O	2.18	0.44
5:A:103:VAL:O	5:A:105:VAL:HG23	2.18	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.53	0.44
1:0:1244:U:H2'	13:J:47:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.18	0.44
40:0:4557:HOH:O	23:T:82:THR:HA	2.17	0.44
6:B:71:VAL:CG1	6:B:296:LEU:HD22	2.48	0.44
7:C:95:GLU:H	7:C:95:GLU:CD	2.26	0.44
8:D:35:ALA:C	8:D:37:ALA:N	2.76	0.44
12:H:55:VAL:HG12	40:H:9540:HOH:O	2.18	0.44
18:O:4:ASN:HA	18:O:5:PRO:HD3	1.90	0.44
27:X:31:ILE:O	27:X:35:GLU:HG3	2.16	0.44
1:0:213:G:N2	1:0:225:G:H2'	2.33	0.43
1:0:556:C:H2'	1:0:557:C:C6	2.53	0.43
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.18	0.43
1:0:1086:A:C6	26:W:11:VAL:HG11	2.52	0.43
1:0:2044:G:OP1	27:X:23:HIS:HE1	2.01	0.43
5:A:132:ASP:HB3	5:A:135:VAL:H	1.83	0.43
7:C:219:ASN:N	7:C:222:ASP:OD1	2.44	0.43
13:J:75:PRO:HB3	13:J:132:LEU:HB3	2.00	0.43
15:L:144:ASP:O	15:L:147:GLU:HB2	2.18	0.43
21:R:61:GLN:NE2	40:R:9449:HOH:O	2.50	0.43
23:T:38:ARG:NH1	23:T:38:ARG:HG3	2.32	0.43
27:X:61:ARG:HG3	27:X:61:ARG:NH1	2.33	0.43
29:Z:30:GLU:HA	29:Z:33:MET:HB3	1.99	0.43
1:0:157:G:H4'	16:M:95:LYS:HE2	1.99	0.43
1:0:338:C:H5''	40:C:9230:HOH:O	2.16	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.53	0.43
1:0:2503:A:OP1	12:H:151:ARG:NH2	2.42	0.43
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.51	0.43
5:A:29:HIS:CD2	5:A:153:ARG:NH1	2.86	0.43
5:A:105:VAL:HG13	5:A:155:THR:O	2.18	0.43
6:B:279:THR:CG2	6:B:280:VAL:N	2.80	0.43
15:L:145:LEU:C	15:L:147:GLU:N	2.76	0.43
19:P:55:LYS:CG	19:P:56:GLY:N	2.80	0.43
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.85	0.43
23:T:30:ASP:O	23:T:33:GLU:HB3	2.18	0.43
23:T:96:VAL:HG13	23:T:97:ARG:N	2.32	0.43
26:W:13:MET:HE2	26:W:18:GLN:N	2.33	0.43
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.98	0.43
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	2.00	0.43
2:9:3057:A:C8	8:D:141:VAL:HG21	2.52	0.43
6:B:41:PHE:HA	6:B:79:MET:HE1	2.00	0.43
6:B:181:ILE:HG22	6:B:186:GLY:HA2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:88:LEU:N	8:D:89:PRO:CD	2.81	0.43
12:H:154:TYR:C	12:H:154:TYR:HD1	2.26	0.43
13:J:80:LYS:NZ	40:J:7377:HOH:O	2.49	0.43
28:Y:216:ARG:HD2	40:Y:9368:HOH:O	2.16	0.43
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.18	0.43
31:2:41:HIS:CD2	31:2:44:ARG:H	2.35	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
1:0:1174:A:H62	1:0:1200:A:H2'	1.83	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2787:C:H5	40:0:5178:HOH:O	2.01	0.43
40:0:5154:HOH:O	5:A:206:ARG:HD3	2.18	0.43
5:A:123:GLY:HA2	5:A:159:VAL:O	2.18	0.43
16:M:72:ALA:HB2	16:M:93:ARG:HG2	2.01	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1884:G:O6	5:A:190:ARG:HD2	2.16	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.17	0.43
2:9:3044:A:O4'	8:D:76:ARG:NE	2.51	0.43
5:A:69:LEU:HD23	5:A:107:ASN:CG	2.43	0.43
6:B:36:PRO:HB3	6:B:174:ARG:HB2	1.99	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.43
7:C:123:LEU:HD23	7:C:123:LEU:HA	1.86	0.43
17:N:11:ARG:CG	17:N:14:ARG:NH1	2.73	0.43
17:N:71:TRP:CE3	17:N:175:LEU:HD22	2.53	0.43
20:Q:59:GLN:HB3	40:Q:6286:HOH:O	2.17	0.43
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.18	0.43
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.18	0.43
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.43
1:0:588:G:O6	26:W:154:ARG:NH1	2.52	0.43
1:0:903:U:O4	15:L:18:HIS:HB2	2.17	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.51	0.43
1:0:1511:U:O2'	1:0:1512:G:H5'	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
1:0:2363:G:O3'	20:Q:11:ARG:NH1	2.51	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.43
1:0:2776:A:H2'	1:0:2777:G:O4'	2.18	0.43
40:0:6985:HOH:O	28:Y:141:THR:HG23	2.19	0.43
7:C:51:TYR:CD1	30:1:56:GLU:HB2	2.54	0.43
9:E:35:TYR:HB2	40:E:5715:HOH:O	2.18	0.43
10:F:11:ASP:O	10:F:14:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:47:ILE:HG21	40:H:9543:HOH:O	2.18	0.43
23:T:103:LEU:C	23:T:105:ASP:H	2.27	0.43
26:W:110:GLN:HE21	26:W:110:GLN:HA	1.84	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.83	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	1.98	0.43
1:0:2856:A:P	27:X:15:ARG:HH22	2.42	0.43
7:C:27:ARG:HD2	18:O:5:PRO:HD2	2.01	0.43
7:C:194:PHE:HA	7:C:234:VAL:HG13	2.01	0.43
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.01	0.43
12:H:56:GLN:HG2	12:H:126:ARG:HG2	2.00	0.43
15:L:12:THR:HG21	15:L:16:GLY:O	2.18	0.43
16:M:24:GLN:O	16:M:28:GLN:HG3	2.19	0.43
16:M:107:ARG:NH1	16:M:107:ARG:CG	2.77	0.43
19:P:13:VAL:HG21	19:P:41:ARG:HG2	2.01	0.43
23:T:79:LEU:HG	23:T:89:ARG:HB2	2.01	0.43
26:W:146:ILE:HD13	26:W:146:ILE:HA	1.92	0.43
30:1:53:LYS:HA	30:1:53:LYS:HD3	1.84	0.43
1:0:830:G:H2'	1:0:831:U:C6	2.54	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.43
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.43
1:0:2015:A:O2'	1:0:2016:U:H5'	2.19	0.43
1:0:2897:C:HO2'	6:B:285:VAL:HA	1.83	0.43
6:B:109:LEU:HD11	6:B:113:LEU:HD11	2.00	0.43
40:C:9167:HOH:O	18:O:3:THR:HG21	2.18	0.43
10:F:49:PHE:CB	10:F:83:LEU:HD11	2.49	0.43
10:F:52:GLU:HG3	10:F:77:VAL:O	2.19	0.43
17:N:67:ALA:C	17:N:69:TYR:H	2.26	0.43
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.52	0.43
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.43
1:0:710:G:N2	1:0:719:C:C2	2.87	0.43
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.43
1:0:1185:U:H4'	33:I:123:ASN:HB3	2.00	0.43
1:0:2676:C:H4'	13:J:70:PHE:HD1	1.83	0.43
40:O:4966:HOH:O	5:A:11:ARG:CZ	2.67	0.43
5:A:97:ALA:C	5:A:131:HIS:HE2	2.24	0.43
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.84	0.43
10:F:26:THR:HG21	10:F:102:GLY:C	2.44	0.43
12:H:166:SER:HB2	12:H:167:PRO:CD	2.48	0.43
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.99	0.43
17:N:74:PRO:HG2	17:N:159:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:52:THR:CG2	24:U:54:THR:HB	2.49	0.43
26:W:108:ARG:HE	26:W:114:PRO:CG	2.32	0.43
1:0:818:A:O2'	29:Z:13:ARG:HD2	2.19	0.43
1:0:821:U:H2'	1:0:822:C:H6	1.84	0.43
1:0:883:U:O2	1:0:883:U:C2'	2.65	0.43
1:0:2515:C:H2'	1:0:2516:G:O4'	2.19	0.43
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.87	0.43
10:F:101:ALA:HA	40:F:5413:HOH:O	2.19	0.43
12:H:2:PRO:HD2	12:H:5:MET:SD	2.58	0.43
13:J:39:VAL:HG21	13:J:107:ASN:ND2	2.34	0.43
14:K:13:GLU:OE1	14:K:44:LEU:HD12	2.19	0.43
19:P:55:LYS:HG2	19:P:56:GLY:N	2.33	0.43
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.49	0.43
19:P:115:SER:O	19:P:116:SER:C	2.62	0.43
21:R:113:HIS:HE1	21:R:144:GLU:CD	2.27	0.43
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.33	0.43
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.54	0.43
1:0:185:G:H4'	1:0:186:A:H4'	2.00	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
1:0:797:A:O4'	29:Z:10:ARG:N	2.51	0.42
1:0:1008:C:H2'	1:0:1009:U:C6	2.54	0.42
1:0:2072:G:N2	40:0:7335:HOH:O	2.50	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.42
1:0:2851:G:H4'	6:B:157:LYS:NZ	2.34	0.42
5:A:207:GLN:O	5:A:208:HIS:HB3	2.19	0.42
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.54	0.42
6:B:102:THR:HG23	6:B:182:VAL:HG12	1.99	0.42
7:C:246:ARG:NH1	7:C:246:ARG:HB3	2.33	0.42
22:S:37:VAL:O	22:S:41:VAL:HG23	2.18	0.42
22:S:57:THR:C	22:S:59:ASP:H	2.27	0.42
25:V:12:THR:OG1	25:V:13:PRO:HD2	2.19	0.42
31:2:10:ARG:HH11	31:2:49:GLU:CD	2.27	0.42
1:0:461:C:N3	1:0:479:G:H5'	2.34	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.52	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:2748:G:H5'	40:0:7972:HOH:O	2.19	0.42
1:0:2866:U:C4	24:U:50:GLU:HB3	2.55	0.42
40:9:5851:HOH:O	17:N:115:VAL:HG13	2.19	0.42
15:L:91:VAL:HG12	15:L:120:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:42:ARG:HA	16:M:43:PRO:HD3	1.87	0.42
26:W:142:ASP:HB3	26:W:145:GLY:H	1.84	0.42
31:2:44:ARG:HD3	31:2:44:ARG:HA	1.78	0.42
33:I:102:VAL:HG23	33:I:140:GLU:O	2.18	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
1:0:709:G:O2'	18:O:25:VAL:CG1	2.67	0.42
1:0:816:G:C6	1:0:817:G:N1	2.87	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.30	0.42
1:0:1315:G:C4	28:Y:212:ARG:HB2	2.55	0.42
