



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:53 PM UTC

PDB ID : 1YIT / pdb_00001yit
Title : Crystal Structure Of Virginiamycin M and S Bound To The 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-13
Resolution : 2.80 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

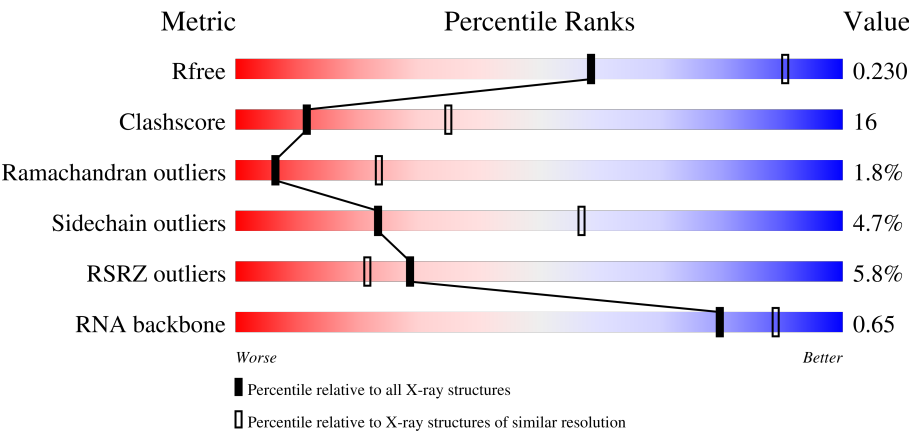
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	3% 58% 31% 5% 6%
2	1	57	65% 33% .
3	2	50	28% 46% 46% 8%
4	3	92	3% 66% 30% .

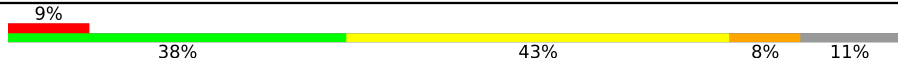
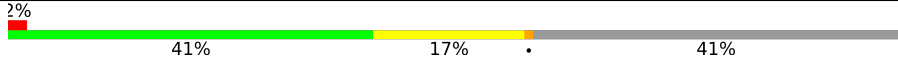
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Mol	Chain	Length	Quality of chain
5	8	7	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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
33	MG	0	8049	-	-	-	X
33	MG	0	8060	-	-	-	X
33	MG	0	8062	-	-	-	X
33	MG	0	8063	-	-	-	X
33	MG	0	8068	-	-	-	X
33	MG	0	8071	-	-	-	X
33	MG	0	8072	-	-	-	X
33	MG	0	8089	-	-	-	X
33	MG	0	8094	-	-	-	X
33	MG	0	8100	-	-	-	X
33	MG	0	8117	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	R	8585	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 91326 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	26349	10873	19054	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called VIRGINIAMYCIN S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	8	7	Total	C	N	O	0	0	0
			60	43	7	10			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	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 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	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 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total	Mg	0	0
			109	109		
33	2	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	1	Total	K	0	0
			1	1		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	73	Total Na 73 73	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

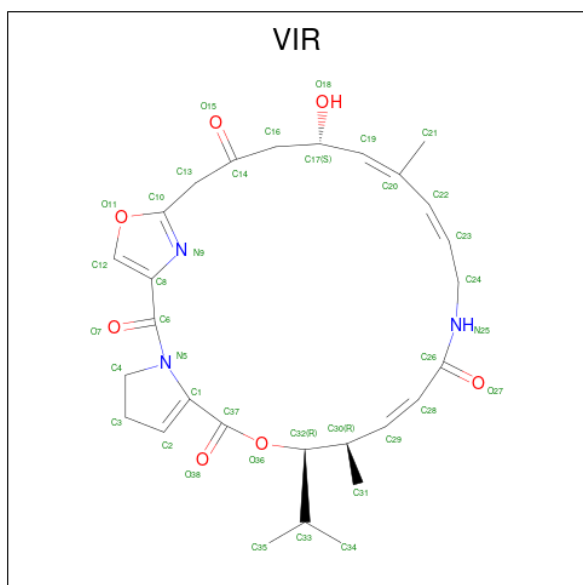
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	3	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0

- Molecule 37 is VIRGINIAMYCIN M1 (CCD ID: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	1	Total C N O 38 28 3 7	0	0

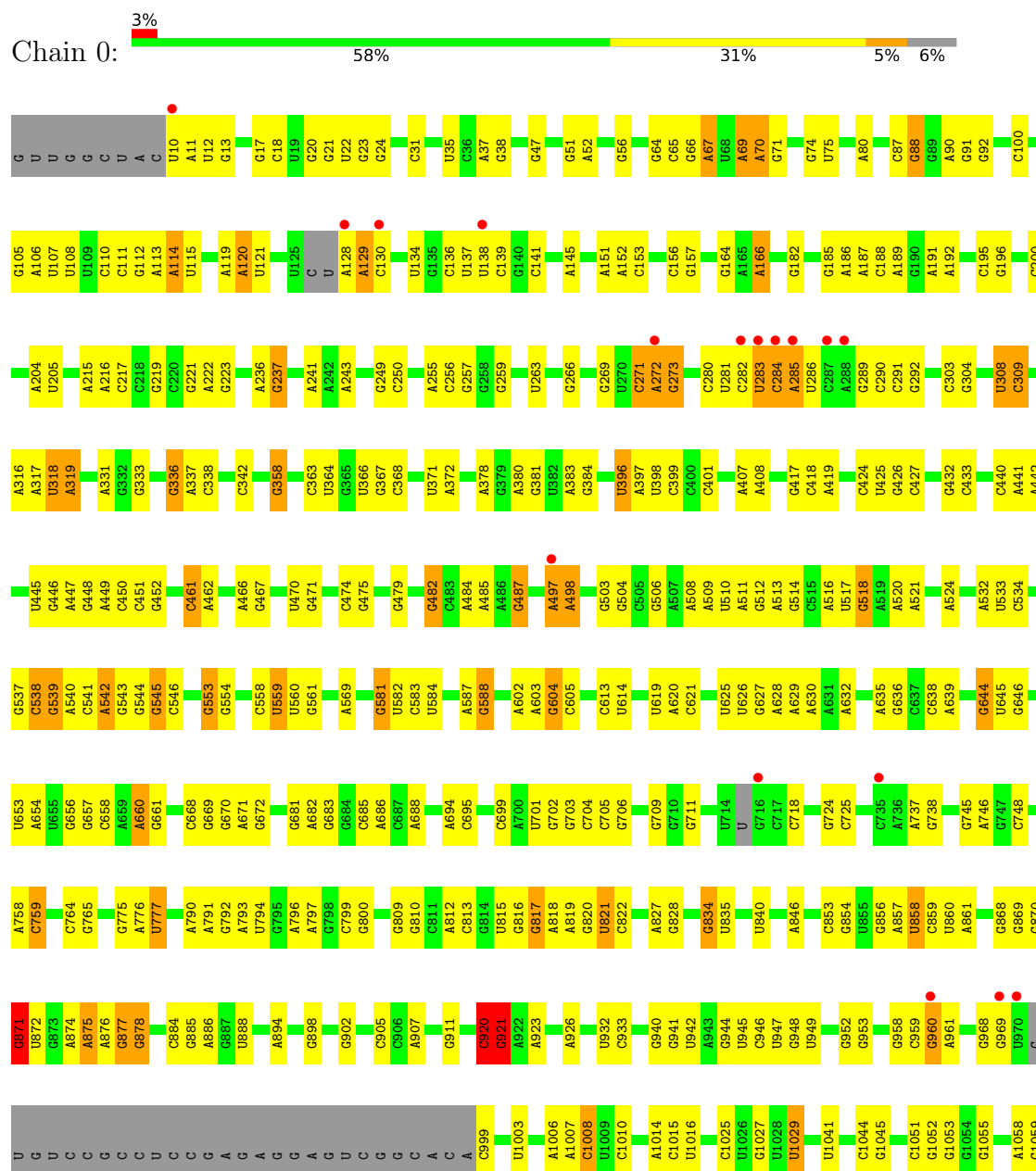
- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

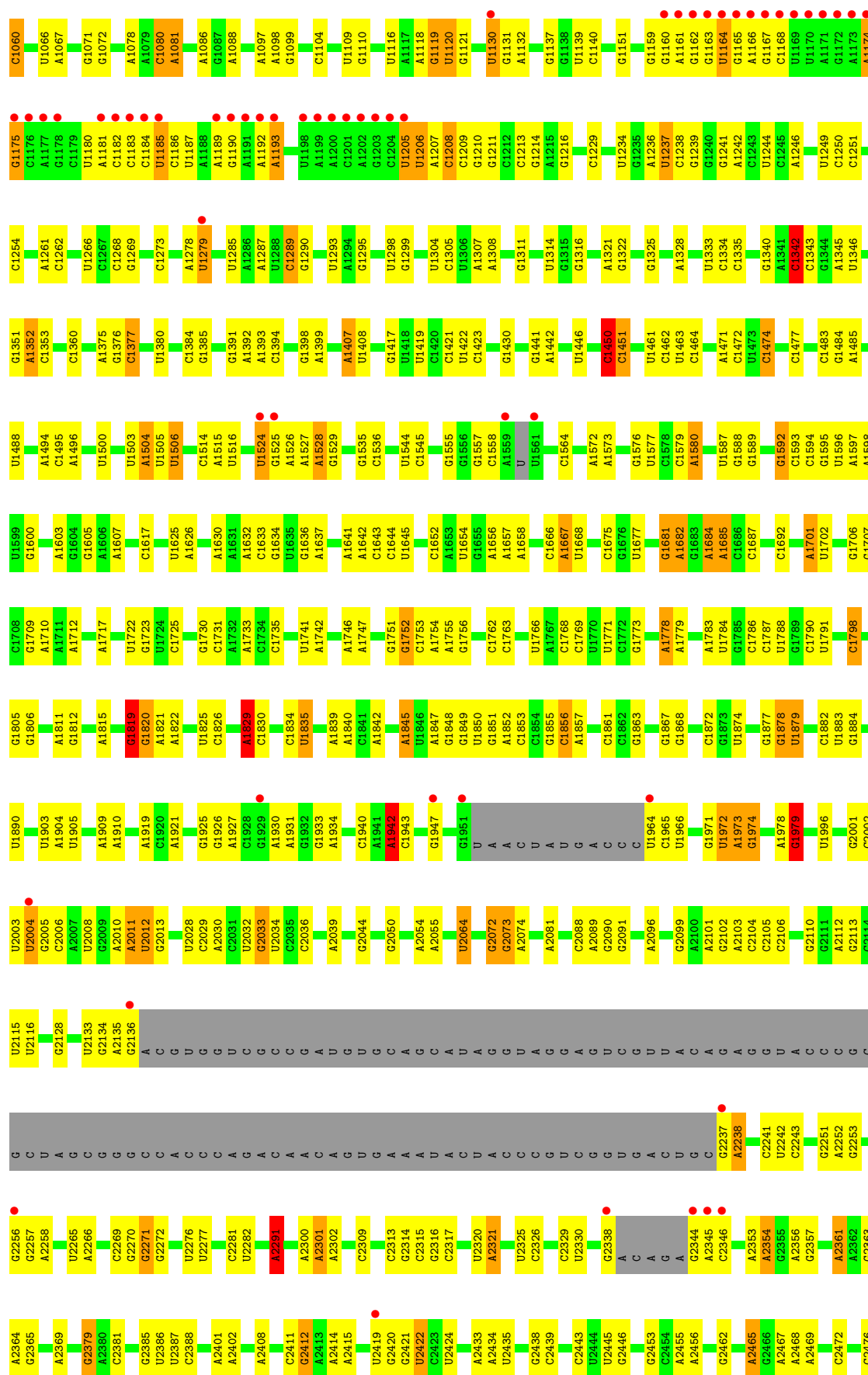
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0
38	O	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0