1:0:1363:G:OP1	7:C:76:ARG:NH2	2.48	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.84	0.42
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
1:0:2663:U:O2	40:0:8435:HOH:O	2.22	0.42
5:A:194:MET:HE3	5:A:199:HIS:CB	2.48	0.42
6:B:54:VAL:O	6:B:55:ASN:C	2.62	0.42
8:D:128:LEU:C	8:D:128:LEU:HD23	2.44	0.42
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.42
31:2:48:ASP:O	31:2:49:GLU:HB2	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:945:U:H2'	1:0:946:C:C6	2.55	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.42
1:0:2415:A:O2'	17:N:29:SER:HB3	2.19	0.42
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.84	0.42
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.85	0.42
11:G:64:ASN:N	11:G:64:ASN:ND2	2.67	0.42
17:N:181:ASP:O	17:N:184:ILE:HG22	2.19	0.42
18:O:98:LEU:O	18:O:102:ILE:HG13	2.19	0.42
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.19	0.42
1:0:1257:C:H2'	1:0:1258:G:O4'	2.19	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.19	0.42
40:0:7289:HOH:O	7:C:175:LYS:HE3	2.19	0.42
13:J:132:LEU:HD23	13:J:132:LEU:HA	1.82	0.42
16:M:167:GLY:O	16:M:171:ARG:HG3	2.20	0.42
18:O:59:VAL:HG21	18:O:111:VAL:HG21	2.02	0.42
19:P:13:VAL:HG11	19:P:40:VAL:HG12	2.01	0.42
21:R:122:GLN:HB3	21:R:138:SER:HB2	2.00	0.42
22:S:33:SER:OG	22:S:36:GLU:HG3	2.19	0.42
22:S:51:GLN:HE21	22:S:53:ASN:ND2	1.90	0.42
23:T:14:ALA:HA	23:T:15:PRO:HD3	1.95	0.42
27:X:20:GLU:CG	27:X:21:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	2.01	0.42
1:0:325:U:H2'	1:0:326:G:H8	1.84	0.42
1:0:710:G:H5'	18:O:25:VAL:CG1	2.49	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.20	0.42
1:0:1574:C:O5'	1:0:1574:C:H6	2.02	0.42
1:0:2248:C:H3'	40:0:5967:HOH:O	2.18	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.42
1:0:2713:G:O2'	1:0:2714:U:H5'	2.20	0.42
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.42
2:9:3004:G:O2'	17:N:44:ARG:NH2	2.53	0.42
5:A:109:GLU:HG2	5:A:116:GLY:H	1.85	0.42
5:A:113:GLY:HA2	5:A:153:ARG:NH2	2.34	0.42
14:K:49:LEU:CD1	14:K:80:ILE:HD13	2.49	0.42
16:M:15:PRO:HA	16:M:20:LEU:HD23	2.02	0.42
27:X:9:VAL:HG13	27:X:88:GLU:CD	2.45	0.42
1:0:107:U:H2'	1:0:108:U:H5'	2.02	0.42
1:0:470:U:O2'	30:1:16:HIS:CD2	2.70	0.42
1:0:564:G:H1'	40:0:6803:HOH:O	2.18	0.42
1:0:1298:U:H2'	1:0:1299:G:H8	1.85	0.42
1:0:1422:U:H2'	1:0:1423:C:C6	2.55	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.20	0.42
2:9:3023:U:O2'	2:9:3024:U:H4'	2.19	0.42
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.85	0.42
13:J:74:ARG:HH12	13:J:76:ASP:CB	2.30	0.42
17:N:36:ALA:HB1	17:N:118:ILE:HD12	2.02	0.42
17:N:82:TYR:CD2	17:N:82:TYR:C	2.97	0.42
18:O:38:ARG:NH1	40:O:7674:HOH:O	2.53	0.42
23:T:12:ARG:NH1	40:T:3035:HOH:O	2.47	0.42
25:V:1:THR:CG2	25:V:2:VAL:N	2.82	0.42
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.83	0.42
29:Z:10:ARG:C	29:Z:12:GLY:H	2.26	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
1:0:271:C:C2	1:0:273:G:O4'	2.73	0.42
1:0:1205:U:C2'	1:0:1206:U:H5''	2.50	0.42
1:0:2821:C:H4'	6:B:116:PRO:HG3	2.01	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
5:A:51:ARG:NH1	5:A:120:ARG:O	2.53	0.42
6:B:17:LYS:O	6:B:260:HIS:CD2	2.70	0.42
7:C:218:VAL:N	40:C:9232:HOH:O	2.52	0.42
10:F:67:ALA:HB1	10:F:72:VAL:O	2.19	0.42
12:H:14:TYR:CD2	12:H:94:VAL:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:6:ARG:NH2	40:L:9444:HOH:O	2.53	0.42
20:Q:8:GLU:C	20:Q:8:GLU:CD	2.88	0.42
20:Q:94:GLN:O	20:Q:95:GLU:HB2	2.20	0.42
27:X:7:GLU:HA	27:X:75:ALA:HA	2.00	0.42
33:I:118:SER:HB2	33:I:123:ASN:HB2	2.02	0.42
1:0:380:A:H2'	40:0:7673:HOH:O	2.19	0.42
1:0:695:C:H2'	1:0:696:C:C6	2.54	0.42
1:0:1733:A:H4'	6:B:212:GLN:HA	2.02	0.42
1:0:2716:G:H5''	6:B:206:THR:CG2	2.45	0.42
2:9:3006:C:H4'	17:N:35:VAL:HG11	2.02	0.42
5:A:33:GLU:OE1	5:A:33:GLU:N	2.36	0.42
6:B:277:GLU:N	6:B:278:PRO:CD	2.82	0.42
10:F:99:THR:O	10:F:99:THR:HG23	2.19	0.42
11:G:23:ILE:O	11:G:27:ILE:HG13	2.20	0.42
12:H:51:VAL:CG1	12:H:53:GLU:O	2.67	0.42
14:K:20:CYS:HB2	14:K:29:LEU:HG	2.01	0.42
15:L:19:LYS:NZ	40:L:9417:HOH:O	2.52	0.42
15:L:133:VAL:HB	40:L:9452:HOH:O	2.19	0.42
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.48	0.42
17:N:173:ASP:O	17:N:177:GLU:HB2	2.20	0.42
22:S:51:GLN:NE2	22:S:53:ASN:HD21	1.90	0.42
29:Z:46:ARG:O	29:Z:57:CYS:HA	2.19	0.42
1:0:1314:U:H2'	40:0:6383:HOH:O	2.20	0.42
1:0:1363:G:P	7:C:76:ARG:HH22	2.43	0.42
1:0:1367:A:H2'	1:0:1368:U:O4'	2.19	0.42
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.42
1:0:1940:C:H4'	40:0:7785:HOH:O	2.19	0.42
1:0:2089:A:O2'	1:0:2090:G:H5'	2.20	0.42
1:0:2456:A:H2'	1:0:2457:U:H6	1.85	0.42
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.42
8:D:10:PHE:CD1	8:D:11:HIS:N	2.88	0.42
11:G:63:ARG:HB2	11:G:66:LEU:HG	2.02	0.42
15:L:104:ASP:HB2	40:L:9460:HOH:O	2.19	0.42
27:X:80:GLU:HB3	40:X:5564:HOH:O	2.19	0.42
32:3:48:ASN:ND2	32:3:50:GLY:H	2.18	0.42
33:I:92:PRO:HD3	40:I:1549:HOH:O	2.19	0.42
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
1:0:1311:G:O2'	1:0:1312:G:H5'	2.20	0.41
1:0:1473:U:O2'	1:0:1474:C:H5''	2.20	0.41
5:A:122:SER:O	5:A:124:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:167:GLU:OE2	8:D:173:GLU:HB3	2.20	0.41
10:F:38:LYS:HZ3	16:M:3:SER:HA	1.85	0.41
22:S:56:ASN:O	31:2:8:LYS:NZ	2.47	0.41
32:3:55:VAL:HB	32:3:56:PRO:HD2	2.02	0.41
32:3:69:TYR:O	32:3:77:ALA:HA	2.19	0.41
1:0:396:U:OP2	32:3:38:ARG:HD2	2.19	0.41
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.46	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.28	0.41
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.41
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.85	0.41
40:0:7460:HOH:O	20:Q:9:GLY:HA2	2.20	0.41
40:0:7470:HOH:O	6:B:264:GLU:HG3	2.19	0.41
5:A:75:GLY:HA2	29:Z:64:PHE:HA	2.02	0.41
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.93	0.41
15:L:144:ASP:HA	15:L:147:GLU:CD	2.45	0.41
21:R:104:PHE:HB3	21:R:109:MET:CE	2.49	0.41
25:V:45:ARG:O	25:V:48:GLU:N	2.53	0.41
32:3:62:THR:HB	40:3:9487:HOH:O	2.20	0.41
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.21	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.35	0.41
7:C:21:VAL:C	7:C:23:GLU:N	2.79	0.41
8:D:146:LYS:O	8:D:147:ALA:C	2.63	0.41
8:D:163:VAL:HA	40:D:6326:HOH:O	2.20	0.41
8:D:170:TYR:CD1	8:D:170:TYR:N	2.89	0.41
12:H:169:GLY:HA3	40:H:9557:HOH:O	2.20	0.41
19:P:16:VAL:CG1	19:P:17:GLY:N	2.83	0.41
26:W:38:THR:HG22	26:W:39:ASP:H	1.85	0.41
33:I:80:LYS:HD3	33:I:86:GLU:O	2.20	0.41
1:0:1086:A:N6	26:W:11:VAL:HG11	2.35	0.41
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.41
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
1:0:1451:C:H5'	1:0:1505:U:C4	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
10:F:117:GLU:C	10:F:119:ARG:N	2.78	0.41
16:M:81:ARG:HG2	16:M:85:ARG:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:14:LEU:HG	18:O:102:ILE:HD11	2.03	0.41
19:P:89:ASN:HB3	19:P:92:GLU:HB2	2.01	0.41
20:Q:28:ARG:HG2	40:Q:4350:HOH:O	2.20	0.41
24:U:47:ARG:HG2	24:U:54:THR:HG21	2.03	0.41
28:Y:154:ARG:CG	28:Y:154:ARG:HH11	2.34	0.41
31:2:36:ASN:C	31:2:38:LYS:H	2.27	0.41
1:0:20:G:H5''	1:0:510:U:O4	2.21	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:790:A:H1'	1:0:1710:A:O2'	2.21	0.41
1:0:1181:A:H2'	1:0:1182:C:H5'	2.03	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.04	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.55	0.41
5:A:29:HIS:CD2	5:A:153:ARG:HH12	2.37	0.41
5:A:53:ALA:HB3	40:A:9591:HOH:O	2.20	0.41
15:L:73:VAL:HG23	15:L:74:THR:N	2.32	0.41
21:R:96:VAL:O	21:R:99:ALA:HB3	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:CG2	2.68	0.41
27:X:20:GLU:CD	27:X:21:PRO:HD2	2.46	0.41
1:0:407:A:H8	40:0:5010:HOH:O	2.03	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
5:A:6:GLY:HA3	40:A:9557:HOH:O	2.20	0.41
5:A:36:ASP:HA	5:A:83:GLY:HA3	2.02	0.41
6:B:81:ALA:HB1	6:B:142:LEU:HD13	2.03	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.67	0.41
8:D:96:SER:C	8:D:98:PHE:H	2.28	0.41
14:K:41:LYS:O	14:K:42:ASN:HB2	2.20	0.41
17:N:170:GLU:O	17:N:174:GLU:HG3	2.21	0.41
26:W:21:LEU:HD22	26:W:26:ILE:HD11	2.02	0.41
29:Z:30:GLU:HG2	29:Z:33:MET:CE	2.51	0.41
33:I:110:GLU:HA	33:I:113:HIS:CD2	2.55	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.41
1:0:447:A:OP1	23:T:1:SER:HB2	2.21	0.41
1:0:1535:G:H2'	1:0:1536:C:C6	2.56	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.21	0.41
2:9:3039:U:O2'	2:9:3042:C:H5	2.03	0.41
5:A:30:ARG:HE	5:A:30:ARG:HB3	1.64	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.03	0.41
6:B:79:MET:C	6:B:80:ARG:HG2	2.44	0.41
15:L:66:VAL:HG23	15:L:67:ARG:N	2.35	0.41
16:M:164:THR:CG2	16:M:166:ALA:H	2.32	0.41
17:N:108:SER:HA	17:N:109:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:45:LEU:CD1	18:O:88:LYS:HD2	2.51	0.41
1:O:1025:C:H5'	26:W:23:MET:O	2.21	0.41
1:O:1076:G:C2	1:O:1084:C:C2	3.09	0.41
1:O:1427:A:N6	1:O:1440:U:H1'	2.33	0.41
1:O:1594:C:O2'	1:O:1607:A:H4'	2.21	0.41
1:O:1849:G:H1'	1:O:2011:A:N1	2.35	0.41
1:O:2335:C:H2'	1:O:2336:G:C8	2.56	0.41
40:O:3646:HOH:O	19:P:91:LYS:HA	2.21	0.41
40:O:4333:HOH:O	23:T:9:LYS:HD2	2.20	0.41
6:B:18:ARG:HE	6:B:256:GLN:NE2	2.19	0.41
6:B:41:PHE:CD1	6:B:79:MET:CE	3.04	0.41
7:C:61:PHE:HB3	40:C:9251:HOH:O	2.20	0.41
10:F:12:LEU:HD23	10:F:12:LEU:O	2.21	0.41
13:J:143:LYS:HA	13:J:145:TRP:CZ3	2.55	0.41
15:L:94:ARG:NH1	15:L:143:THR:HG21	2.36	0.41
15:L:124:ASP:OD1	15:L:149:ARG:NH2	2.54	0.41
16:M:76:ARG:HG3	16:M:88:VAL:HG21	2.03	0.41
21:R:33:ARG:NH1	40:R:9452:HOH:O	2.51	0.41
25:V:43:PRO:O	25:V:46:ILE:HG22	2.19	0.41
26:W:5:VAL:O	26:W:52:VAL:HG23	2.20	0.41
29:Z:39:CYS:HA	29:Z:40:PRO:HD3	1.97	0.41
31:2:11:LEU:HD23	31:2:11:LEU:HA	1.91	0.41
31:2:39:ARG:HG2	40:2:3143:HOH:O	2.21	0.41
1:O:271:C:H41	1:O:378:A:H2	1.68	0.41
1:O:284:C:H4'	1:O:285:A:H8	1.86	0.41
1:O:392:U:H5''	16:M:193:LYS:HB3	2.01	0.41
1:O:737:A:C8	1:O:737:A:H3'	2.56	0.41
1:O:875:A:C2	5:A:194:MET:SD	3.14	0.41
1:O:1181:A:H4'	33:I:92:PRO:HG2	2.03	0.41
1:O:1414:A:H2'	1:O:1415:G:O4'	2.20	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.21	0.41
1:O:1882:C:OP1	5:A:192:VAL:HG23	2.21	0.41
1:O:2336:G:H1'	40:D:5675:HOH:O	2.20	0.41
1:O:2748:G:H4'	1:O:2749:U:H5'	2.02	0.41
1:O:2819:C:O4'	6:B:96:PRO:HB2	2.21	0.41
1:O:2820:A:H2'	1:O:2821:C:C6	2.56	0.41
40:O:3421:HOH:O	6:B:252:PRO:HD3	2.21	0.41
5:A:65:ARG:HG2	5:A:65:ARG:NH1	2.36	0.41
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.33	0.41
6:B:27:ASN:HD22	6:B:27:ASN:H	1.69	0.41
8:D:23:VAL:O	8:D:23:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:84:MET:HB2	9:E:131:LEU:HB2	2.03	0.41
10:F:79:GLN:HB2	10:F:82:ASP:OD2	2.21	0.41
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.99	0.41
14:K:107:THR:HG22	14:K:108:GLU:CG	2.44	0.41
17:N:24:LEU:HD13	20:Q:26:PRO:HB3	2.02	0.41
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.47	0.41
19:P:134:VAL:O	19:P:137:LEU:HB3	2.21	0.41
23:T:81:LYS:HD2	23:T:87:VAL:HG11	2.03	0.41
26:W:54:PHE:CZ	26:W:140:LYS:HB2	2.55	0.41
27:X:45:GLU:HG3	40:X:6178:HOH:O	2.21	0.41
29:Z:36:ASP:HB3	29:Z:45:ASP:O	2.21	0.41
33:I:93:GLN:HA	33:I:96:PHE:CE2	2.54	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.21	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.36	0.41
1:0:2767:C:OP1	6:B:318:ASN:ND2	2.54	0.41
1:0:2828:G:H2'	1:0:2829:G:O4'	2.21	0.41
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.41
15:L:120:LEU:HD12	15:L:133:VAL:HG21	2.02	0.41
18:O:14:LEU:HD23	18:O:102:ILE:HD11	2.02	0.41
21:R:68:HIS:CD2	21:R:76:ASP:HB2	2.56	0.41
24:U:17:THR:HG21	40:U:3194:HOH:O	2.21	0.41
26:W:4:LEU:HD23	26:W:54:PHE:HB3	2.03	0.41
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.56	0.41
30:1:28:HIS:O	30:1:32:LYS:N	2.49	0.41
31:2:20:ARG:HG3	31:2:21:VAL:H	1.86	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.40
1:0:556:C:H2'	1:0:557:C:H6	1.86	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.40
1:0:1724:U:H5''	40:0:4311:HOH:O	2.19	0.40
1:0:1816:C:H2'	1:0:1817:U:O4'	2.21	0.40
1:0:2720:C:O2	14:K:87:ARG:NH2	2.54	0.40
40:0:9644:HOH:O	15:L:30:ARG:HD2	2.20	0.40
5:A:135:VAL:O	5:A:135:VAL:HG13	2.21	0.40
7:C:57:PRO:O	7:C:58:ALA:C	2.64	0.40
7:C:72:LYS:HG2	7:C:77:ALA:HA	2.02	0.40
7:C:140:VAL:HG12	7:C:141:SER:N	2.36	0.40
25:V:1:THR:OG1	25:V:2:VAL:N	2.53	0.40
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.36	0.40
1:0:1119:G:C6	1:0:1244:U:C5	3.09	0.40
1:0:2329:C:O2'	1:0:2330:U:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2361:A:H2'	1:0:2362:A:O4'	2.21	0.40
1:0:2748:G:C5'	40:0:7972:HOH:O	2.69	0.40
5:A:38:ILE:HD13	5:A:38:ILE:HA	1.92	0.40
6:B:183:GLU:O	6:B:184:ASP:C	2.64	0.40
6:B:278:PRO:HD3	6:B:294:TYR:CE2	2.56	0.40
8:D:21:VAL:HA	8:D:131:THR:O	2.21	0.40
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.51	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.92	0.40
17:N:37:ARG:HD3	17:N:37:ARG:HA	1.69	0.40
20:Q:43:ILE:HG13	20:Q:52:PHE:CZ	2.56	0.40
26:W:4:LEU:CD1	26:W:24:LEU:HD13	2.51	0.40
1:0:120:A:H2'	1:0:120:A:N3	2.37	0.40
1:0:1589:G:N2	1:0:1605:G:H1'	2.35	0.40
1:0:1829:A:C8	1:0:1885:A:C8	3.09	0.40
1:0:2101:A:H5'	7:C:63:SER:HB3	2.04	0.40
1:0:2824:C:C5'	1:0:2825:C:H5'	2.51	0.40
5:A:43:VAL:O	5:A:44:ASP:HB2	2.21	0.40
6:B:60:SER:HA	6:B:61:PRO:HD3	1.92	0.40
6:B:81:ALA:O	6:B:186:GLY:HA3	2.22	0.40
6:B:279:THR:HG23	6:B:280:VAL:N	2.35	0.40
7:C:84:VAL:HG12	7:C:85:LYS:HG2	2.04	0.40
8:D:67:ASP:O	8:D:69:ILE:HG13	2.21	0.40
8:D:91:ALA:HB2	8:D:106:PHE:CD2	2.56	0.40
12:H:79:GLU:C	12:H:80:GLU:HG3	2.46	0.40
17:N:152:GLU:C	17:N:154:LEU:N	2.77	0.40
23:T:18:GLU:O	23:T:21:LYS:HG2	2.22	0.40
25:V:8:ILE:CG2	25:V:59:ILE:HG13	2.51	0.40
25:V:42:ASN:HB3	40:V:7247:HOH:O	2.21	0.40
28:Y:96:GLU:O	28:Y:235:GLU:HA	2.21	0.40
28:Y:115:ARG:NE	40:Y:9353:HOH:O	2.55	0.40
28:Y:187:VAL:CG1	28:Y:205:ILE:HG12	2.51	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
1:0:1235:G:C1'	13:J:63:ILE:HG23	2.51	0.40
1:0:1299:G:N2	40:0:5226:HOH:O	2.53	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.21	0.40
40:0:7989:HOH:O	32:3:60:LYS:HG3	2.21	0.40
6:B:62:ARG:CB	6:B:65:MET:HE3	2.52	0.40
12:H:76:GLU:C	12:H:77:LEU:HD23	2.46	0.40
18:O:59:VAL:HG23	18:O:111:VAL:HG23	2.02	0.40
1:0:423:A:O2'	1:0:424:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:1081:A:H5''	40:0:3742:HOH:O	2.21	0.40
1:0:1626:A:H2'	1:0:1627:G:C5'	2.52	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.04	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
2:9:3002:U:OP2	2:9:3003:A:H5'	2.22	0.40
2:9:3008:G:OP1	17:N:23:ARG:NH1	2.51	0.40
2:9:3091:C:H2'	2:9:3092:G:O4'	2.22	0.40
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.52	0.40
7:C:57:PRO:HG2	7:C:73:LEU:CD1	2.51	0.40
8:D:25:MET:HE1	8:D:40:ILE:HD11	2.02	0.40
11:G:16:LYS:O	11:G:20:VAL:HG23	2.22	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
13:J:103:VAL:HG12	40:J:5907:HOH:O	2.21	0.40
14:K:125:ALA:C	14:K:127:ALA:N	2.80	0.40
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.03	0.40
17:N:138:ASP:O	17:N:139:TRP:C	2.65	0.40
21:R:61:GLN:CD	40:R:9449:HOH:O	2.65	0.40
30:1:25:LYS:CG	31:2:49:GLU:H	2.35	0.40
32:3:30:GLN:HE21	32:3:30:GLN:HB3	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	9	14
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	8	12
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	16	25
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	4	4
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	4	4
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	3	3
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	25
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	9	13
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	24	37
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	1	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	7	10
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	2	2
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	4	5
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	18
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	3	3
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	8	12