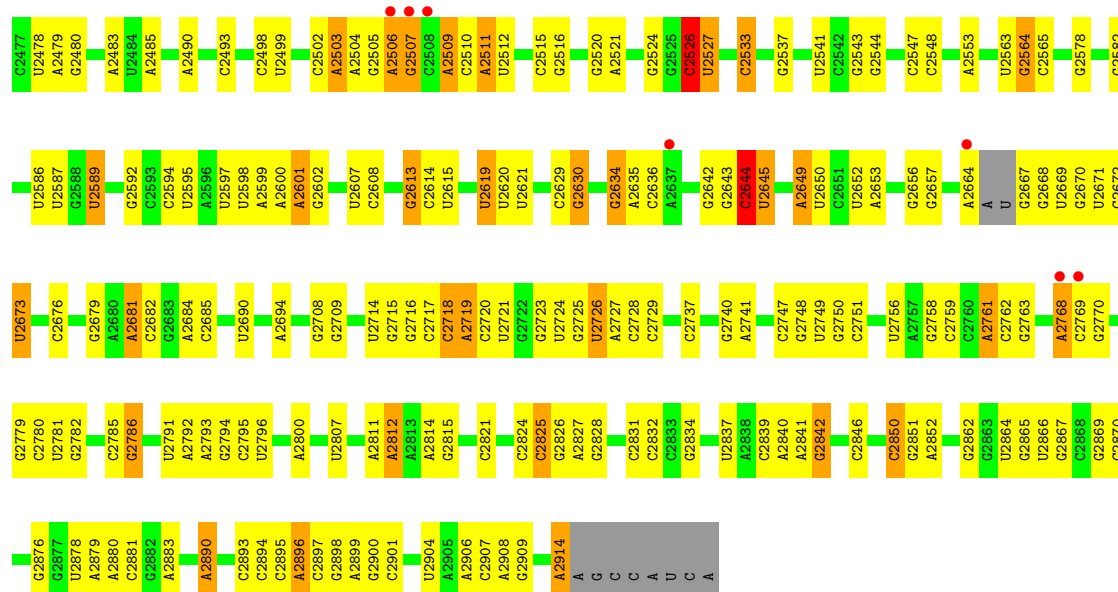
3 Residue-property plots

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







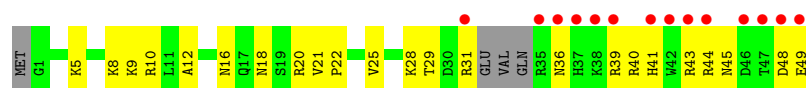
• Molecule 2: 50S RIBOSOMAL PROTEIN L37E

Chain 1: 65% 33% .



• Molecule 3: 50S RIBOSOMAL PROTEIN L39E

Chain 2: 28% 46% 46% 8%



• Molecule 4: 50S RIBOSOMAL PROTEIN L44E

Chain 3: 3% 66% 30% .



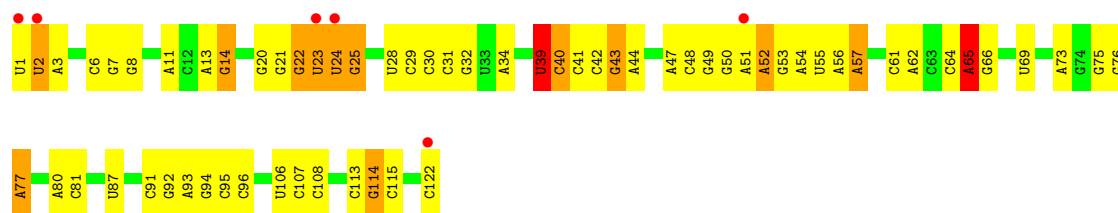
• Molecule 5: VIRGINIAMYCIN S1

Chain 8: 43% 43% 14%

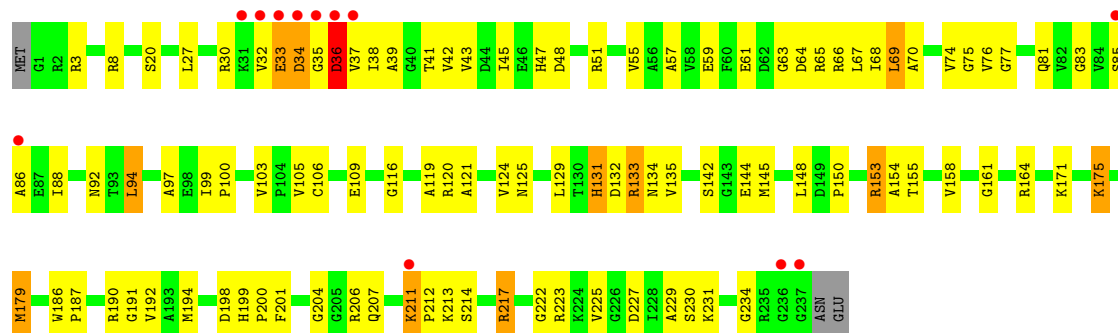


• Molecule 6: 5S RIBOSOMAL RNA

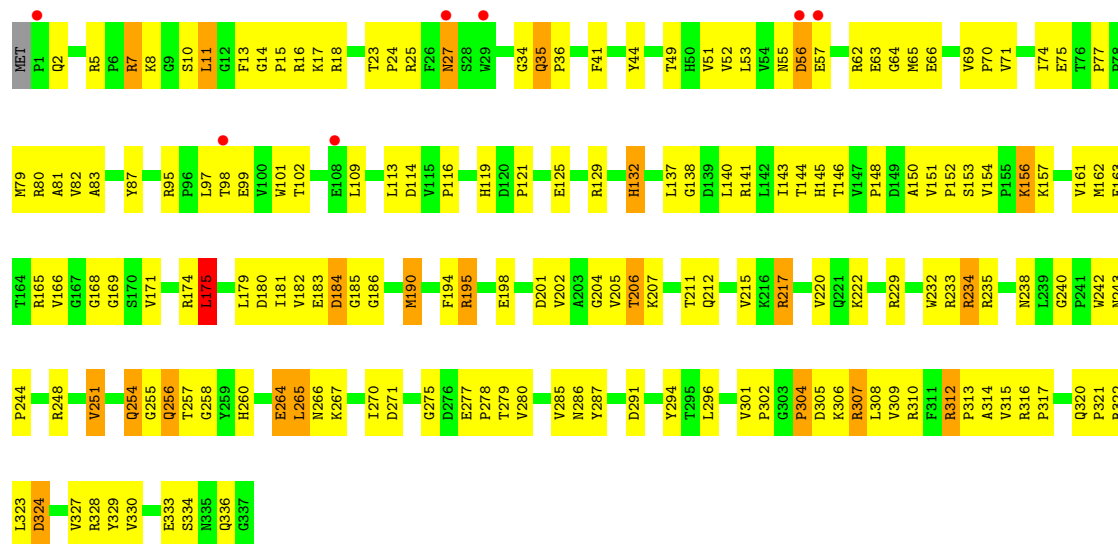
Chain 9: 5% 48% 41% 10% .



• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

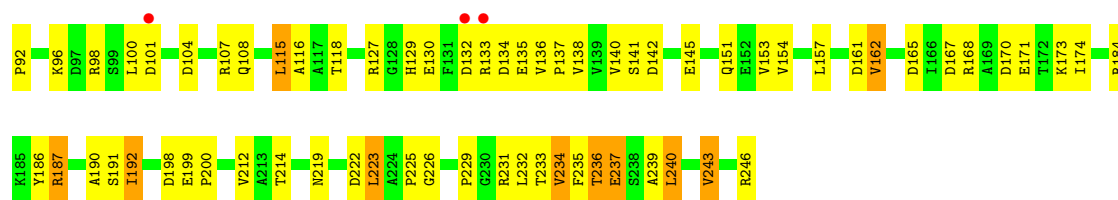


• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

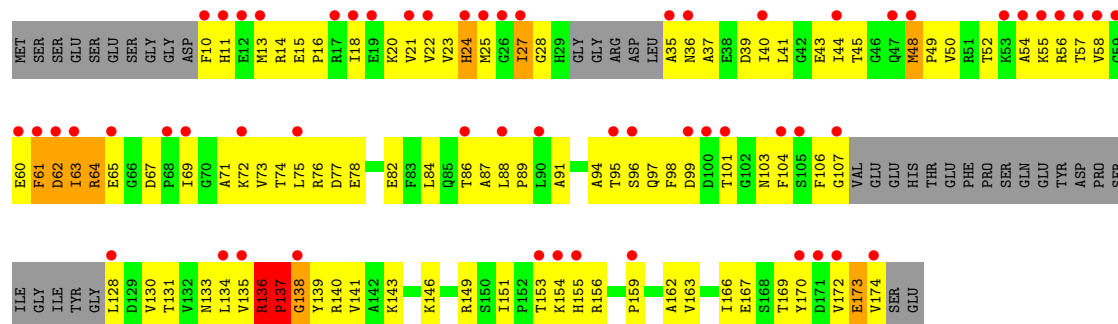


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

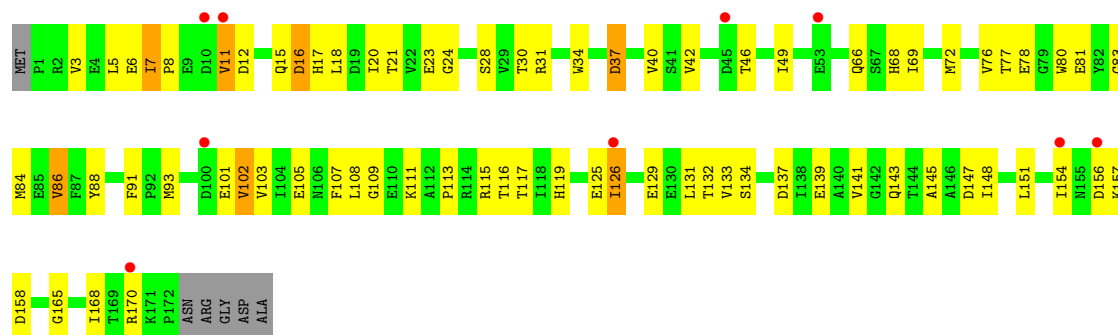




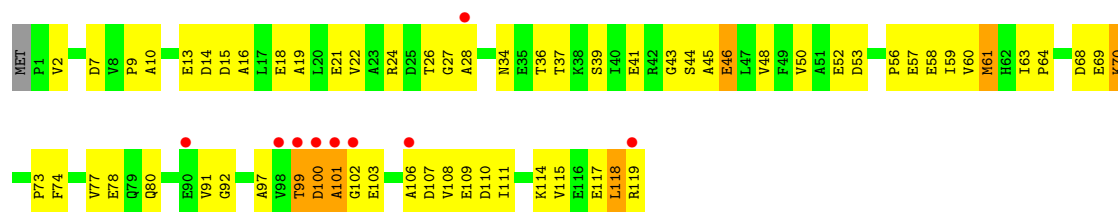
• Molecule 10: 50S RIBOSOMAL PROTEIN L5P