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO

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Mol	Chain	Res	Type
10	F	101	ALA
12	H	166	SER
13	J	143	LYS
15	L	80	ASP
17	N	154	LEU
17	N	184	ILE
29	Z	81	ARG
5	A	37	VAL
6	B	34	GLY
8	D	27	ILE
8	D	61	PHE
8	D	65	GLU
12	H	168	ALA
15	L	143	THR
16	M	83	SER
23	T	53	GLY
25	V	43	PRO
29	Z	20	ARG
31	2	37	HIS
33	I	129	VAL
5	A	86	ALA
6	B	185	GLY
8	D	28	GLY
8	D	56	ARG
8	D	164	ALA
10	F	71	GLY
17	N	183	ASP
23	T	46	ASP
5	A	34	ASP
7	C	8	LEU
7	C	58	ALA
8	D	171	ASP
12	H	16	ARG
12	H	81	GLY
13	J	5	GLU
13	J	7	ASP
17	N	65	ASP
17	N	155	GLU
17	N	162	ASP
8	D	77	ASP
10	F	100	ASP
14	K	126	SER

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Mol	Chain	Res	Type
17	N	164	ASP
17	N	167	ASP
29	Z	42	CYS
32	3	56	PRO
6	B	2	GLN
8	D	16	PRO
13	J	65	ASN
17	N	68	GLU
25	V	40	PRO
25	V	2	VAL
6	B	181	ILE
33	I	73	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%)	165 (92%)	14 (8%)	11	20
6	B	282/283 (100%)	262 (93%)	20 (7%)	13	23
7	C	193/193 (100%)	174 (90%)	19 (10%)	7	12
8	D	117/148 (79%)	114 (97%)	3 (3%)	40	63
9	E	152/156 (97%)	146 (96%)	6 (4%)	28	48
10	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	29	49
13	J	118/121 (98%)	109 (92%)	9 (8%)	12	21
14	K	106/106 (100%)	98 (92%)	8 (8%)	12	21
15	L	113/127 (89%)	110 (97%)	3 (3%)	39	62
16	M	158/158 (100%)	154 (98%)	4 (2%)	42	64
17	N	149/150 (99%)	141 (95%)	8 (5%)	20	35
18	O	93/94 (99%)	91 (98%)	2 (2%)	45	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	P	113/117 (97%)	109 (96%)	4 (4%)	32	53
20	Q	79/80 (99%)	74 (94%)	5 (6%)	16	29
21	R	117/122 (96%)	114 (97%)	3 (3%)	40	63
22	S	71/74 (96%)	70 (99%)	1 (1%)	59	79
23	T	105/106 (99%)	99 (94%)	6 (6%)	18	33
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	48	70
26	W	130/130 (100%)	125 (96%)	5 (4%)	29	49
27	X	66/74 (89%)	61 (92%)	5 (8%)	12	21
28	Y	120/196 (61%)	109 (91%)	11 (9%)	8	14
29	Z	60/68 (88%)	58 (97%)	2 (3%)	33	55
30	1	46/47 (98%)	45 (98%)	1 (2%)	45	67
31	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
32	3	79/79 (100%)	76 (96%)	3 (4%)	29	49
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2942 (95%)	151 (5%)	22	39

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

Mol	Chain	Res	Type
5	A	3	ARG
5	A	26	ASP
5	A	33	GLU
5	A	36	ASP
5	A	55	VAL
5	A	62	ASP
5	A	94	LEU
5	A	131	HIS
5	A	151	GLN
5	A	165	THR
5	A	175	LYS
5	A	179	MET
5	A	206	ARG
5	A	217	ARG
6	B	11	LEU
6	B	27	ASN
6	B	71	VAL

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Mol	Chain	Res	Type
6	B	82	VAL
6	B	84	LEU
6	B	98	THR
6	B	103	ASP
6	B	113	LEU
6	B	149	ASP
6	B	162	MET
6	B	175	LEU
6	B	190	MET
6	B	195	ARG
6	B	251	VAL
6	B	254	GLN
6	B	265	LEU
6	B	277	GLU
6	B	279	THR
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	16	VAL
7	C	67	GLN
7	C	76	ARG
7	C	78	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	50	VAL
8	D	137	PRO
9	E	7	ILE
9	E	86	VAL
9	E	102	VAL

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Mol	Chain	Res	Type
9	E	108	LEU
9	E	155	ASN
9	E	156	ASP
10	F	12	LEU
10	F	46	GLU
12	H	18	GLU
12	H	84	LYS
12	H	88	ARG
12	H	154	TYR
12	H	159	PRO
13	J	7	ASP
13	J	39	VAL
13	J	45	VAL
13	J	46	ILE
13	J	52	GLN
13	J	74	ARG
13	J	93	ARG
13	J	127	ILE
13	J	131	THR
14	K	4	LEU
14	K	10	GLN
14	K	44	LEU
14	K	56	SER
14	K	84	ASP
14	K	98	VAL
14	K	100	GLU
14	K	107	THR
15	L	35	ARG
15	L	43	HIS
15	L	140	VAL
16	M	46	LEU
16	M	93	ARG
16	M	99	ARG
16	M	164	THR
17	N	12	ARG
17	N	17	ARG
17	N	26	LEU
17	N	49	THR
17	N	65	ASP
17	N	127	LEU
17	N	139	TRP
17	N	152	GLU

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Mol	Chain	Res	Type
18	O	43	VAL
18	O	111	VAL
19	P	21	VAL
19	P	52	LYS
19	P	98	ILE
19	P	117	SER
20	Q	11	ARG
20	Q	16	ASN
20	Q	18	PRO
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	132	ARG
21	R	143	VAL
22	S	10	VAL
23	T	5	ASP
23	T	39	ASN
23	T	48	VAL
23	T	80	GLU
23	T	89	ARG
23	T	96	VAL
25	V	65	ASP
26	W	26	ILE
26	W	35	VAL
26	W	78	ASP
26	W	122	ARG
26	W	146	ILE
27	X	56	GLU
27	X	72	VAL
27	X	79	GLU
27	X	82	GLU
27	X	85	VAL
28	Y	103	THR
28	Y	141	THR
28	Y	144	ARG
28	Y	154	ARG
28	Y	163	THR
28	Y	174	VAL
28	Y	187	VAL
28	Y	189	ASN
28	Y	200	THR
28	Y	231	PRO

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Mol	Chain	Res	Type
28	Y	235	GLU
29	Z	44	GLU
29	Z	78	THR
30	1	47	ASP
31	2	18	ASN
32	3	40	ARG
32	3	56	PRO
32	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	5	GLN
5	A	29	HIS
5	A	125	ASN
5	A	188	ASN
5	A	199	HIS
5	A	218	ASN
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	178	GLN
8	D	47	GLN
8	D	103	ASN
8	D	133	ASN
9	E	106	ASN
9	E	143	GLN
10	F	80	GLN
11	G	64	ASN
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	92	HIS
12	H	128	GLN
12	H	170	ASN

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Mol	Chain	Res	Type
13	J	25	GLN
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	77	HIS
16	M	170	ASN
17	N	22	GLN
17	N	93	GLN
17	N	107	ASN
17	N	140	GLN
17	N	153	GLN
18	O	100	GLN
18	O	110	HIS
19	P	50	GLN
19	P	66	GLN
19	P	73	HIS
19	P	88	GLN
19	P	101	GLN
19	P	118	GLN
20	Q	40	HIS
21	R	22	GLN
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
21	R	122	GLN
21	R	140	GLN
22	S	44	GLN
22	S	51	GLN
22	S	53	ASN
22	S	55	GLN
22	S	75	GLN
23	T	11	GLN
23	T	37	GLN
23	T	39	ASN
23	T	43	ASN
24	U	39	ASN

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Mol	Chain	Res	Type
24	U	48	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	59	GLN
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	22	ASN
28	Y	119	GLN
28	Y	133	HIS
28	Y	134	HIS
28	Y	149	GLN
28	Y	153	GLN
28	Y	189	ASN
29	Z	41	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	18	GLN
32	3	30	GLN
32	3	48	ASN
33	I	104	GLN
33	I	113	HIS
33	I	123	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	240 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	256 (8%)	33 (1%)

All (256) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	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	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
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

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Mol	Chain	Res	Type
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	581	G
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	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	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

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Mol	Chain	Res	Type
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
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	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1528	A
1	0	1592	G

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Mol	Chain	Res	Type
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1686	C
1	0	1692	C
1	0	1693	A
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	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
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
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

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Mol	Chain	Res	Type
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
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	2467	A
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
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
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	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U

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Mol	Chain	Res	Type
1	0	2648	U
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
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	2783	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
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
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A

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Mol	Chain	Res	Type
2	9	3114	G
2	9	3122	C
4	5	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
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	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2852	A
2	9	3065	A

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

8 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	19,22,23	0.29	0	25,31,34	0.36	0
1	1MA	0	628	1,36	21,25,26	0.74	1 (4%)	30,37,40	0.79	1 (3%)
3	HFA	4	77	3	10,11,12	0.97	1 (10%)	11,13,15	0.31	0
1	UR3	0	2619	1,38	19,22,23	0.46	0	26,32,35	0.70	1 (3%)
3	PPU	4	76	1,3	23,26,41	0.42	0	29,38,60	0.78	1 (3%)
4	ACA	5	78	4	6,7,8	2.04	1 (16%)	5,6,8	0.91	0
1	PSU	0	2621	1	18,21,22	1.62	2 (11%)	21,30,33	1.35	3 (14%)
1	OMG	0	2588	1,3	23,26,27	0.36	0	32,38,41	0.39	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	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1,36	-	2/7/25/26	0/3/3/3
3	HFA	4	77	3	-	0/5/6/8	0/1/1/1
1	UR3	0	2619	1,38	-	0/7/25/26	0/2/2/2
3	PPU	4	76	1,3	-	0/11/29/44	0/3/3/4
4	ACA	5	78	4	-	0/5/5/6	-
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	0/9/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.08	1.43	1.36
4	5	78	ACA	C3-C2	-4.60	1.32	1.52
1	0	2621	PSU	C6-C5	3.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	628	1MA	C6-N6	2.56	1.34	1.28
3	4	77	HFA	OA-CA	2.39	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.42	120.48	118.17
1	0	2621	PSU	C6-N1-C2	-3.11	119.80	122.69
3	4	76	PPU	C2-N1-C6	2.88	118.88	111.83
1	0	628	1MA	N1-C2-N3	2.80	129.32	126.00
1	0	2619	UR3	C4-N3-C2	2.72	126.76	124.58
1	0	2621	PSU	O2-C2-N1	2.65	125.52	122.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	3	0
1	0	2619	UR3	1	0
3	4	76	PPU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	76:A	O3'	77:PHE	C	1.60