• Molecule 11: 50S RIBOSOMAL PROTEIN L6P

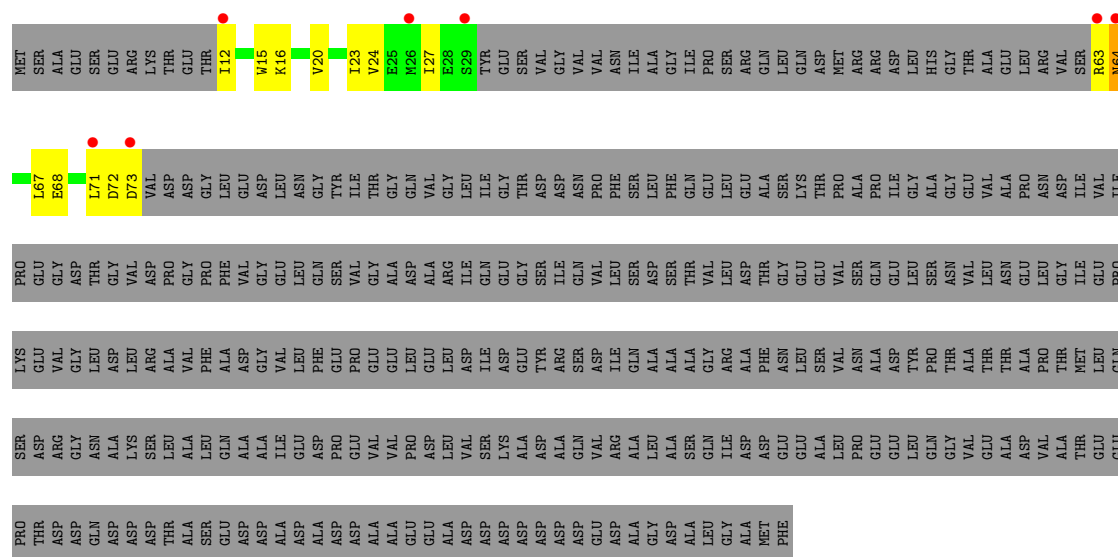


• Molecule 12: 50S RIBOSOMAL PROTEIN L7AE

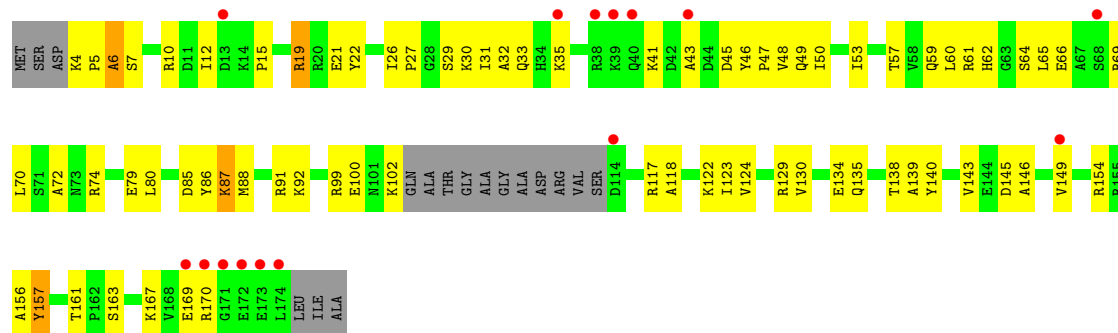


• Molecule 13: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

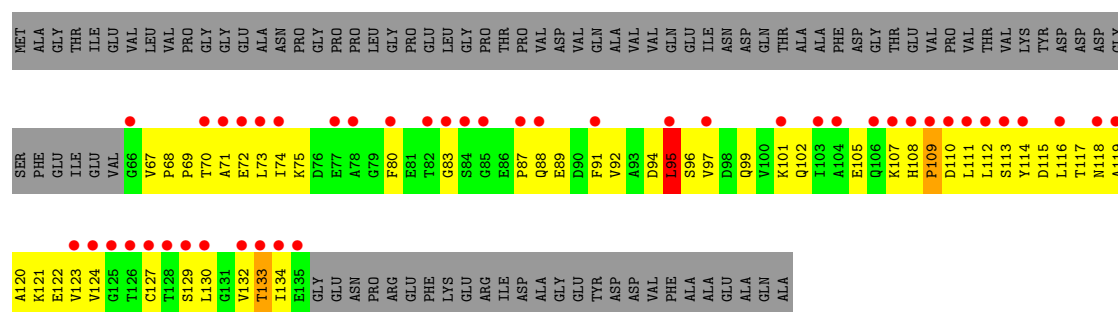




• Molecule 14: 50S RIBOSOMAL PROTEIN L10E

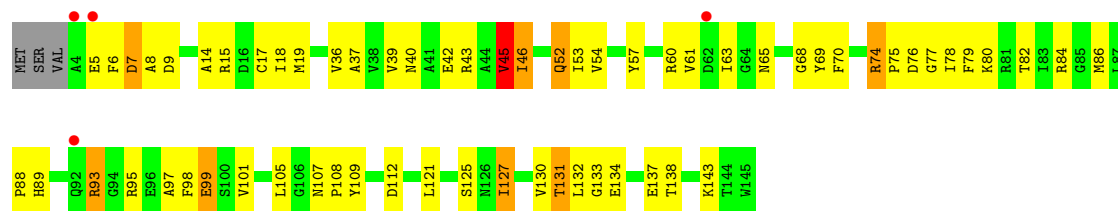


• Molecule 15: 50S RIBOSOMAL PROTEIN L11P

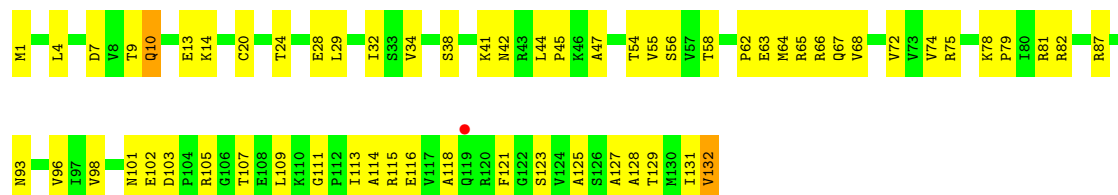


• Molecule 16: 50S RIBOSOMAL PROTEIN L13P

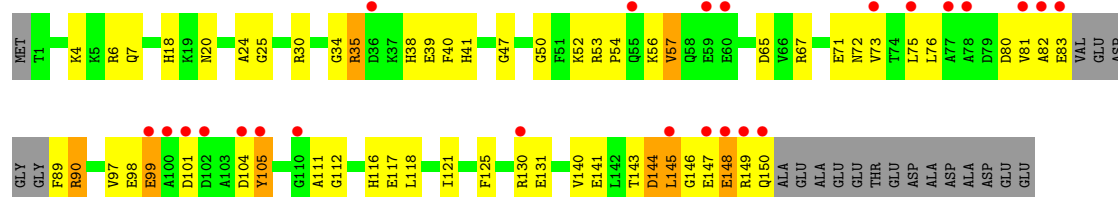




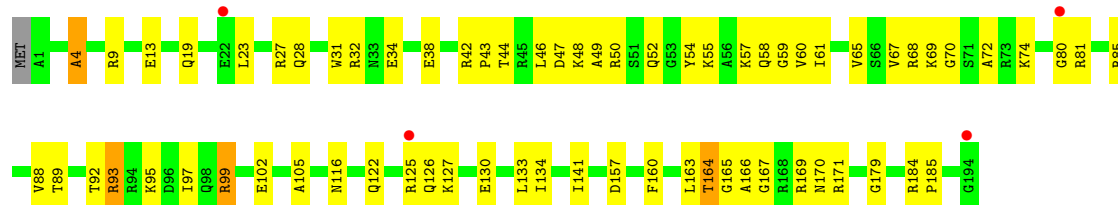
• Molecule 17: 50S RIBOSOMAL PROTEIN L14P



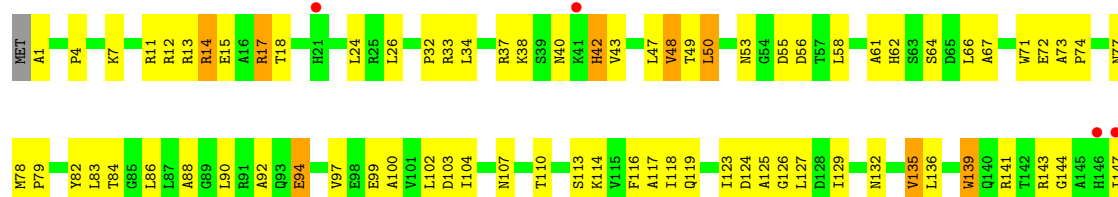
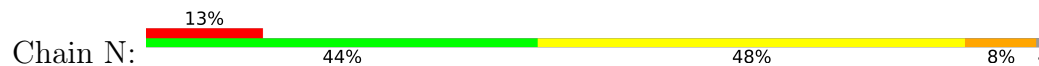
• Molecule 18: 50S RIBOSOMAL PROTEIN L15P

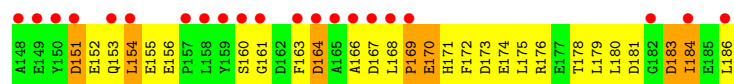


• Molecule 19: 50S RIBOSOMAL PROTEIN L15E

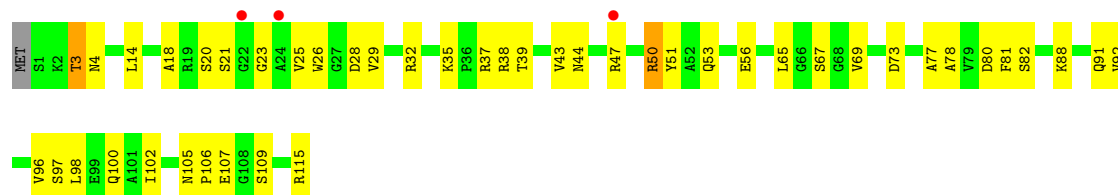


• Molecule 20: 50S RIBOSOMAL PROTEIN L18P

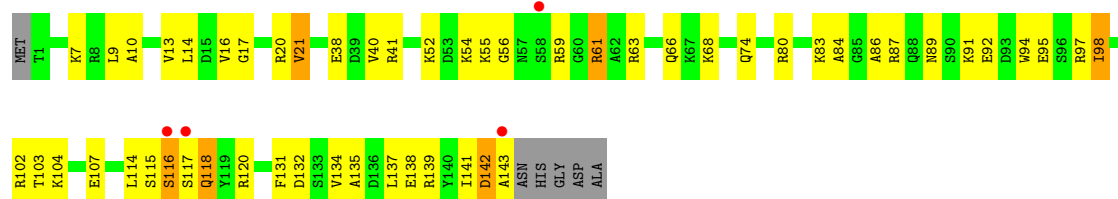




• Molecule 21: 50S RIBOSOMAL PROTEIN L18E



• Molecule 22: 50S RIBOSOMAL PROTEIN L19E



• Molecule 23: 50S RIBOSOMAL PROTEIN L21E



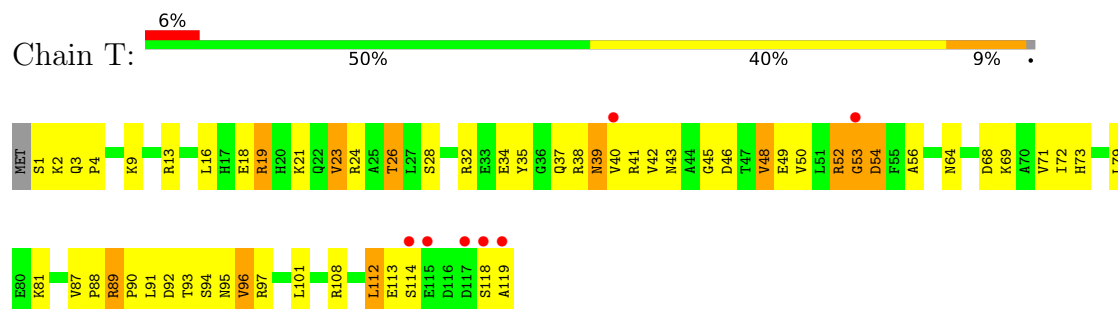
• Molecule 24: 50S RIBOSOMAL PROTEIN L22P



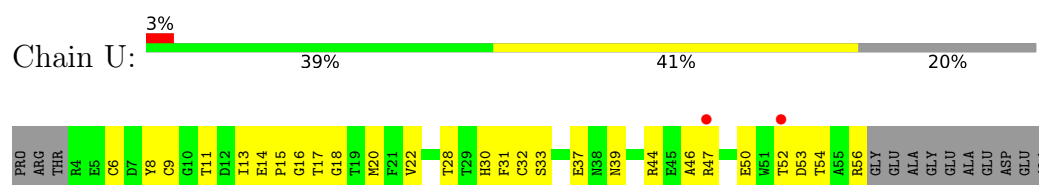
• Molecule 25: 50S RIBOSOMAL PROTEIN L23P



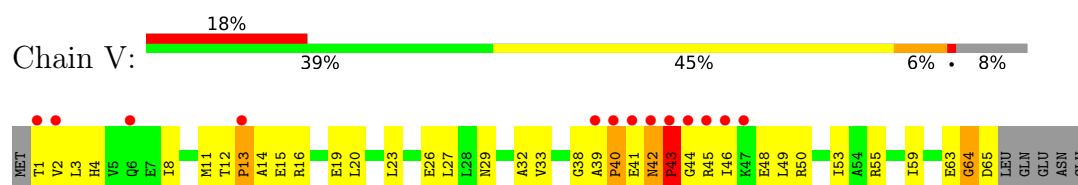
- Molecule 26: 50S RIBOSOMAL PROTEIN L24P



- Molecule 27: 50S RIBOSOMAL PROTEIN L24E



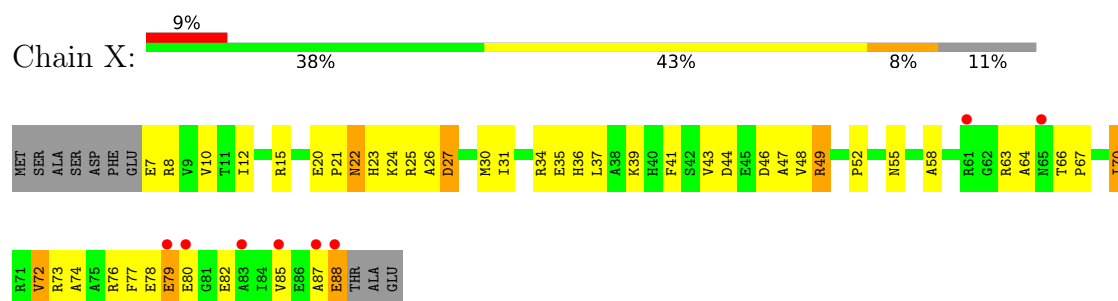
- Molecule 28: 50S RIBOSOMAL PROTEIN L29P



- Molecule 29: 50S RIBOSOMAL PROTEIN L30P



- Molecule 30: 50S RIBOSOMAL PROTEIN L31E



- Molecule 31: 50S RIBOSOMAL PROTEIN L32E

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.58Å 299.76Å 573.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.80 29.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.99-2.80) 93.9 (29.99-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.221 0.208 , 0.230	Depositor DCC
R_{free} test set	4117 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	91326	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: VIR, MG, NA, OMG, 1MA, PSU, UR3, MHV, K, OMU, CD, MEA, MHW, 004, CL, DBB

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	0.37	0/65958	0.60	20/102869 (0.0%)
2	1	0.44	0/438	0.92	1/578 (0.2%)
3	2	0.43	0/401	0.78	0/529
4	3	0.37	0/771	0.84	4/1024 (0.4%)
5	8	1.19	0/13	1.35	0/15
6	9	0.36	0/2904	0.60	3/4526 (0.1%)
7	A	0.42	0/1786	0.99	9/2408 (0.4%)
8	B	0.42	0/2690	0.99	16/3652 (0.4%)
9	C	0.46	0/1884	0.99	5/2551 (0.2%)
10	D	0.36	0/1111	0.90	8/1498 (0.5%)
11	E	0.39	0/1382	0.88	2/1880 (0.1%)
12	F	0.38	0/901	0.86	1/1224 (0.1%)
13	G	0.36	0/241	0.79	0/324
14	H	0.41	0/1302	0.95	4/1743 (0.2%)
15	I	0.36	0/526	0.90	2/716 (0.3%)
16	J	0.44	0/1136	0.95	4/1530 (0.3%)
17	K	0.41	0/1001	0.99	3/1347 (0.2%)
18	L	0.38	0/1130	0.97	7/1509 (0.5%)
19	M	0.42	0/1582	0.93	6/2117 (0.3%)
20	N	0.36	0/1474	1.02	9/1999 (0.5%)
21	O	0.43	0/874	0.93	6/1181 (0.5%)
22	P	0.41	0/1147	0.86	1/1528 (0.1%)
23	Q	0.46	0/749	1.03	2/1005 (0.2%)
24	R	0.46	0/1172	0.97	5/1578 (0.3%)
25	S	0.37	0/648	0.88	3/875 (0.3%)
26	T	0.39	0/958	0.95	4/1289 (0.3%)
27	U	0.39	0/417	0.91	1/562 (0.2%)
28	V	0.38	0/502	1.01	4/675 (0.6%)
29	W	0.48	0/1219	1.04	4/1655 (0.2%)
30	X	0.45	0/664	1.00	4/895 (0.4%)
31	Y	0.44	0/1146	0.93	2/1536 (0.1%)
32	Z	0.34	0/589	0.87	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98716	0.71	140/147605 (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	38
6	9	0	4
All	All	0	42

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	135	VAL	N-CA-C	-10.16	103.25	113.10
22	P	118	GLN	N-CA-C	-8.75	100.93	111.69
23	Q	17	LYS	N-CA-C	-8.72	98.76	109.83
7	A	222	GLY	N-CA-C	-8.10	104.84	114.48
1	0	1942	A	C5'-C4'-C3'	8.06	128.09	116.00
30	X	22	ASN	N-CA-C	7.95	120.66	111.11
1	0	2644	C	C2'-C3'-O3'	7.90	121.35	109.50
14	H	163	SER	N-CA-C	-7.89	98.80	110.48
20	N	153	GLN	N-CA-C	-7.82	102.56	113.20
16	J	112	ASP	N-CA-C	-7.66	99.14	110.48
31	Y	143	TRP	N-CA-C	7.53	121.26	109.96
18	L	145	LEU	N-CA-C	-7.34	103.21	111.07
8	B	157	LYS	N-CA-C	-7.23	105.07	114.04
11	E	11	VAL	N-CA-C	7.19	120.25	109.17
29	W	143	THR	N-CA-C	-7.15	103.82	112.54
8	B	222	LYS	N-CA-C	-7.12	99.38	110.42
7	A	48	ASP	CA-C-N	6.91	126.61	119.56
7	A	48	ASP	C-N-CA	6.91	126.61	119.56
9	C	78	ARG	N-CA-C	6.90	117.69	108.38
20	N	13	ARG	N-CA-C	-6.86	104.54	113.12
28	V	42	ASN	CA-C-N	6.74	128.26	119.84
28	V	42	ASN	C-N-CA	6.74	128.26	119.84
19	M	89	THR	N-CA-C	6.73	118.27	111.07
20	N	169	PRO	N-CA-C	-6.72	105.76	114.03
20	N	151	ASP	N-CA-C	-6.63	105.05	113.01
6	9	39	U	N1-C1'-C2'	6.60	121.90	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	25	ASN	N-CA-C	6.53	120.52	111.90
19	M	70	GLY	N-CA-C	6.49	120.01	111.70
8	B	175	LEU	N-CA-C	-6.49	104.13	111.14
18	L	47	GLY	N-CA-C	6.37	118.60	111.85
24	R	141	VAL	N-CA-C	6.36	117.64	108.48
19	M	13	GLU	N-CA-C	-6.31	105.06	112.89
20	N	48	VAL	N-CA-C	6.29	117.65	108.53
18	L	148	GLU	N-CA-C	-6.21	105.83	113.41
1	0	2291	A	N9-C1'-C2'	6.18	121.27	112.00
26	T	54	ASP	N-CA-C	-6.15	105.74	113.18
8	B	265	LEU	N-CA-C	6.11	118.80	110.55
26	T	52	ARG	N-CA-C	6.10	123.80	110.80
24	R	137	ASN	N-CA-C	6.09	119.47	110.46
25	S	27	ALA	N-CA-C	-6.05	98.87	108.73
1	0	871	G	C5'-C4'-O4'	-6.04	100.74	109.80
1	0	1504	A	N9-C1'-C2'	6.02	121.03	112.00
9	C	186	TYR	N-CA-C	6.02	118.98	110.14
10	D	136	ARG	CA-C-N	6.01	127.36	119.84
10	D	136	ARG	C-N-CA	6.01	127.36	119.84
2	1	43	ALA	N-CA-C	-6.01	104.81	111.36
1	0	920	C	C2'-C3'-O3'	-5.97	104.74	113.70
8	B	114	ASP	N-CA-C	-5.95	101.32	109.71
10	D	62	ASP	N-CA-C	-5.92	105.37	112.59
1	0	834	G	C2'-C3'-O3'	-5.91	104.83	113.70
24	R	122	GLN	N-CA-C	-5.91	98.89	108.41
1	0	2526	C	N1-C1'-C2'	5.87	120.81	112.00
26	T	34	GLU	N-CA-C	5.87	117.68	111.28
21	O	50	ARG	N-CA-C	5.86	117.47	111.14
1	0	1120	U	C5'-C4'-C3'	-5.85	107.22	116.00
17	K	111	GLY	CA-C-N	5.85	127.15	119.84
17	K	111	GLY	C-N-CA	5.85	127.15	119.84
21	O	69	VAL	N-CA-C	5.85	116.90	108.48
1	0	1819	G	C5'-C4'-C3'	5.85	124.77	116.00
10	D	15	GLU	CA-C-N	5.82	127.12	119.84
10	D	15	GLU	C-N-CA	5.82	127.12	119.84
29	W	68	THR	N-CA-C	5.80	117.68	111.36
12	F	118	LEU	N-CA-C	-5.75	106.31	113.15
1	0	2726	U	N1-C1'-C2'	5.75	120.62	112.00
9	C	192	ILE	N-CA-C	5.74	117.01	109.21
8	B	156	LYS	N-CA-C	5.61	117.93	110.53
20	N	14	ARG	N-CA-C	-5.61	105.07	111.07
10	D	151	ILE	N-CA-C	5.58	114.42	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	96	SER	N-CA-C	-5.57	103.03	110.55
6	9	39	U	C4'-C3'-O3'	-5.57	104.65	113.00
6	9	65	A	N9-C1'-C2'	5.57	120.35	112.00
31	Y	183	GLU	N-CA-C	-5.55	100.25	109.46
21	O	82	SER	N-CA-C	-5.50	102.86	110.35
18	L	7	GLN	N-CA-C	5.50	118.19	111.82
15	I	116	LEU	N-CA-C	-5.48	105.69	112.38
1	0	1592	G	N9-C1'-C2'	5.48	120.22	112.00
25	S	57	THR	N-CA-C	5.48	118.23	110.50
4	3	55	VAL	CA-C-N	5.46	126.67	119.84
4	3	55	VAL	C-N-CA	5.46	126.67	119.84
4	3	43	ASN	N-CA-C	5.44	119.18	112.54
8	B	151	VAL	CA-C-N	5.44	124.63	118.97
8	B	151	VAL	C-N-CA	5.44	124.63	118.97
23	Q	13	LYS	N-CA-C	5.43	117.96	111.71
19	M	125	ARG	N-CA-C	5.38	119.62	112.30
20	N	42	HIS	N-CA-C	5.36	117.56	109.41
10	D	48	MET	N-CA-C	5.35	116.43	109.64
18	L	20	ASN	N-CA-C	5.34	120.93	110.56
19	M	4	ALA	N-CA-C	-5.34	105.35	111.07
9	C	167	ASP	N-CA-C	-5.33	106.03	112.54
28	V	64	GLY	N-CA-C	-5.32	107.28	116.01
7	A	198	ASP	N-CA-C	5.32	119.83	113.23
24	R	3	SER	N-CA-C	-5.28	101.26	109.24
14	H	10	ARG	N-CA-C	5.27	118.96	112.54
29	W	69	ARG	N-CA-C	5.27	120.36	112.94
4	3	67	LEU	N-CA-C	5.26	118.16	109.85
8	B	242	TRP	N-CA-C	-5.25	105.47	111.14
9	C	89	ALA	N-CA-C	5.25	117.42	111.02
21	O	4	ASN	CA-C-N	5.25	124.88	119.05
21	O	4	ASN	C-N-CA	5.25	124.88	119.05
1	0	2673	U	N1-C1'-C2'	5.24	119.86	112.00
7	A	133	ARG	N-CA-C	-5.23	106.90	113.28
1	0	1261	A	N9-C1'-C2'	5.20	119.81	112.00
25	S	31	ARG	N-CA-C	-5.20	106.62	113.17
30	X	80	GLU	N-CA-C	-5.19	107.08	113.41
24	R	34	GLU	N-CA-C	5.19	117.84	111.82
1	0	534	C	N1-C1'-C2'	5.17	119.76	112.00
8	B	154	VAL	CA-C-N	5.17	124.79	119.05
8	B	154	VAL	C-N-CA	5.17	124.79	119.05
30	X	79	GLU	N-CA-C	5.17	117.82	111.82
27	U	16	GLY	N-CA-C	-5.15	106.64	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	45	VAL	N-CA-C	5.15	117.15	108.81
8	B	324	ASP	CA-C-N	5.14	125.07	119.78
8	B	324	ASP	C-N-CA	5.14	125.07	119.78
1	0	874	A	C4'-C3'-O3'	-5.13	105.30	113.00
18	L	57	VAL	N-CA-C	-5.12	107.98	112.90
1	0	2301	A	N9-C1'-C2'	5.12	119.68	112.00
7	A	38	ILE	N-CA-C	5.12	117.00	109.63
7	A	148	LEU	N-CA-C	5.11	117.44	109.52
20	N	170	GLU	N-CA-C	-5.10	105.80	111.36
28	V	46	ILE	N-CA-C	-5.10	104.67	111.05
26	T	48	VAL	N-CA-C	5.10	115.71	108.42
1	0	1504	A	C4'-C3'-O3'	-5.09	105.36	113.00
18	L	144	ASP	N-CA-C	-5.09	105.81	111.36
7	A	213	LYS	N-CA-C	5.09	117.73	111.82
7	A	8	ARG	N-CA-C	-5.08	105.83	111.36
8	B	143	ILE	N-CA-C	-5.07	102.96	109.30
14	H	161	THR	N-CA-C	5.07	119.84	113.25
8	B	161	VAL	N-CA-C	5.05	115.37	107.99
30	X	12	ILE	N-CA-C	5.05	112.86	107.76
16	J	9	ASP	N-CA-C	-5.04	105.97	111.82
1	0	1450	C	C2'-C3'-O3'	-5.04	106.14	113.70
14	H	6	ALA	N-CA-C	-5.04	106.65	112.89
8	B	217	ARG	N-CA-C	5.03	116.84	111.36
16	J	68	GLY	N-CA-C	5.02	118.91	112.18
1	0	921	G	N9-C1'-C2'	5.02	119.52	112.00
11	E	37	ASP	N-CA-C	5.01	119.25	113.38
10	D	36	ASN	N-CA-C	-5.01	107.23	113.19
19	M	74	LYS	N-CA-C	5.01	117.97	109.76
21	O	43	VAL	N-CA-C	5.00	115.79	108.53
17	K	54	THR	N-CA-C	-5.00	102.12	110.17