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%)	-0.20	73 (2%) 56 52	24, 49, 93, 153	0
2	9	122/122 (100%)	0.45	5 (4%) 41 37	41, 69, 93, 152	0
3	4	2/4 (50%)	-0.27	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	0.48	1 (25%) 2 1	55, 57, 58, 66	0
5	A	237/240 (98%)	0.49	14 (5%) 28 24	31, 54, 86, 106	0
6	B	337/338 (99%)	0.50	12 (3%) 46 42	31, 55, 79, 93	0
7	C	246/246 (100%)	0.41	8 (3%) 49 45	27, 49, 70, 87	0
8	D	140/177 (79%)	2.15	63 (45%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.85	10 (5%) 29 25	44, 66, 86, 92	0
10	F	119/120 (99%)	1.02	14 (11%) 9 6	49, 74, 100, 112	0
11	G	29/348 (8%)	1.73	11 (37%) 1 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.87	15 (9%) 14 11	47, 65, 96, 103	0
13	J	142/145 (97%)	0.44	5 (3%) 47 43	37, 52, 72, 93	0
14	K	132/132 (100%)	0.26	1 (0%) 82 80	37, 48, 71, 84	0
15	L	145/165 (87%)	0.93	22 (15%) 5 4	29, 69, 112, 121	0
16	M	194/194 (100%)	0.72	26 (13%) 7 5	37, 48, 85, 93	0
17	N	186/187 (99%)	1.13	29 (15%) 5 4	49, 68, 112, 119	0
18	O	115/116 (99%)	0.73	4 (3%) 47 43	40, 59, 73, 81	0
19	P	143/149 (95%)	0.58	8 (5%) 30 26	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.35	2 (2%) 63 59	42, 52, 67, 76	0
21	R	150/155 (96%)	0.05	1 (0%) 84 81	33, 47, 66, 75	0
22	S	81/85 (95%)	0.62	3 (3%) 45 41	43, 61, 84, 97	0
23	T	119/120 (99%)	0.87	11 (9%) 14 12	41, 59, 85, 110	0
24	U	53/66 (80%)	0.53	1 (1%) 66 62	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.37	13 (20%) 3 2	56, 78, 115, 120	0
26	W	154/154 (100%)	0.50	5 (3%) 50 46	40, 53, 74, 82	0
27	X	82/92 (89%)	0.69	7 (8%) 16 13	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.25	3 (2%) 63 59	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.90	29 (39%) 1 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.11	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.36	12 (26%) 1 1	41, 68, 96, 102	0
32	3	92/92 (100%)	0.59	3 (3%) 49 45	41, 61, 73, 86	0
33	I	70/162 (43%)	3.25	56 (80%) 0 0	111, 124, 142, 144	0
All	All	6652/7484 (88%)	0.35	467 (7%) 22 19	24, 54, 100, 153	0

All (467) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	133	THR	9.7
25	V	1	THR	9.6
16	M	70	GLY	9.0
8	D	63	ILE	7.9
8	D	10	PHE	6.9
8	D	57	THR	6.6
17	N	166	ALA	6.5
33	I	79	ILE	6.5
33	I	118	SER	6.4
16	M	74	LYS	6.4
2	9	3001	U	6.3
8	D	107	GLY	6.2
33	I	76	ALA	6.2
17	N	154	LEU	5.9
29	Z	11	SER	5.9
23	T	117	ASP	5.8
8	D	90	LEU	5.7
29	Z	12	GLY	5.7
23	T	119	ALA	5.6
25	V	2	VAL	5.6
1	0	1161	A	5.6
17	N	168	LEU	5.5
31	2	49	GLU	5.5
33	I	88	GLY	5.5
29	Z	22	SER	5.4

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Mol	Chain	Res	Type	RSRZ
8	D	174	VAL	5.4
16	M	78	LYS	5.3
16	M	79	ALA	5.3
1	0	2645	U	5.2
33	I	137	VAL	5.1
16	M	80	GLY	5.1
29	Z	21	VAL	5.1
15	L	82	ALA	5.0
25	V	39	ALA	5.0
33	I	129	VAL	5.0
16	M	71	SER	5.0
33	I	138	THR	4.9
8	D	172	VAL	4.9
9	E	45	ASP	4.9
33	I	96	PHE	4.9
25	V	40	PRO	4.8
33	I	78	LEU	4.8
11	G	26	MET	4.7
29	Z	10	ARG	4.7
33	I	117	LEU	4.7
2	9	3002	U	4.7
33	I	90	GLY	4.6
1	0	10	U	4.6
13	J	70	PHE	4.6
16	M	72	ALA	4.6
8	D	55	LYS	4.6
16	M	82	ARG	4.5
6	B	1	PRO	4.5
29	Z	16	ALA	4.5
8	D	171	ASP	4.5
29	Z	18	TYR	4.4
33	I	132	CYS	4.4
33	I	85	PHE	4.4
16	M	87	GLY	4.4
33	I	134	SER	4.3
31	2	47	THR	4.3
31	2	42	TRP	4.3
10	F	102	GLY	4.3
27	X	88	GLU	4.2
15	L	81	VAL	4.2
31	2	37	HIS	4.2
33	I	75	THR	4.2