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1681	G	Sidechain
1	0	1829	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	22	U	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	521	A	Sidechain
1	0	619	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	888	U	Sidechain
6	9	39	U	Sidechain
6	9	65	A	Sidechain
6	9	87	U	Sidechain
6	9	94	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	872	0
2	1	431	0	426	23	0
3	2	396	0	413	24	0
4	3	755	0	728	22	0
5	8	60	0	46	1	0
6	9	2599	0	1325	70	0
7	A	1753	0	1766	130	0
8	B	2625	0	2533	168	0
9	C	1859	0	1816	109	0
10	D	1094	0	1085	97	0
11	E	1357	0	1266	70	0
12	F	890	0	843	55	0
13	G	240	0	231	17	0
14	H	1282	0	1292	77	0
15	I	519	0	500	54	0
16	J	1120	0	1098	69	0
17	K	992	0	1031	63	0
18	L	1118	0	1076	50	0
19	M	1558	0	1566	61	0
20	N	1445	0	1401	110	0
21	O	865	0	873	30	0
22	P	1136	0	1123	55	0
23	Q	735	0	729	22	0
24	R	1149	0	1122	60	0
25	S	641	0	605	24	0
26	T	950	0	923	55	0
27	U	410	0	364	29	0
28	V	499	0	511	39	0
29	W	1196	0	1137	114	0
30	X	654	0	653	45	0
31	Y	1130	0	1133	44	0
32	Z	578	0	540	45	0
33	0	109	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	1	0	0	0	0
35	0	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	38	0	34	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
All	All	91326	0	59999	2398	0

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

All (2398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	21:O:3:THR:HG22	1.23	1.16
1:0:871:G:H5'	1:0:871:G:H8	1.13	1.14
9:C:236:THR:HG22	9:C:239:ALA:H	1.13	1.07
1:0:21:G:H5'	24:R:2:ILE:HA	1.40	1.04
1:0:871:G:H5'	1:0:871:G:C8	1.92	1.04
6:9:6:C:H5''	20:N:37:ARG:HH12	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:G:H5''	28:V:50:ARG:HH12	1.20	1.03
1:O:1242:A:H5'	16:J:82:THR:HG23	1.41	1.03
26:T:71:VAL:HG11	26:T:90:PRO:HB3	1.37	1.02
1:O:156:C:H5''	19:M:171:ARG:HD3	1.37	1.01
1:O:870:G:H2'	1:O:871:G:H5''	1.42	1.01
31:Y:187:VAL:HG23	31:Y:192:ASP:HB2	1.42	1.01
14:H:59:GLN:HE21	14:H:129:ARG:HE	1.08	0.99
10:D:154:LYS:H	10:D:154:LYS:HD2	1.26	0.98
29:W:5:VAL:HG11	29:W:153:MET:HE1	1.44	0.97
32:Z:46:ARG:HD2	32:Z:59:TYR:HB2	1.47	0.97
1:O:1751:G:H2'	1:O:1752:G:H5''	1.44	0.96
6:9:6:C:H5''	20:N:37:ARG:NH1	1.78	0.96
29:W:72:PRO:HG2	29:W:77:ALA:HB3	1.48	0.95
1:O:1119:G:H2'	16:J:52:GLN:NE2	1.80	0.95
6:9:76:G:H3'	6:9:77:A:H5''	1.47	0.95
17:K:10:GLN:H	17:K:10:GLN:NE2	1.65	0.94
10:D:57:THR:HG23	10:D:63:ILE:HA	1.49	0.94
7:A:211:LYS:HB3	7:A:212:PRO:HD2	1.50	0.93
6:9:56:A:H2'	6:9:57:A:H5''	1.48	0.93
1:O:2717:C:H2'	1:O:2718:C:H5''	1.51	0.93
16:J:74:ARG:HB3	16:J:74:ARG:HH11	1.34	0.93
15:I:127:CYS:HB3	15:I:132:VAL:HB	1.50	0.93
26:T:9:LYS:HE3	26:T:13:ARG:NH1	1.84	0.92
1:O:545:G:H5'	1:O:545:G:H8	1.34	0.92
8:B:320:GLN:HE21	8:B:321:PRO:HD2	1.34	0.92
4:3:60:LYS:HG3	4:3:61:PRO:HD2	1.51	0.91
22:P:115:SER:H	22:P:118:GLN:HE21	0.91	0.91
1:O:2890:A:H1'	27:U:56:ARG:NH2	1.85	0.91
22:P:59:ARG:HH22	22:P:66:GLN:HE22	0.95	0.91
9:C:127:ARG:NH2	9:C:225:PRO:HG2	1.85	0.91
9:C:78:ARG:HH11	9:C:78:ARG:HG3	1.32	0.91
1:O:1116:U:HO2'	1:O:1118:A:H2	0.91	0.91
29:W:137:GLN:HE21	29:W:141:HIS:HE1	1.15	0.90
30:X:37:LEU:HD13	30:X:85:VAL:HG21	1.53	0.90
1:O:2506:A:HO2'	1:O:2507:G:H8	1.15	0.90
7:A:191:GLY:HA2	7:A:194:MET:HE2	1.51	0.90
29:W:149:LEU:HG	29:W:153:MET:HE2	1.52	0.90
7:A:35:GLY:O	7:A:36:ASP:HB3	1.71	0.90
1:O:1119:G:H2'	16:J:52:GLN:HE22	1.30	0.90
1:O:1160:G:H5'	1:O:1161:A:H5'	1.54	0.90
1:O:1474:C:H6	1:O:1474:C:H5'	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:10:GLN:HE21	17:K:10:GLN:N	1.69	0.89
22:P:115:SER:N	22:P:118:GLN:HE21	1.71	0.89
24:R:17:MET:HE1	24:R:19:ARG:NH2	1.88	0.89
4:3:25:VAL:HG22	4:3:68:LYS:HG3	1.54	0.89
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.89
9:C:1:MET:HG2	9:C:2:GLN:H	1.37	0.88
17:K:10:GLN:H	17:K:10:GLN:HE21	0.89	0.88
1:0:870:G:C2'	1:0:871:G:H5''	2.04	0.87
8:B:179:LEU:O	8:B:183:GLU:HG2	1.75	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.56	0.87
1:0:1187:U:HO2'	1:0:1189:A:H2	1.21	0.87
10:D:63:ILE:HG13	10:D:64:ARG:H	1.38	0.87
22:P:59:ARG:NH2	22:P:66:GLN:HE22	1.73	0.87
7:A:100:PRO:HG2	7:A:103:VAL:HG21	1.55	0.87
17:K:98:VAL:CG1	17:K:102:GLU:HA	2.05	0.86
29:W:13:MET:HE2	29:W:18:GLN:HA	1.57	0.86
8:B:190:MET:HE2	8:B:194:PHE:CD1	2.11	0.86
1:0:2533:C:H5'	1:0:2533:C:H6	1.40	0.86
8:B:162:MET:HE1	8:B:308:LEU:HD21	1.58	0.85
14:H:32:ALA:HB3	14:H:69:ARG:HH12	1.40	0.85
14:H:59:GLN:NE2	14:H:129:ARG:HE	1.74	0.85
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.85
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.85
29:W:6:GLN:HB2	29:W:26:ILE:HD12	1.59	0.84
1:0:2756:U:H3	1:0:2896:A:H2	1.25	0.84
16:J:93:ARG:HB3	16:J:93:ARG:HH11	1.41	0.84
19:M:102:GLU:OE1	19:M:164:THR:HG21	1.76	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.84
1:0:1593:C:H5'	22:P:116:SER:O	1.77	0.84
16:J:19:MET:HE3	16:J:132:LEU:HD11	1.60	0.83
7:A:88:ILE:HD13	7:A:100:PRO:HD3	1.57	0.83
24:R:18:LEU:HB2	24:R:143:VAL:HG13	1.60	0.83
14:H:102:LYS:HD3	14:H:122:LYS:HD3	1.60	0.83
25:S:57:THR:HG22	25:S:59:ASP:H	1.44	0.83
29:W:4:LEU:HD23	29:W:54:PHE:HB3	1.59	0.83
1:0:559:U:H6	1:0:559:U:H5'	1.43	0.83
1:0:656:G:H5'	21:O:3:THR:CG2	2.07	0.83
12:F:58:GLU:HA	12:F:61:MET:HE2	1.61	0.83
20:N:164:ASP:OD1	20:N:167:ASP:HA	1.78	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.79	0.82
12:F:91:VAL:HG12	12:F:92:GLY:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:14:LEU:HD23	21:O:102:ILE:HD11	1.60	0.82
8:B:55:ASN:HB3	8:B:63:GLU:HA	1.60	0.82
22:P:115:SER:H	22:P:118:GLN:NE2	1.75	0.82
22:P:59:ARG:HH22	22:P:66:GLN:NE2	1.78	0.82
1:O:1118:A:H8	1:O:1118:A:H3'	1.44	0.81
26:T:101:LEU:HD13	26:T:112:LEU:HD11	1.63	0.81
28:V:12:THR:HG22	28:V:15:GLU:HG3	1.61	0.81
8:B:201:ASP:HB2	8:B:312:ARG:HD2	1.63	0.81
9:C:236:THR:HG22	9:C:239:ALA:N	1.94	0.81
1:O:1118:A:H3'	1:O:1118:A:C8	2.16	0.81
1:O:1666:C:O2'	1:O:1667:A:H5''	1.81	0.80
7:A:153:ARG:HB2	7:A:153:ARG:HH11	1.45	0.80
31:Y:187:VAL:HG23	31:Y:192:ASP:CB	2.11	0.80
1:O:1164:U:H3	1:O:1192:A:H2	1.29	0.80
1:O:2768:A:H2'	1:O:2769:C:O4'	1.82	0.80
30:X:76:ARG:HH11	30:X:76:ARG:HG3	1.45	0.80
32:Z:37:HIS:HB2	32:Z:47:VAL:HB	1.64	0.80
8:B:304:PRO:HD2	8:B:307:ARG:HD2	1.64	0.80
1:O:1667:A:H8	1:O:1667:A:H5'	1.46	0.80
1:O:1701:A:H4'	1:O:1702:U:H5''	1.63	0.80
1:O:56:G:H5''	28:V:50:ARG:NH1	1.95	0.80
10:D:25:MET:HE2	10:D:41:LEU:HG	1.63	0.80
14:H:41:LYS:HE2	14:H:45:ASP:HB3	1.64	0.79
7:A:179:MET:HA	7:A:179:MET:HE3	1.63	0.79
20:N:7:LYS:HE3	23:Q:21:ARG:O	1.83	0.79
1:O:2291:A:C8	1:O:2309:C:H5'	2.18	0.79
8:B:320:GLN:NE2	8:B:321:PRO:HD2	1.96	0.79
17:K:29:LEU:HB3	17:K:55:VAL:HG11	1.64	0.79
8:B:62:ARG:HA	8:B:65:MET:HE3	1.63	0.79
10:D:28:GLY:HA2	10:D:69:ILE:HG23	1.65	0.79
20:N:48:VAL:CG1	20:N:55:ASP:HB3	2.14	0.78
29:W:81:ASP:OD1	29:W:92:ASP:HB2	1.82	0.78
8:B:18:ARG:HG3	8:B:256:GLN:HG3	1.65	0.78
17:K:118:ALA:HA	17:K:125:ALA:HB2	1.64	0.78
19:M:99:ARG:HD2	19:M:167:GLY:HA2	1.63	0.78
1:O:541:C:C2'	1:O:542:A:H5''	2.14	0.78
13:G:68:GLU:O	13:G:72:ASP:HB2	1.83	0.78
1:O:877:G:H5'	1:O:878:G:OP1	1.84	0.78
7:A:36:ASP:OD2	7:A:85:SER:HB2	1.83	0.78
29:W:13:MET:HE3	29:W:17:ILE:HG22	1.65	0.77
29:W:13:MET:HE2	29:W:18:GLN:CA	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:91:VAL:HG12	12:F:92:GLY:H	1.47	0.77
1:0:2812:A:H2	1:0:2814:A:H62	1.32	0.77
2:1:25:LYS:HD2	3:2:49:GLU:H	1.50	0.77
6:9:48:C:H4'	20:N:141:ARG:HH21	1.50	0.77
29:W:21:LEU:HD22	29:W:26:ILE:CD1	2.15	0.77
10:D:58:VAL:HB	10:D:62:ASP:HB3	1.67	0.76
1:0:1160:G:C5'	1:0:1161:A:H5'	2.14	0.76
1:0:2679:G:H2'	1:0:2681:A:OP2	1.86	0.76
16:J:75:PRO:HG2	16:J:105:LEU:HD21	1.67	0.76
30:X:72:VAL:HG22	30:X:85:VAL:HG12	1.66	0.76
20:N:132:ASN:O	20:N:135:VAL:HG12	1.86	0.76
1:0:1684:A:H1'	3:2:43:ARG:HH22	1.51	0.75
17:K:98:VAL:HG11	17:K:102:GLU:HA	1.68	0.75
1:0:1205:U:H2'	1:0:1206:U:H5''	1.67	0.75
9:C:76:ARG:HB3	9:C:76:ARG:NH1	2.01	0.75
9:C:98:ARG:HG2	9:C:98:ARG:HH11	1.51	0.75
1:0:1116:U:H3	1:0:1246:A:H62	1.33	0.75
1:0:1206:U:H5'	1:0:1206:U:H6	1.51	0.75
1:0:542:A:H5'	1:0:542:A:H8	1.52	0.75
8:B:238:ASN:HD22	8:B:240:GLY:H	1.34	0.75
1:0:1205:U:H2'	1:0:1206:U:C5'	2.17	0.74
12:F:63:ILE:HB	12:F:64:PRO:HD3	1.67	0.74
2:1:8:GLN:HE22	2:1:11:LYS:NZ	1.84	0.74
1:0:21:G:C5'	24:R:2:ILE:HA	2.16	0.74
1:0:871:G:H8	1:0:871:G:C5'	1.98	0.74
1:0:2716:G:H5''	8:B:206:THR:HG21	1.68	0.74
1:0:541:C:H2'	1:0:542:A:C5'	2.17	0.74
6:9:14:G:H5'	6:9:14:G:H8	1.51	0.74
8:B:162:MET:HG3	8:B:310:ARG:HD3	1.69	0.74
29:W:21:LEU:HD21	29:W:48:VAL:HG11	1.70	0.74
6:9:56:A:C2'	6:9:57:A:H5''	2.18	0.74
24:R:14:ALA:HB3	24:R:147:LEU:HB2	1.70	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.73
8:B:258:GLY:H	8:B:260:HIS:CE1	2.06	0.73
8:B:264:GLU:HG2	8:B:267:LYS:HE2	1.68	0.73
27:U:20:MET:HE2	27:U:30:HIS:NE2	2.03	0.73
1:0:545:G:H5'	1:0:545:G:C8	2.21	0.73
1:0:2908:A:H2'	1:0:2909:G:O4'	1.87	0.73
12:F:2:VAL:HG22	12:F:57:GLU:OE1	1.88	0.73
1:0:450:C:OP1	9:C:184:ARG:NH2	2.22	0.73
12:F:34:ASN:HA	19:M:4:ALA:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:12:ILE:HG23	14:H:129:ARG:CZ	2.19	0.73
9:C:78:ARG:HG3	9:C:78:ARG:NH1	2.01	0.73
1:O:1603:A:H5'	1:O:1605:G:O4'	1.89	0.73
7:A:191:GLY:HA2	7:A:194:MET:CE	2.19	0.73
1:O:1474:C:H5'	1:O:1474:C:C6	2.23	0.73
1:O:2502:C:H2'	1:O:2503:A:H5'	1.70	0.73
20:N:47:LEU:HD11	20:N:127:LEU:HD21	1.71	0.73
1:O:2578:G:H5'	1:O:2578:G:H8	1.52	0.73
17:K:74:VAL:CG1	17:K:113:ILE:HG12	2.19	0.73
29:W:88:THR:HG22	29:W:89:ASP:H	1.52	0.72
1:O:2533:C:H5'	1:O:2533:C:C6	2.23	0.72