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Mol	Chain	Res	Type	RSRZ
8	D	53	LYS	4.2
23	T	118	SER	4.2
5	A	37	VAL	4.2
16	M	81	ARG	4.2
8	D	61	PHE	4.2
8	D	106	PHE	4.2
1	0	1173	A	4.1
17	N	165	ALA	4.1
27	X	65	ASN	4.1
16	M	75	ARG	4.1
8	D	54	ALA	4.1
31	2	48	ASP	4.1
11	G	12	ILE	4.1
16	M	88	VAL	4.1
25	V	43	PRO	4.0
33	I	93	GLN	4.0
33	I	135	LEU	4.0
22	S	81	ILE	4.0
29	Z	29	ILE	4.0
1	0	2748	G	4.0
33	I	139	ILE	4.0
33	I	121	LEU	4.0
29	Z	14	PHE	3.9
15	L	77	ALA	3.9
16	M	86	GLN	3.9
12	H	168	ALA	3.9
1	0	1477	C	3.9
17	N	95	ALA	3.9
33	I	83	ALA	3.9
5	A	36	ASP	3.9
16	M	73	ARG	3.9
31	2	44	ARG	3.9
29	Z	82	SER	3.9
1	0	1476	A	3.9
8	D	35	ALA	3.9
5	A	237	GLY	3.9
12	H	40	ALA	3.8
33	I	109	ALA	3.8
33	I	116	LEU	3.8
33	I	72	VAL	3.8
33	I	89	SER	3.8
27	X	87	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
16	M	83	SER	3.7
9	E	10	ASP	3.7
8	D	131	THR	3.7
1	0	2345	A	3.7
8	D	69	ILE	3.7
17	N	167	ASP	3.7
31	2	38	LYS	3.7
16	M	89	THR	3.7
8	D	135	VAL	3.6
1	0	1162	G	3.6
1	0	138	U	3.6
33	I	125	ALA	3.6
33	I	105	VAL	3.5
13	J	4	ALA	3.5
17	N	137	ALA	3.5
11	G	63	ARG	3.5
2	9	3024	U	3.5
16	M	77	HIS	3.5
1	0	1172	G	3.5
15	L	91	VAL	3.5
15	L	78	ALA	3.5
19	P	18	LYS	3.5
15	L	148	GLU	3.4
33	I	81	ASP	3.4
15	L	146	GLY	3.4
2	9	3023	U	3.4
29	Z	20	ARG	3.4
1	0	737	A	3.4
11	G	71	LEU	3.4
17	N	134	ASP	3.4
16	M	84	LYS	3.4
19	P	143	ALA	3.4
16	M	76	ARG	3.4
23	T	116	ASP	3.4
33	I	80	LYS	3.4
18	O	23	GLY	3.4
1	0	1164	U	3.3
1	0	2769	C	3.3
16	M	85	ARG	3.3
33	I	74	PRO	3.3
33	I	82	GLU	3.3
18	O	22	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
8	D	44	ILE	3.3
12	H	111	ASP	3.2
29	Z	34	ASN	3.2
1	0	2747	C	3.2
22	S	1	SER	3.2
8	D	128	LEU	3.2
8	D	134	LEU	3.2
33	I	77	GLU	3.2
33	I	114	PRO	3.2
17	N	163	PHE	3.1
9	E	172	PRO	3.1
33	I	100	LEU	3.1
1	0	514	G	3.1
1	0	1524	U	3.1
23	T	114	SER	3.1
8	D	59	GLY	3.1
1	0	1175	G	3.1
33	I	128	VAL	3.1
15	L	55	GLN	3.1
28	Y	235	GLU	3.1
7	C	63	SER	3.1
12	H	112	GLY	3.1
15	L	150	GLN	3.1
1	0	1981	A	3.1
17	N	169	PRO	3.1
31	2	46	ASP	3.1
9	E	154	ILE	3.1
8	D	52	THR	3.0
33	I	87	THR	3.0
8	D	167	GLU	3.0
8	D	62	ASP	3.0
33	I	126	LYS	3.0
8	D	40	ILE	3.0
8	D	58	VAL	3.0
10	F	8	VAL	3.0
33	I	97	VAL	3.0
29	Z	17	ARG	3.0
29	Z	42	CYS	3.0
27	X	85	VAL	3.0
25	V	41	GLU	3.0
8	D	89	PRO	3.0
17	N	158	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
7	C	132	ASP	3.0
1	0	497	A	3.0
29	Z	41	ASN	3.0
29	Z	15	GLY	3.0
31	2	41	HIS	2.9
17	N	157	PRO	2.9
6	B	56	ASP	2.9
1	0	1177	A	2.9
17	N	161	GLY	2.9
15	L	83	GLU	2.9
1	0	1192	A	2.9
6	B	57	GLU	2.9
1	0	1169	U	2.9
8	D	141	VAL	2.9
17	N	1	ALA	2.9
33	I	92	PRO	2.9
33	I	124	ALA	2.9
10	F	17	LEU	2.9
15	L	145	LEU	2.9
6	B	2	GLN	2.9
8	D	170	TYR	2.9
17	N	159	TYR	2.9
33	I	119	TYR	2.9
17	N	76	GLY	2.9
15	L	149	ARG	2.8
8	D	154	LYS	2.8
1	0	1204	C	2.8
15	L	143	THR	2.8
12	H	137	TYR	2.8
12	H	169	GLY	2.8
17	N	5	ARG	2.8
23	T	36	GLY	2.8
1	0	271	C	2.8
8	D	56	ARG	2.8
16	M	69	LYS	2.8
5	A	35	GLY	2.8
8	D	11	HIS	2.8
5	A	38	ILE	2.8
29	Z	40	PRO	2.8
33	I	102	VAL	2.8
6	B	183	GLU	2.8
32	3	41	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
11	G	29	SER	2.7
12	H	66	ARG	2.7
1	0	1165	G	2.7
1	0	1951	G	2.7
29	Z	43	GLY	2.7
8	D	50	VAL	2.7
33	I	140	GLU	2.7
33	I	111	GLN	2.7
15	L	102	ASP	2.7
11	G	27	ILE	2.7
33	I	123	ASN	2.7
8	D	93	LEU	2.7
16	M	68	ARG	2.7
15	L	99	GLU	2.7
8	D	26	GLY	2.7
1	0	2237	G	2.7
1	0	284	C	2.7
17	N	186	LEU	2.7
29	Z	19	GLY	2.6
11	G	23	ILE	2.6
1	0	1186	C	2.6
12	H	146	VAL	2.6
15	L	93	VAL	2.6
13	J	5	GLU	2.6
17	N	160	SER	2.6
10	F	101	ALA	2.6
25	V	36	ALA	2.6
1	0	1170	U	2.6
17	N	164	ASP	2.6
8	D	68	PRO	2.6
29	Z	23	ARG	2.6
5	A	32	VAL	2.6
14	K	132	VAL	2.6
1	0	288	A	2.6
1	0	1176	C	2.6
1	0	1964	U	2.6
8	D	104	PHE	2.6
9	E	87	PHE	2.6
8	D	36	ASN	2.6
29	Z	26	VAL	2.6
19	P	58	SER	2.6
1	0	1171	A	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1184	C	2.6
9	E	12	ASP	2.6
27	X	84	ILE	2.6
13	J	6	PHE	2.6
8	D	88	LEU	2.6
17	N	180	LEU	2.6
8	D	130	VAL	2.6
16	M	1	ALA	2.6
33	I	112	LYS	2.6
1	0	1199	A	2.6
5	A	26	ASP	2.5
17	N	162	ASP	2.5
26	W	86	GLU	2.5
33	I	94	GLU	2.5
1	0	510	U	2.5
33	I	106	LYS	2.5
8	D	169	THR	2.5
8	D	12	GLU	2.5
20	Q	95	GLU	2.5
23	T	115	GLU	2.5
1	0	1929	G	2.5
15	L	100	ALA	2.5
8	D	105	SER	2.5
8	D	137	PRO	2.5
1	0	128	A	2.5
1	0	441	A	2.5
7	C	101	ASP	2.5
19	P	111	GLU	2.5
1	0	735	C	2.5
1	0	2004	U	2.5
1	0	960	G	2.5
1	0	1163	G	2.5
27	X	83	ALA	2.5
9	E	53	GLU	2.5
29	Z	59	TYR	2.5
33	I	108	ILE	2.5
1	0	2511	A	2.5
8	D	155	HIS	2.5
29	Z	46	ARG	2.5
1	0	1525	G	2.5
1	0	2344	G	2.5
15	L	65	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
17	N	172	PHE	2.4
1	0	1168	C	2.4
8	D	73	VAL	2.4
8	D	173	GLU	2.4
1	0	1160	G	2.4
1	0	1523	G	2.4
8	D	18	ILE	2.4
10	F	105	ASP	2.4
11	G	73	ASP	2.4
6	B	119	HIS	2.4
28	Y	236	VAL	2.4
5	A	211	LYS	2.4
9	E	6	GLU	2.4
9	E	7	ILE	2.4
10	F	118	LEU	2.4
5	A	192	VAL	2.4
10	F	2	VAL	2.4
1	0	1181	A	2.4
1	0	1193	A	2.4
1	0	2768	A	2.4
8	D	74	THR	2.4
8	D	101	THR	2.4
12	H	32	LYS	2.4
1	0	999	C	2.4
20	Q	18	PRO	2.4
13	J	46	ILE	2.4
17	N	147	ILE	2.4
29	Z	37	HIS	2.4
1	0	1203	G	2.4
7	C	61	PHE	2.4
8	D	37	ALA	2.4
11	G	70	ALA	2.4
16	M	194	ALA	2.4
6	B	108	GLU	2.4
33	I	122	THR	2.3
33	I	131	THR	2.3
15	L	75	LEU	2.3
29	Z	45	ASP	2.3
8	D	132	VAL	2.3
33	I	98	ALA	2.3
10	F	9	PRO	2.3
21	R	150	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	0	1202	A	2.3
5	A	205	GLY	2.3
31	2	39	ARG	2.3
1	0	1625	U	2.3
9	E	20	ILE	2.3
10	F	111	ILE	2.3
1	0	1153	C	2.3
18	O	24	ALA	2.3
1	0	1190	G	2.3
25	V	44	GLY	2.3
25	V	46	ILE	2.3
29	Z	33	MET	2.3
10	F	60	VAL	2.3
19	P	92	GLU	2.3
10	F	16	ALA	2.3
8	D	86	THR	2.3
1	0	358	G	2.3
15	L	80	ASP	2.3
8	D	60	GLU	2.3
29	Z	79	VAL	2.3
8	D	138	GLY	2.2
25	V	3	LEU	2.2
6	B	33	ASP	2.2
22	S	19	ASP	2.2
26	W	91	ASP	2.2
12	H	167	PRO	2.2
23	T	40	VAL	2.2
12	H	170	ASN	2.2
12	H	138	CYS	2.2
11	G	72	ASP	2.2
26	W	16	ASP	2.2
33	I	120	ASP	2.2
1	0	2419	U	2.2
24	U	4	ARG	2.2
26	W	26	ILE	2.2
27	X	61	ARG	2.2
10	F	1	PRO	2.2
33	I	113	HIS	2.2
2	9	3122	C	2.2
32	3	62	THR	2.2
8	D	102	GLY	2.2
12	H	62	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
23	T	53	GLY	2.2
8	D	65	GLU	2.2
7	C	246	ARG	2.2
28	Y	216	ARG	2.2
33	I	73	PRO	2.2
1	0	1967	U	2.2
4	5	77	PHE	2.2
1	0	1197	G	2.1
8	D	166	ILE	2.1
19	P	110	ASP	2.1
19	P	116	SER	2.1
29	Z	24	ARG	2.1
25	V	65	ASP	2.1
5	A	31	LYS	2.1
15	L	97	VAL	2.1
1	0	272	A	2.1
1	0	1166	A	2.1
23	T	82	THR	2.1
5	A	33	GLU	2.1
16	M	90	ARG	2.1
16	M	107	ARG	2.1
1	0	1182	C	2.1
1	0	1196	C	2.1
6	B	180	ASP	2.1
5	A	84	VAL	2.1
15	L	57	VAL	2.1
17	N	43	VAL	2.1
17	N	139	TRP	2.1
1	0	1188	A	2.1
5	A	206	ARG	2.1
26	W	108	ARG	2.1
31	2	35	ARG	2.1
7	C	135	GLU	2.1
32	3	92	GLU	2.1
12	H	36	LYS	2.1
1	0	1950	G	2.1
8	D	51	ARG	2.1
25	V	38	GLY	2.1
29	Z	13	ARG	2.1
17	N	138	ASP	2.1
23	T	5	ASP	2.1
12	H	140	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
7	C	76	ARG	2.0
7	C	133	ARG	2.0
8	D	87	ALA	2.0
31	2	43	ARG	2.0
19	P	114	LEU	2.0
25	V	42	ASN	2.0
8	D	66	GLY	2.0
17	N	94	GLU	2.0
18	O	99	GLU	2.0
1	0	1279	U	2.0
1	0	1189	A	2.0
1	0	1200	A	2.0
8	D	29	HIS	2.0
6	B	171	VAL	2.0
11	G	69	ARG	2.0
10	F	104	ALA	2.0
8	D	72	LYS	2.0
17	N	71	TRP	2.0
6	B	120	ASP	2.0
6	B	139	ASP	2.0
10	F	15	ASP	2.0