1:O:272:A:H5'	1:O:273:G:OP2	1.88	0.72
20:N:169:PRO:O	20:N:172:PHE:HB3	1.90	0.72
8:B:41:PHE:CD1	8:B:79:MET:HE2	2.23	0.72
1:O:2837:U:H1'	8:B:307:ARG:HH12	1.53	0.72
6:9:114:G:O6	20:N:11:ARG:HD3	1.89	0.72
12:F:58:GLU:CD	19:M:27:ARG:HH22	1.97	0.72
29:W:65:VAL:HA	29:W:68:THR:HG22	1.72	0.72
1:O:111:C:O2'	2:1:20:ARG:HG2	1.90	0.71
1:O:447:A:OP1	26:T:2:LYS:HG2	1.89	0.71
1:O:2506:A:O2'	1:O:2507:G:H8	1.72	0.71
6:9:73:A:H61	6:9:108:C:H42	1.38	0.71
7:A:81:GLN:HB2	7:A:92:ASN:ND2	2.05	0.71
3:2:41:HIS:H	3:2:45:ASN:HD22	1.36	0.71
19:M:164:THR:HG22	19:M:167:GLY:H	1.55	0.71
1:O:1751:G:C2'	1:O:1752:G:H5''	2.19	0.71
6:9:92:G:H2'	6:9:93:A:C8	2.25	0.71
1:O:2502:C:C2'	1:O:2503:A:H5'	2.21	0.71
7:A:36:ASP:HB2	7:A:83:GLY:HA3	1.73	0.71
22:P:135:ALA:HB1	22:P:139:ARG:HH12	1.53	0.71
30:X:78:GLU:HG2	30:X:79:GLU:H	1.54	0.71
1:O:1160:G:H5'	1:O:1161:A:C5'	2.20	0.71
6:9:75:G:H1	6:9:106:U:H3	1.35	0.71
10:D:22:VAL:HG22	10:D:74:THR:HG22	1.71	0.71
11:E:84:MET:HE1	11:E:148:ILE:CD1	2.21	0.71
1:O:236:A:H4'	1:O:237:G:H5'	1.72	0.71
1:O:2320:U:H4'	1:O:2321:A:O4'	1.91	0.71
15:I:97:VAL:HG12	15:I:101:LYS:HE3	1.73	0.71
29:W:21:LEU:HD21	29:W:48:VAL:CG1	2.20	0.71
1:O:470:U:O2'	2:1:16:HIS:HD2	1.74	0.71
1:O:1925:G:H5'	4:3:29:ARG:HH12	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:76:ARG:HB3	9:C:76:ARG:HH11	1.55	0.71
9:C:115:LEU:HD13	9:C:223:LEU:HD21	1.72	0.71
8:B:162:MET:CE	8:B:308:LEU:HD21	2.19	0.70
1:O:1118:A:H62	1:O:1244:U:H3	1.38	0.70
8:B:98:THR:HG22	8:B:99:GLU:H	1.56	0.70
19:M:28:GLN:O	19:M:32:ARG:HG3	1.90	0.70
6:9:28:U:H5'	20:N:40:ASN:ND2	2.07	0.70
20:N:154:LEU:C	20:N:156:GLU:H	1.99	0.70
28:V:12:THR:HG22	28:V:15:GLU:CG	2.20	0.70
29:W:137:GLN:HE21	29:W:141:HIS:CE1	2.05	0.70
8:B:212:GLN:HB2	8:B:257:THR:HG21	1.74	0.70
10:D:135:VAL:HG21	10:D:139:TYR:CD1	2.26	0.70
14:H:49:GLN:HE21	14:H:140:TYR:HE2	1.40	0.70
1:O:1666:C:H2'	1:O:1667:A:H5'	1.73	0.70
9:C:236:THR:H	9:C:239:ALA:HB3	1.57	0.70
17:K:74:VAL:HG11	17:K:113:ILE:HG12	1.73	0.70
9:C:235:PHE:HE2	9:C:243:VAL:HG21	1.57	0.70
16:J:93:ARG:HB3	16:J:93:ARG:NH1	2.06	0.70
24:R:8:ALA:HB1	24:R:13:THR:HG21	1.72	0.70
8:B:27:ASN:HD22	8:B:27:ASN:H	1.39	0.70
16:J:74:ARG:HH11	16:J:74:ARG:CB	2.03	0.70
24:R:39:THR:HB	24:R:42:GLU:HG3	1.74	0.69
1:O:338:C:H4'	9:C:174:ILE:CD1	2.22	0.69
15:I:120:ALA:O	15:I:124:VAL:HG23	1.92	0.69
27:U:9:CYS:HA	27:U:52:THR:HG23	1.75	0.69
6:9:2:U:OP2	6:9:3:A:H5'	1.92	0.69
1:O:1181:A:H5'	15:I:89:GLU:OE2	1.92	0.69
18:L:67:ARG:O	18:L:71:GLU:HG3	1.92	0.69
26:T:16:LEU:HA	26:T:19:ARG:HG3	1.74	0.69
29:W:88:THR:HG23	29:W:110:GLN:HB3	1.73	0.69
1:O:553:G:P	31:Y:204:ARG:HH22	2.16	0.69
1:O:338:C:H4'	9:C:174:ILE:HD11	1.75	0.69
8:B:71:VAL:HG11	8:B:296:LEU:HB3	1.74	0.69
29:W:6:GLN:HG2	29:W:29:VAL:HA	1.75	0.69
11:E:3:VAL:HG22	11:E:49:ILE:HB	1.74	0.69
1:O:1119:G:H22	1:O:1246:A:H2	1.40	0.69
1:O:2054:A:N3	24:R:128:ARG:NH2	2.40	0.69
1:O:1834:C:H2'	1:O:1840:A:N6	2.08	0.68
25:S:57:THR:HG22	25:S:59:ASP:N	2.07	0.68
1:O:69:A:H5'	1:O:69:A:C8	2.28	0.68
1:O:2346:C:O2'	10:D:52:THR:HG21	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2364:A:H5''	23:Q:15:LYS:HD3	1.75	0.68
22:P:115:SER:OG	22:P:118:GLN:HG3	1.94	0.68
25:S:77:VAL:O	25:S:80:ARG:HG2	1.94	0.68
1:O:2690:U:O2'	11:E:111:LYS:HE3	1.94	0.68
9:C:246:ARG:HB3	9:C:246:ARG:NH1	2.07	0.68
11:E:8:PRO:HB2	11:E:11:VAL:HG23	1.74	0.68
11:E:137:ASP:OD1	11:E:139:GLU:HB2	1.93	0.68
19:M:60:VAL:C	19:M:61:ILE:HD12	2.19	0.68
7:A:105:VAL:HG11	7:A:154:ALA:HB1	1.76	0.68
7:A:200:PRO:HG2	7:A:225:VAL:HG21	1.75	0.68
22:P:103:THR:O	22:P:107:GLU:HG3	1.93	0.68
1:O:2629:C:H41	7:A:206:ARG:HH21	1.39	0.68
19:M:48:LYS:HE3	19:M:52:GLN:NE2	2.08	0.68
7:A:164:ARG:HA	32:Z:69:TYR:CE1	2.28	0.68
26:T:52:ARG:HB2	26:T:95:ASN:HB3	1.75	0.68
17:K:14:LYS:HB2	17:K:45:PRO:HG2	1.75	0.68
7:A:199:HIS:HD2	7:A:201:PHE:H	1.42	0.67
20:N:48:VAL:HG11	20:N:55:ASP:HB3	1.75	0.67
7:A:105:VAL:HG13	7:A:155:THR:O	1.94	0.67
9:C:246:ARG:HB3	9:C:246:ARG:HH11	1.57	0.67
17:K:74:VAL:HG12	17:K:75:ARG:HG3	1.76	0.67
1:O:1116:U:O2'	1:O:1118:A:H2	1.69	0.67
1:O:1189:A:H1'	1:O:1209:C:H1'	1.76	0.67
3:2:36:ASN:HB3	3:2:39:ARG:HE	1.59	0.67
6:9:39:U:H1'	6:9:44:A:H61	1.59	0.67
10:D:58:VAL:HG12	10:D:60:GLU:HG2	1.77	0.67
24:R:111:ILE:HG23	24:R:145:LEU:HD11	1.76	0.67
1:O:1189:A:H1'	1:O:1209:C:C1'	2.23	0.67
1:O:1632:A:H2'	1:O:1633:C:H5'	1.77	0.67
13:G:64:ASN:HD22	13:G:64:ASN:N	1.90	0.67
24:R:99:ALA:HB1	24:R:109:MET:CE	2.23	0.67
28:V:39:ALA:N	28:V:40:PRO:HD2	2.09	0.67
6:9:6:C:C5'	20:N:37:ARG:NH1	2.55	0.67
11:E:37:ASP:OD1	16:J:125:SER:HB3	1.94	0.67
7:A:190:ARG:NH2	7:A:207:GLN:OE1	2.28	0.67
8:B:305:ASP:O	8:B:306:LYS:HB2	1.94	0.67
32:Z:78:THR:O	32:Z:81:ARG:HB2	1.95	0.67
1:O:447:A:P	26:T:1:SER:HB2	2.35	0.67
11:E:81:GLU:HG2	11:E:134:SER:HB3	1.76	0.67
1:O:2769:C:O2'	1:O:2770:G:H5'	1.95	0.67
8:B:132:HIS:NE2	8:B:171:VAL:HG23	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:84:MET:HE1	11:E:148:ILE:HD13	1.76	0.66
27:U:14:GLU:O	27:U:17:THR:HB	1.94	0.66
21:O:47:ARG:HH11	21:O:47:ARG:HG3	1.59	0.66
31:Y:189:ASN:C	31:Y:189:ASN:HD22	2.04	0.66
32:Z:10:ARG:HG3	32:Z:11:SER:H	1.60	0.66
1:O:657:G:OP1	9:C:27:ARG:NH2	2.28	0.66
6:9:29:C:H2'	6:9:30:C:H5'	1.76	0.66
8:B:314:ALA:HB3	8:B:317:PRO:HG3	1.78	0.66
10:D:146:LYS:NZ	20:N:107:ASN:HD21	1.94	0.66
30:X:44:ASP:HB3	30:X:46:ASP:OD1	1.95	0.66
1:O:1641:A:H2'	1:O:1642:A:H5'	1.77	0.66
1:O:2769:C:C2'	1:O:2770:G:H5'	2.26	0.66
14:H:48:VAL:HA	14:H:170:ARG:O	1.94	0.66
24:R:99:ALA:HB1	24:R:109:MET:HE3	1.78	0.66
29:W:6:GLN:HB2	29:W:26:ILE:CD1	2.26	0.66
24:R:104:PHE:HB2	24:R:109:MET:HE2	1.77	0.66
26:T:71:VAL:CG1	26:T:90:PRO:HB3	2.21	0.66
1:O:1328:A:OP1	31:Y:169:ARG:HD2	1.94	0.66
1:O:506:G:H22	1:O:509:A:H5''	1.61	0.66
1:O:1119:G:N2	1:O:1246:A:C2	2.60	0.66
1:O:1819:G:H2'	1:O:1820:G:H4'	1.78	0.66
8:B:66:GLU:OE1	8:B:328:ARG:HD2	1.96	0.66
30:X:47:ALA:HB1	30:X:82:GLU:HB3	1.75	0.66
1:O:1183:C:N4	1:O:1184:C:H41	1.94	0.66
7:A:94:LEU:HD23	7:A:94:LEU:N	2.11	0.66
1:O:1187:U:O2'	1:O:1189:A:H2	1.78	0.65
12:F:91:VAL:CG1	12:F:92:GLY:H	2.10	0.65
7:A:217:ARG:HG2	7:A:229:ALA:HB2	1.77	0.65
29:W:48:VAL:HG12	29:W:52:VAL:HB	1.78	0.65
9:C:142:ASP:OD1	9:C:237:GLU:HB3	1.97	0.65
8:B:56:ASP:OD1	8:B:322:ARG:HB3	1.97	0.65
16:J:19:MET:HE2	16:J:79:PHE:HA	1.77	0.65
3:2:41:HIS:HD2	3:2:44:ARG:H	1.45	0.65
11:E:84:MET:HE2	11:E:133:VAL:HG23	1.79	0.65
20:N:61:ALA:HB3	20:N:88:ALA:HB2	1.78	0.65
29:W:21:LEU:HD22	29:W:26:ILE:HD13	1.78	0.65
7:A:164:ARG:HA	32:Z:69:TYR:HE1	1.62	0.65
20:N:17:ARG:HB3	20:N:17:ARG:HH11	1.61	0.65
29:W:65:VAL:HA	29:W:68:THR:CG2	2.26	0.65
1:O:69:A:H5'	1:O:69:A:H8	1.62	0.65
8:B:141:ARG:HG2	8:B:165:ARG:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:115:LEU:HD21	9:C:243:VAL:HG13	1.77	0.65
16:J:107:ASN:C	16:J:107:ASN:HD22	2.05	0.65
1:O:2420:G:O2'	1:O:2421:G:H5'	1.96	0.65
1:O:2780:C:H1'	11:E:143:GLN:HE21	1.61	0.65
6:9:29:C:O3'	10:D:138:GLY:HA2	1.97	0.65
14:H:12:ILE:O	14:H:12:ILE:HG22	1.97	0.65
14:H:62:HIS:HA	14:H:65:LEU:HD23	1.79	0.65
27:U:52:THR:HG22	27:U:54:THR:H	1.61	0.65
1:O:1234:U:N3	8:B:244:PRO:HB3	2.12	0.64
1:O:1377:C:H5'	1:O:1377:C:H6	1.62	0.64
6:9:13:A:O2'	6:9:14:G:H5''	1.97	0.64
10:D:50:VAL:O	10:D:71:ALA:HA	1.97	0.64
12:F:37:THR:O	12:F:41:GLU:HG3	1.98	0.64
16:J:74:ARG:O	16:J:78:ILE:HG12	1.97	0.64
28:V:39:ALA:C	28:V:41:GLU:H	2.06	0.64
1:O:1964:U:H2'	1:O:1964:U:O2	1.97	0.64
1:O:656:G:C5'	21:O:3:THR:HG22	2.15	0.64
2:1:21:ARG:HD2	2:1:37:CYS:SG	2.37	0.64
8:B:125:GLU:O	8:B:129:ARG:HG3	1.97	0.64
6:9:6:C:C5'	20:N:37:ARG:HH12	2.02	0.64
11:E:137:ASP:O	11:E:141:VAL:HG23	1.97	0.64
20:N:34:LEU:HA	20:N:47:LEU:HD23	1.78	0.64
7:A:153:ARG:HH11	7:A:153:ARG:CB	2.11	0.64
13:G:27:ILE:HD13	13:G:71:LEU:HD23	1.78	0.64
31:Y:106:THR:HG23	31:Y:107:PRO:HD2	1.79	0.64
1:O:1973:A:H5'	1:O:1973:A:H8	1.61	0.64
1:O:2548:C:OP2	8:B:5:ARG:NH2	2.31	0.64
28:V:38:GLY:C	28:V:40:PRO:HD2	2.23	0.64
20:N:176:ARG:O	20:N:180:LEU:HD13	1.98	0.64
14:H:146:ALA:O	14:H:149:VAL:HG12	1.98	0.64
1:O:2850:C:H6	1:O:2850:C:H5'	1.63	0.64
7:A:43:VAL:HG21	7:A:59:GLU:HG3	1.79	0.64
7:A:121:ALA:O	7:A:124:VAL:HG22	1.98	0.64