33	I	95	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACA	5	78	8/9	0.90	0.32	66,72,83,86	0
3	HFA	4	77	11/12	0.94	0.12	42,44,47,48	0
1	OMG	0	2588	24/25	0.96	0.08	31,34,39,41	0
1	PSU	0	2621	20/21	0.97	0.07	36,38,43,43	0
3	PPU	4	76	24/38	0.97	0.07	41,44,45,49	0
1	1MA	0	628	23/24	0.97	0.07	32,35,37,38	0
1	UR3	0	2619	21/22	0.97	0.08	39,42,45,48	0
1	OMU	0	2587	21/22	0.98	0.07	32,37,40,40	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	SR	0	9529	1/1	0.58	0.24	131,131,131,131	0
34	MG	0	8047	1/1	0.61	0.39	107,107,107,107	0
34	MG	0	8052	1/1	0.68	0.26	99,99,99,99	0
34	MG	0	8072	1/1	0.69	0.34	89,89,89,89	0
34	MG	0	8050	1/1	0.69	0.16	89,89,89,89	0
36	NA	0	9122	1/1	0.71	0.45	90,90,90,90	0
34	MG	0	8013	1/1	0.71	0.23	25,25,25,25	0
36	NA	0	9184	1/1	0.76	0.34	87,87,87,87	0
38	SR	0	9501	1/1	0.78	0.19	159,159,159,159	0
36	NA	0	9185	1/1	0.78	0.37	54,54,54,54	0
36	NA	S	9112	1/1	0.79	0.13	80,80,80,80	0
36	NA	0	9182	1/1	0.79	0.21	90,90,90,90	0
36	NA	9	9183	1/1	0.79	0.26	75,75,75,75	0
36	NA	0	9164	1/1	0.80	0.29	61,61,61,61	0
38	SR	0	9547	1/1	0.80	0.26	194,194,194,194	0
38	SR	B	9521	1/1	0.80	0.48	200,200,200,200	0
34	MG	9	8095	1/1	0.81	0.24	55,55,55,55	0
34	MG	0	8024	1/1	0.81	0.31	86,86,86,86	0
36	NA	0	9152	1/1	0.82	0.41	83,83,83,83	0
34	MG	0	8055	1/1	0.82	0.27	97,97,97,97	0
36	NA	0	9169	1/1	0.82	0.42	116,116,116,116	0
38	SR	0	9500	1/1	0.83	0.38	200,200,200,200	0
34	MG	0	8065	1/1	0.83	0.23	107,107,107,107	0
34	MG	0	8092	1/1	0.83	0.25	77,77,77,77	0
36	NA	0	9177	1/1	0.83	0.30	77,77,77,77	0
34	MG	0	8101	1/1	0.83	0.18	80,80,80,80	0
36	NA	0	9171	1/1	0.84	0.18	61,61,61,61	0
34	MG	0	8014	1/1	0.84	0.26	73,73,73,73	0
34	MG	0	8108	1/1	0.84	0.27	103,103,103,103	0
36	NA	0	9126	1/1	0.84	0.28	63,63,63,63	0
36	NA	0	9175	1/1	0.85	0.22	55,55,55,55	0
36	NA	0	9140	1/1	0.85	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	NA	0	9173	1/1	0.85	0.11	69,69,69,69	0
36	NA	0	9129	1/1	0.86	0.20	72,72,72,72	0
36	NA	0	9181	1/1	0.86	0.15	54,54,54,54	0
34	MG	0	8040	1/1	0.86	0.26	92,92,92,92	0
38	SR	0	9484	1/1	0.87	0.12	149,149,149,149	0
34	MG	0	8094	1/1	0.87	0.24	72,72,72,72	0
36	NA	0	9135	1/1	0.87	0.16	55,55,55,55	0
34	MG	0	8059	1/1	0.87	0.15	84,84,84,84	0
36	NA	D	9151	1/1	0.87	0.16	68,68,68,68	0
34	MG	0	8093	1/1	0.87	0.12	49,49,49,49	0
36	NA	0	9174	1/1	0.88	0.23	65,65,65,65	0
38	SR	0	9537	1/1	0.88	0.20	157,157,157,157	0
36	NA	0	9178	1/1	0.88	0.33	54,54,54,54	0
36	NA	0	9168	1/1	0.88	0.33	69,69,69,69	0
36	NA	R	9186	1/1	0.89	0.16	80,80,80,80	0
34	MG	0	8022	1/1	0.89	0.25	112,112,112,112	0
36	NA	0	9125	1/1	0.89	0.19	92,92,92,92	0
36	NA	0	9170	1/1	0.89	0.26	77,77,77,77	0
34	MG	5	8118	1/1	0.89	0.23	45,45,45,45	0
36	NA	0	9172	1/1	0.89	0.31	76,76,76,76	0
36	NA	0	9154	1/1	0.89	0.17	54,54,54,54	0
36	NA	0	9113	1/1	0.89	0.10	60,60,60,60	0
36	NA	0	9166	1/1	0.89	0.25	74,74,74,74	0
34	MG	0	8102	1/1	0.90	0.10	68,68,68,68	0
34	MG	0	8025	1/1	0.90	0.23	27,27,27,27	0
34	MG	0	8061	1/1	0.90	0.17	87,87,87,87	0
34	MG	0	8084	1/1	0.90	0.34	89,89,89,89	0
35	K	0	9002	1/1	0.90	0.12	88,88,88,88	0
34	MG	0	8090	1/1	0.90	0.15	68,68,68,68	0
38	SR	9	9588	1/1	0.90	0.10	143,143,143,143	0
36	NA	0	9116	1/1	0.90	0.40	52,52,52,52	0
39	CD	Z	9203	1/1	0.90	0.10	84,84,84,84	0
36	NA	0	9106	1/1	0.91	0.31	44,44,44,44	0
34	MG	0	8107	1/1	0.91	0.21	65,65,65,65	0
34	MG	0	8091	1/1	0.91	0.10	64,64,64,64	0
38	SR	0	9459	1/1	0.91	0.12	103,103,103,103	0
36	NA	0	9161	1/1	0.91	0.26	68,68,68,68	0
34	MG	0	8116	1/1	0.91	0.07	64,64,64,64	0
36	NA	0	9165	1/1	0.91	0.21	45,45,45,45	0
36	NA	0	9179	1/1	0.91	0.27	121,121,121,121	0
36	NA	0	9124	1/1	0.91	0.24	50,50,50,50	0
34	MG	0	8051	1/1	0.91	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	SR	0	9581	1/1	0.91	0.10	130,130,130,130	0
34	MG	0	8082	1/1	0.91	0.35	82,82,82,82	0
35	K	0	9001	1/1	0.91	0.37	74,74,74,74	0
34	MG	0	8103	1/1	0.91	0.13	67,67,67,67	0
34	MG	0	8113	1/1	0.92	0.10	52,52,52,52	0
36	NA	0	9128	1/1	0.92	0.11	49,49,49,49	0
36	NA	0	9162	1/1	0.92	0.17	52,52,52,52	0
34	MG	0	8045	1/1	0.92	0.19	72,72,72,72	0
34	MG	T	8073	1/1	0.92	0.13	43,43,43,43	0
38	SR	9	9503	1/1	0.92	0.08	122,122,122,122	0
38	SR	0	9482	1/1	0.92	0.38	135,135,135,135	0
36	NA	0	9107	1/1	0.92	0.13	71,71,71,71	0
36	NA	0	9111	1/1	0.92	0.13	63,63,63,63	0
36	NA	0	9114	1/1	0.93	0.14	65,65,65,65	0
34	MG	0	8097	1/1	0.93	0.13	57,57,57,57	0
36	NA	0	9101	1/1	0.93	0.07	46,46,46,46	0
36	NA	0	9141	1/1	0.93	0.12	73,73,73,73	0
36	NA	0	9143	1/1	0.93	0.14	40,40,40,40	0
34	MG	0	8099	1/1	0.93	0.10	75,75,75,75	0
34	MG	A	8066	1/1	0.93	0.11	57,57,57,57	0
36	NA	0	9155	1/1	0.93	0.13	60,60,60,60	0
36	NA	0	9157	1/1	0.93	0.18	47,47,47,47	0
38	SR	0	9590	1/1	0.93	0.12	131,131,131,131	0
38	SR	0	9626	1/1	0.93	0.47	154,154,154,154	0
36	NA	J	9146	1/1	0.93	0.06	55,55,55,55	0
34	MG	0	8114	1/1	0.93	0.12	83,83,83,83	0
34	MG	0	8042	1/1	0.93	0.07	48,48,48,48	0
37	CL	0	9316	1/1	0.93	0.23	78,78,78,78	0
38	SR	0	9468	1/1	0.94	0.10	128,128,128,128	0
36	NA	0	9150	1/1	0.94	0.09	47,47,47,47	0
34	MG	0	8106	1/1	0.94	0.08	51,51,51,51	0
38	SR	0	9490	1/1	0.94	0.18	116,116,116,116	0
38	SR	0	9495	1/1	0.94	0.07	111,111,111,111	0
34	MG	0	8037	1/1	0.94	0.07	46,46,46,46	0
34	MG	0	8060	1/1	0.94	0.12	82,82,82,82	0
38	SR	0	9505	1/1	0.94	0.20	106,106,106,106	0
34	MG	0	8083	1/1	0.94	0.08	53,53,53,53	0
34	MG	0	8067	1/1	0.94	0.10	40,40,40,40	0
36	NA	0	9120	1/1	0.94	0.11	61,61,61,61	0
34	MG	0	8089	1/1	0.94	0.12	61,61,61,61	0
34	MG	0	8104	1/1	0.94	0.05	57,57,57,57	0
37	CL	0	9311	1/1	0.94	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	NA	0	9149	1/1	0.94	0.13	49,49,49,49	0
37	CL	A	9309	1/1	0.94	0.26	66,66,66,66	0
38	SR	0	9452	1/1	0.94	0.11	106,106,106,106	0
38	SR	H	9486	1/1	0.94	0.24	125,125,125,125	0
36	NA	0	9167	1/1	0.94	0.18	65,65,65,65	0
38	SR	0	9455	1/1	0.95	0.07	88,88,88,88	0
36	NA	0	9158	1/1	0.95	0.13	66,66,66,66	0
38	SR	0	9465	1/1	0.95	0.06	107,107,107,107	0
36	NA	0	9159	1/1	0.95	0.26	58,58,58,58	0
36	NA	0	9131	1/1	0.95	0.08	47,47,47,47	0
36	NA	0	9132	1/1	0.95	0.10	68,68,68,68	0
36	NA	0	9134	1/1	0.95	0.07	47,47,47,47	0
34	MG	0	8115	1/1	0.95	0.08	59,59,59,59	0
36	NA	0	9139	1/1	0.95	0.08	43,43,43,43	0
34	MG	0	8054	1/1	0.95	0.07	63,63,63,63	0
34	MG	0	8063	1/1	0.95	0.08	65,65,65,65	0
38	SR	0	9509	1/1	0.95	0.07	95,95,95,95	0
36	NA	0	9102	1/1	0.95	0.25	63,63,63,63	0
38	SR	0	9532	1/1	0.95	0.11	120,120,120,120	0
36	NA	Q	9148	1/1	0.95	0.05	49,49,49,49	0
38	SR	0	9539	1/1	0.95	0.38	157,157,157,157	0
34	MG	0	8085	1/1	0.95	0.12	63,63,63,63	0
38	SR	0	9570	1/1	0.95	0.12	111,111,111,111	0
34	MG	0	8075	1/1	0.95	0.07	47,47,47,47	0
36	NA	0	9110	1/1	0.95	0.20	46,46,46,46	0
36	NA	0	9127	1/1	0.95	0.16	60,60,60,60	0
34	MG	0	8043	1/1	0.95	0.06	52,52,52,52	0
37	CL	J	9301	1/1	0.95	0.21	60,60,60,60	0
37	CL	L	9310	1/1	0.95	0.09	58,58,58,58	0
37	CL	N	9307	1/1	0.95	0.10	65,65,65,65	0
39	CD	O	9205	1/1	0.95	0.13	132,132,132,132	0
34	MG	2	8076	1/1	0.95	0.10	64,64,64,64	0
36	NA	0	9130	1/1	0.96	0.06	50,50,50,50	0
36	NA	0	9105	1/1	0.96	0.05	44,44,44,44	0
37	CL	0	9315	1/1	0.96	0.09	52,52,52,52	0
34	MG	0	8039	1/1	0.96	0.06	49,49,49,49	0
38	SR	0	9504	1/1	0.96	0.06	108,108,108,108	0
37	CL	0	9322	1/1	0.96	0.41	61,61,61,61	0
38	SR	0	9508	1/1	0.96	0.06	97,97,97,97	0
34	MG	Y	8109	1/1	0.96	0.10	45,45,45,45	0
38	SR	0	9515	1/1	0.96	0.27	100,100,100,100	0
38	SR	0	9517	1/1	0.96	0.07	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	SR	0	9522	1/1	0.96	0.05	114,114,114,114	0
34	MG	0	8046	1/1	0.96	0.04	39,39,39,39	0
36	NA	0	9156	1/1	0.96	0.12	57,57,57,57	0
38	SR	0	9534	1/1	0.96	0.29	111,111,111,111	0
36	NA	0	9138	1/1	0.96	0.08	62,62,62,62	0
37	CL	3	9304	1/1	0.96	0.07	61,61,61,61	0
38	SR	0	9405	1/1	0.96	0.09	59,59,59,59	0
38	SR	0	9433	1/1	0.96	0.09	75,75,75,75	0
34	MG	0	8057	1/1	0.96	0.08	77,77,77,77	0
38	SR	0	9585	1/1	0.96	0.06	94,94,94,94	0
36	NA	C	9104	1/1	0.96	0.06	33,33,33,33	0
34	MG	0	8058	1/1	0.96	0.08	41,41,41,41	0
34	MG	0	8110	1/1	0.96	0.16	45,45,45,45	0
36	NA	M	9147	1/1	0.96	0.07	42,42,42,42	0
38	SR	0	9475	1/1	0.96	0.06	83,83,83,83	0
38	SR	F	9595	1/1	0.96	0.07	109,109,109,109	0
38	SR	0	9477	1/1	0.96	0.06	86,86,86,86	0
34	MG	0	8080	1/1	0.96	0.14	57,57,57,57	0
36	NA	0	9163	1/1	0.96	0.09	73,73,73,73	0
36	NA	0	9115	1/1	0.97	0.12	41,41,41,41	0
38	SR	0	9467	1/1	0.97	0.06	86,86,86,86	0
34	MG	0	8031	1/1	0.97	0.06	49,49,49,49	0
37	CL	B	9319	1/1	0.97	0.21	54,54,54,54	0
36	NA	0	9117	1/1	0.97	0.05	51,51,51,51	0
37	CL	J	9302	1/1	0.97	0.07	53,53,53,53	0
38	SR	0	9560	1/1	0.97	0.08	101,101,101,101	0
38	SR	0	9568	1/1	0.97	0.04	80,80,80,80	0
37	CL	J	9321	1/1	0.97	0.06	66,66,66,66	0
34	MG	0	8041	1/1	0.97	0.05	55,55,55,55	0
37	CL	M	9318	1/1	0.97	0.06	41,41,41,41	0
36	NA	0	9108	1/1	0.97	0.04	34,34,34,34	0
38	SR	0	9601	1/1	0.97	0.09	119,119,119,119	0
37	CL	Y	9320	1/1	0.97	0.06	47,47,47,47	0
34	MG	0	8112	1/1	0.97	0.04	46,46,46,46	0
34	MG	0	8098	1/1	0.97	0.06	45,45,45,45	0
38	SR	A	9497	1/1	0.97	0.05	96,96,96,96	0
37	CL	0	9312	1/1	0.97	0.08	57,57,57,57	0
34	MG	0	8021	1/1	0.97	0.06	56,56,56,56	0
38	SR	0	9454	1/1	0.97	0.05	82,82,82,82	0
34	MG	0	8019	1/1	0.97	0.05	51,51,51,51	0
37	CL	0	9317	1/1	0.97	0.07	52,52,52,52	0
34	MG	0	8002	1/1	0.98	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8027	1/1	0.98	0.12	36,36,36,36	0
38	SR	0	9483	1/1	0.98	0.04	77,77,77,77	0
36	NA	0	9118	1/1	0.98	0.16	66,66,66,66	0
38	SR	0	9488	1/1	0.98	0.04	86,86,86,86	0
34	MG	0	8088	1/1	0.98	0.03	28,28,28,28	0
36	NA	0	9160	1/1	0.98	0.14	46,46,46,46	0
36	NA	R	9137	1/1	0.98	0.03	36,36,36,36	0
34	MG	0	8068	1/1	0.98	0.14	48,48,48,48	0
37	CL	O	9308	1/1	0.98	0.13	67,67,67,67	0
37	CL	R	9306	1/1	0.98	0.05	45,45,45,45	0
38	SR	0	9506	1/1	0.98	0.11	68,68,68,68	0
34	MG	0	8117	1/1	0.98	0.07	46,46,46,46	0
37	CL	0	9303	1/1	0.98	0.08	53,53,53,53	0
37	CL	0	9305	1/1	0.98	0.07	61,61,61,61	0
38	SR	0	9417	1/1	0.98	0.03	63,63,63,63	0
38	SR	0	9421	1/1	0.98	0.05	78,78,78,78	0
38	SR	0	9429	1/1	0.98	0.04	72,72,72,72	0
38	SR	0	9530	1/1	0.98	0.04	72,72,72,72	0
38	SR	0	9431	1/1	0.98	0.04	65,65,65,65	0
34	MG	0	8070	1/1	0.98	0.04	24,24,24,24	0
38	SR	0	9438	1/1	0.98	0.04	70,70,70,70	0
38	SR	0	9442	1/1	0.98	0.04	66,66,66,66	0
38	SR	0	9545	1/1	0.98	0.05	85,85,85,85	0
38	SR	0	9445	1/1	0.98	0.03	57,57,57,57	0
38	SR	0	9446	1/1	0.98	0.06	88,88,88,88	0
38	SR	0	9566	1/1	0.98	0.08	80,80,80,80	0
38	SR	0	9447	1/1	0.98	0.04	73,73,73,73	0
34	MG	0	8029	1/1	0.98	0.10	35,35,35,35	0
37	CL	0	9313	1/1	0.98	0.07	59,59,59,59	0
37	CL	0	9314	1/1	0.98	0.10	51,51,51,51	0
38	SR	0	9456	1/1	0.98	0.04	67,67,67,67	0
34	MG	0	8030	1/1	0.98	0.04	37,37,37,37	0
38	SR	0	9461	1/1	0.98	0.05	82,82,82,82	0
38	SR	0	9629	1/1	0.98	0.04	75,75,75,75	0
38	SR	9	9481	1/1	0.98	0.04	89,89,89,89	0
38	SR	0	9462	1/1	0.98	0.04	74,74,74,74	0
38	SR	0	9464	1/1	0.98	0.06	81,81,81,81	0
38	SR	A	9437	1/1	0.98	0.04	70,70,70,70	0
34	MG	0	8004	1/1	0.98	0.03	35,35,35,35	0
38	SR	B	9458	1/1	0.98	0.06	82,82,82,82	0
38	SR	0	9466	1/1	0.98	0.14	96,96,96,96	0
34	MG	0	8032	1/1	0.98	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8096	1/1	0.98	0.08	41,41,41,41	0
38	SR	S	9470	1/1	0.98	0.07	101,101,101,101	0
38	SR	0	9469	1/1	0.98	0.05	85,85,85,85	0
34	MG	0	8044	1/1	0.98	0.04	35,35,35,35	0
38	SR	0	9426	1/1	0.99	0.03	71,71,71,71	0
38	SR	0	9489	1/1	0.99	0.04	94,94,94,94	0
38	SR	0	9427	1/1	0.99	0.03	56,56,56,56	0
36	NA	0	9136	1/1	0.99	0.09	34,34,34,34	0
34	MG	0	8028	1/1	0.99	0.03	37,37,37,37	0
38	SR	0	9432	1/1	0.99	0.07	68,68,68,68	0
34	MG	0	8017	1/1	0.99	0.07	31,31,31,31	0
38	SR	0	9434	1/1	0.99	0.04	64,64,64,64	0
38	SR	0	9435	1/1	0.99	0.03	76,76,76,76	0
34	MG	0	8008	1/1	0.99	0.08	16,16,16,16	0
38	SR	0	9440	1/1	0.99	0.05	72,72,72,72	0
38	SR	0	9441	1/1	0.99	0.03	68,68,68,68	0
34	MG	0	8020	1/1	0.99	0.03	36,36,36,36	0
38	SR	0	9443	1/1	0.99	0.03	63,63,63,63	0
38	SR	0	9444	1/1	0.99	0.05	55,55,55,55	0
34	MG	0	8009	1/1	0.99	0.02	21,21,21,21	0
36	NA	0	9123	1/1	0.99	0.07	52,52,52,52	0
34	MG	0	8036	1/1	0.99	0.03	65,65,65,65	0
38	SR	0	9449	1/1	0.99	0.03	67,67,67,67	0
38	SR	0	9450	1/1	0.99	0.05	72,72,72,72	0
38	SR	0	9451	1/1	0.99	0.03	60,60,60,60	0
34	MG	0	8012	1/1	0.99	0.09	39,39,39,39	0
38	SR	0	9453	1/1	0.99	0.04	72,72,72,72	0
34	MG	0	8038	1/1	0.99	0.11	25,25,25,25	0
34	MG	0	8003	1/1	0.99	0.03	35,35,35,35	0
34	MG	0	8074	1/1	0.99	0.10	27,27,27,27	0
38	SR	0	9457	1/1	0.99	0.03	51,51,51,51	0
34	MG	0	8001	1/1	0.99	0.06	22,22,22,22	0
34	MG	0	8079	1/1	0.99	0.04	33,33,33,33	0
34	MG	0	8056	1/1	0.99	0.06	44,44,44,44	0
34	MG	0	8026	1/1	0.99	0.05	30,30,30,30	0
38	SR	0	9408	1/1	0.99	0.02	36,36,36,36	0
38	SR	0	9411	1/1	0.99	0.04	43,43,43,43	0
38	SR	0	9412	1/1	0.99	0.02	45,45,45,45	0
38	SR	0	9413	1/1	0.99	0.02	49,49,49,49	0
38	SR	A	9436	1/1	0.99	0.07	60,60,60,60	0
38	SR	0	9414	1/1	0.99	0.03	57,57,57,57	0
38	SR	0	9474	1/1	0.99	0.04	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8015	1/1	0.99	0.02	35,35,35,35	0
38	SR	0	9420	1/1	0.99	0.07	70,70,70,70	0
38	SR	0	9478	1/1	0.99	0.02	77,77,77,77	0
38	SR	0	9480	1/1	0.99	0.04	93,93,93,93	0
38	SR	L	9409	1/1	0.99	0.02	37,37,37,37	0
38	SR	R	9418	1/1	0.99	0.04	57,57,57,57	0
34	MG	K	8069	1/1	0.99	0.05	25,25,25,25	0
38	SR	1	9460	1/1	0.99	0.02	52,52,52,52	0
38	SR	3	9439	1/1	0.99	0.04	72,72,72,72	0
38	SR	0	9423	1/1	0.99	0.05	64,64,64,64	0
38	SR	0	9425	1/1	0.99	0.05	56,56,56,56	0
39	CD	1	9202	1/1	0.99	0.07	54,54,54,54	0
39	CD	3	9204	1/1	0.99	0.06	64,64,64,64	0
38	SR	0	9407	1/1	1.00	0.04	47,47,47,47	0
38	SR	0	9430	1/1	1.00	0.02	49,49,49,49	0
34	MG	0	8005	1/1	1.00	0.04	29,29,29,29	0
38	SR	0	9473	1/1	1.00	0.09	82,82,82,82	0
38	SR	0	9498	1/1	1.00	0.04	63,63,63,63	0
38	SR	0	9422	1/1	1.00	0.02	58,58,58,58	0
38	SR	0	9410	1/1	1.00	0.03	41,41,41,41	0
38	SR	1	9419	1/1	1.00	0.03	40,40,40,40	0
38	SR	0	9424	1/1	1.00	0.03	49,49,49,49	0
38	SR	0	9448	1/1	1.00	0.03	63,63,63,63	0
38	SR	0	9415	1/1	1.00	0.02	56,56,56,56	0
39	CD	U	9201	1/1	1.00	0.02	53,53,53,53	0
38	SR	0	9416	1/1	1.00	0.04	43,43,43,43	0
38	SR	0	9406	1/1	1.00	0.02	35,35,35,35	0
38	SR	0	9428	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.