8:B:51:VAL:HG13	8:B:53:LEU:HD13	1.80	0.64
12:F:50:VAL:HG13	12:F:60:VAL:HG11	1.80	0.64
18:L:143:THR:HG22	18:L:144:ASP:N	2.12	0.64
1:O:944:G:H21	29:W:44:MET:CE	2.11	0.63
6:9:69:U:OP1	20:N:4:PRO:HG3	1.98	0.63
10:D:63:ILE:HG13	10:D:64:ARG:N	2.11	0.63
16:J:6:PHE:HB3	16:J:109:TYR:OH	1.98	0.63
24:R:119:VAL:HG21	24:R:142:ASP:CG	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:544:G:H2'	1:0:545:G:H5''	1.81	0.63
14:H:26:ILE:HA	14:H:123:ILE:HG21	1.78	0.63
24:R:18:LEU:HD12	24:R:143:VAL:HG11	1.80	0.63
1:0:1058:A:H2'	1:0:1060:C:H5''	1.80	0.63
1:0:1130:U:H2'	1:0:1131:G:O4'	1.99	0.63
1:0:2851:G:O2'	1:0:2852:A:H5'	1.98	0.63
15:I:102:GLN:HA	15:I:105:GLU:OE2	1.99	0.63
1:0:281:U:H2'	1:0:282:C:O4'	1.98	0.63
1:0:399:C:H5'	19:M:179:GLY:O	1.99	0.63
8:B:248:ARG:O	8:B:251:VAL:HG13	1.99	0.63
14:H:30:LYS:H	14:H:62:HIS:CD2	2.17	0.63
20:N:164:ASP:CG	20:N:167:ASP:HA	2.24	0.63
1:0:2036:C:O4'	17:K:44:LEU:HG	1.98	0.63
1:0:2563:U:H2'	1:0:2565:C:O5'	1.99	0.63
20:N:47:LEU:CD1	20:N:97:VAL:HG11	2.29	0.63
21:O:50:ARG:HD2	21:O:51:TYR:CE1	2.33	0.63
24:R:17:MET:HE1	24:R:19:ARG:CZ	2.29	0.63
29:W:22:GLU:HG2	29:W:27:HIS:CD2	2.34	0.63
1:0:709:G:O2'	21:O:25:VAL:HG12	1.99	0.63
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.63
25:S:42:GLU:HG2	25:S:49:VAL:HG23	1.80	0.63
27:U:52:THR:HG22	27:U:54:THR:N	2.13	0.63
9:C:7:ASP:OD2	9:C:9:ASP:HB2	1.99	0.62
8:B:132:HIS:HB2	8:B:137:LEU:HD22	1.81	0.62
13:G:23:ILE:O	13:G:27:ILE:HG13	1.98	0.62
16:J:130:VAL:HG12	16:J:131:THR:N	2.14	0.62
29:W:21:LEU:HD22	29:W:26:ILE:HD11	1.81	0.62
8:B:5:ARG:HD2	8:B:8:LYS:NZ	2.15	0.62
9:C:72:LYS:HG2	9:C:77:ALA:HA	1.81	0.62
16:J:57:TYR:O	16:J:61:VAL:HG23	1.99	0.62
12:F:69:GLU:O	12:F:70:LYS:HG2	2.00	0.62
14:H:30:LYS:H	14:H:62:HIS:HD2	1.45	0.62
30:X:43:VAL:HG12	30:X:44:ASP:N	2.14	0.62
6:9:14:G:H5'	6:9:14:G:C8	2.34	0.62
1:0:156:C:H5''	19:M:171:ARG:CD	2.23	0.62
1:0:1053:G:OP1	14:H:15:PRO:HG3	1.99	0.62
25:S:33:SER:OG	25:S:36:GLU:HG3	2.00	0.62
1:0:645:U:OP2	18:L:4:LYS:HE2	1.99	0.62
8:B:312:ARG:HD3	8:B:315:VAL:HG13	1.81	0.62
11:E:6:GLU:HA	11:E:46:THR:HG22	1.82	0.62
14:H:12:ILE:HG23	14:H:129:ARG:NE	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:71:VAL:HG11	26:T:90:PRO:CB	2.21	0.62
7:A:76:VAL:HG23	32:Z:63:LYS:HB3	1.81	0.61
10:D:54:ALA:HB2	10:D:69:ILE:HD12	1.82	0.61
1:O:902:G:N7	18:L:18:HIS:HD2	1.98	0.61
1:O:1299:G:O6	18:L:6:ARG:HD3	1.99	0.61
1:O:1741:U:H5'	1:O:1742:A:OP1	2.00	0.61
6:9:48:C:H4'	20:N:141:ARG:NH2	2.15	0.61
15:I:119:ALA:O	15:I:123:VAL:HG23	2.00	0.61
16:J:19:MET:CE	16:J:132:LEU:HD11	2.30	0.61
30:X:76:ARG:HG3	30:X:76:ARG:NH1	2.14	0.61
1:O:1835:U:C5	1:O:1840:A:N7	2.63	0.61
10:D:84:LEU:HA	10:D:87:ALA:HB3	1.82	0.61
12:F:91:VAL:CG1	12:F:92:GLY:N	2.62	0.61
22:P:135:ALA:HB1	22:P:139:ARG:NH1	2.14	0.61
24:R:39:THR:HG23	24:R:107:GLU:O	2.01	0.61
29:W:38:THR:HG22	29:W:39:ASP:N	2.14	0.61
1:O:2414:A:H2'	1:O:2415:A:C8	2.35	0.61
7:A:199:HIS:CD2	7:A:201:PHE:H	2.17	0.61
1:O:681:G:N3	1:O:681:G:H5'	2.15	0.61
18:L:143:THR:HG22	18:L:145:LEU:H	1.64	0.61
1:O:871:G:C8	1:O:871:G:C5'	2.77	0.61
11:E:125:GLU:HB2	11:E:132:THR:HG23	1.82	0.61
16:J:75:PRO:HG2	16:J:105:LEU:CD2	2.30	0.61
20:N:154:LEU:O	20:N:155:GLU:HB3	2.00	0.61
12:F:61:MET:HB3	19:M:19:GLN:OE1	2.00	0.61
14:H:32:ALA:HB3	14:H:69:ARG:NH1	2.14	0.61
15:I:73:LEU:HD12	15:I:107:LYS:HZ2	1.66	0.61
20:N:119:GLN:O	20:N:123:ILE:HG13	2.00	0.61
20:N:152:GLU:C	20:N:154:LEU:H	2.09	0.61
23:Q:26:PRO:O	23:Q:30:VAL:HG22	2.01	0.61
1:O:1477:C:H5'	1:O:1868:G:C5'	2.31	0.61
1:O:2649:A:H5'	1:O:2649:A:H8	1.65	0.61
20:N:47:LEU:HD13	20:N:97:VAL:HG11	1.82	0.61
29:W:68:THR:HG23	29:W:69:ARG:HG2	1.83	0.61
1:O:1118:A:C8	1:O:1118:A:C3'	2.81	0.60
1:O:1168:C:H5'	15:I:83:GLY:HA3	1.83	0.60
1:O:1667:A:H5'	1:O:1667:A:C8	2.34	0.60
1:O:2265:U:H2'	1:O:2266:A:C8	2.36	0.60
8:B:254:GLN:HG2	8:B:255:GLY:N	2.15	0.60
32:Z:57:CYS:SG	32:Z:59:TYR:HB3	2.41	0.60
7:A:105:VAL:CG1	7:A:154:ALA:HB1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:19:MET:HE1	16:J:78:ILE:HG22	1.83	0.60
1:O:2827:A:H2'	1:O:2828:G:O4'	2.01	0.60
18:L:73:VAL:HG11	18:L:118:LEU:HD21	1.83	0.60
11:E:84:MET:HE2	11:E:133:VAL:CG2	2.32	0.60
16:J:107:ASN:HD21	16:J:109:TYR:HB2	1.65	0.60
1:O:1701:A:H4'	1:O:1702:U:C5'	2.30	0.60
1:O:1701:A:H5''	1:O:1702:U:H3'	1.83	0.60
1:O:2270:G:H4'	7:A:223:ARG:HH12	1.66	0.60
4:3:70:ARG:HG2	4:3:77:ALA:HB2	1.82	0.60
10:D:63:ILE:CG1	10:D:64:ARG:H	2.10	0.60
11:E:11:VAL:HG12	11:E:12:ASP:N	2.16	0.60
13:G:16:LYS:O	13:G:20:VAL:HG23	2.01	0.60
14:H:27:PRO:HD3	14:H:123:ILE:HG22	1.84	0.60
20:N:176:ARG:HE	20:N:180:LEU:HD21	1.65	0.60
24:R:82:GLU:O	24:R:86:LYS:HG3	2.01	0.60
1:O:2468:A:H61	4:3:48:ASN:HD21	1.49	0.60
8:B:271:ASP:HB3	8:B:296:LEU:HD12	1.83	0.60
24:R:12:THR:HG22	24:R:149:GLU:OE1	2.01	0.60
1:O:796:A:HO2'	32:Z:10:ARG:N	1.99	0.60
1:O:1080:C:H4'	1:O:1081:A:OP1	2.02	0.60
24:R:132:ARG:HG2	24:R:133:ALA:N	2.17	0.60
29:W:13:MET:CE	29:W:17:ILE:HG22	2.29	0.60
1:O:797:A:C4'	32:Z:10:ARG:N	2.65	0.60
7:A:211:LYS:HB3	7:A:212:PRO:CD	2.30	0.60
9:C:115:LEU:O	9:C:118:THR:HB	2.02	0.60
22:P:115:SER:O	22:P:117:SER:N	2.31	0.60
29:W:88:THR:HG23	29:W:110:GLN:NE2	2.17	0.60
1:O:1285:U:H4'	29:W:74:GLU:OE1	2.02	0.60
16:J:107:ASN:ND2	16:J:109:TYR:H	1.99	0.60
1:O:558:C:H2'	1:O:559:U:C5'	2.32	0.59
2:1:8:GLN:HE22	2:1:11:LYS:HZ2	1.50	0.59
12:F:14:ASP:O	12:F:18:GLU:HG3	2.02	0.59
24:R:18:LEU:HD12	24:R:143:VAL:CG1	2.32	0.59
29:W:13:MET:HE3	29:W:17:ILE:CG2	2.32	0.59
1:O:259:G:H21	19:M:58:GLN:NE2	2.00	0.59
1:O:1589:G:N2	1:O:1605:G:H1'	2.16	0.59
7:A:161:GLY:O	32:Z:68:SER:HB2	2.02	0.59
10:D:146:LYS:NZ	20:N:107:ASN:ND2	2.49	0.59
8:B:190:MET:HE2	8:B:194:PHE:HD1	1.66	0.59
11:E:7:ILE:HD11	11:E:11:VAL:C	2.27	0.59
13:G:64:ASN:N	13:G:64:ASN:ND2	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:62:PRO:HG3	17:K:65:ARG:NH2	2.18	0.59
22:P:134:VAL:O	22:P:137:LEU:HB3	2.02	0.59
31:Y:151:SER:HB3	31:Y:154:ARG:HB3	1.83	0.59
3:2:22:PRO:HG2	3:2:25:VAL:CG2	2.32	0.59
14:H:49:GLN:HG3	14:H:140:TYR:CE2	2.37	0.59
22:P:7:LYS:HD3	22:P:21:VAL:CG2	2.32	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
1:0:2694:A:H4'	11:E:91:PHE:HE1	1.66	0.59
12:F:27:GLY:HA3	12:F:101:ALA:O	2.02	0.59
23:Q:18:PRO:O	23:Q:21:ARG:HB2	2.03	0.59
11:E:116:THR:HG22	11:E:151:LEU:HD22	1.84	0.59
11:E:133:VAL:HG12	11:E:141:VAL:HG13	1.85	0.59
22:P:61:ARG:HH11	22:P:61:ARG:HB2	1.68	0.59
29:W:21:LEU:HD13	29:W:26:ILE:HD11	1.84	0.59
29:W:73:LEU:HD22	29:W:111:GLY:HA2	1.85	0.59
1:0:660:A:H4'	1:0:661:G:O5'	2.03	0.59
10:D:25:MET:HE1	10:D:37:ALA:O	2.02	0.59
12:F:52:GLU:HG3	12:F:77:VAL:O	2.03	0.59
17:K:82:ARG:NH2	17:K:115:ARG:HG2	2.18	0.59
29:W:4:LEU:CD2	29:W:54:PHE:HB3	2.31	0.59
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.59
7:A:33:GLU:OE1	7:A:33:GLU:N	2.35	0.59
31:Y:189:ASN:HA	31:Y:217:ILE:HD11	1.84	0.59
1:0:2408:A:H4'	4:3:15:ASN:O	2.03	0.59
7:A:88:ILE:O	7:A:88:ILE:HG22	2.02	0.59
15:I:129:SER:O	15:I:130:LEU:HD23	2.03	0.59
19:M:134:ILE:HG23	19:M:141:ILE:HD13	1.85	0.59
20:N:38:LYS:HD2	20:N:114:LYS:HE3	1.85	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.03	0.58
8:B:275:GLY:O	8:B:291:ASP:HA	2.03	0.58
8:B:280:VAL:HG13	8:B:333:GLU:O	2.02	0.58
12:F:19:ALA:O	12:F:22:VAL:HG22	2.02	0.58
16:J:39:VAL:HG12	16:J:40:ASN:ND2	2.18	0.58
30:X:25:ARG:HD3	30:X:64:ALA:O	2.01	0.58
30:X:30:MET:HE1	30:X:58:ALA:HB3	1.85	0.58
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.58
1:0:1733:A:H4'	8:B:212:GLN:HA	1.85	0.58
17:K:55:VAL:HG12	17:K:56:SER:N	2.19	0.58
26:T:26:THR:HA	26:T:39:ASN:HB3	1.85	0.58
30:X:72:VAL:HG22	30:X:85:VAL:CG1	2.32	0.58
1:0:583:C:H2'	1:0:584:U:H6	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O2'	23:Q:11:ARG:HG3	2.03	0.58
1:0:2629:C:N4	7:A:206:ARG:HH21	2.01	0.58
2:1:25:LYS:O	2:1:25:LYS:HG2	2.02	0.58
19:M:164:THR:HG22	19:M:166:ALA:N	2.18	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.34	0.58
16:J:131:THR:HG22	16:J:134:GLU:H	1.68	0.58
20:N:100:ALA:O	20:N:129:ILE:HG23	2.03	0.58
30:X:10:VAL:HG11	30:X:36:HIS:HE1	1.69	0.58
1:0:256:C:H2'	1:0:257:G:O4'	2.03	0.58
1:0:1603:A:H5''	1:0:1605:G:H5'	1.86	0.58
1:0:2779:G:H21	11:E:143:GLN:NE2	2.01	0.58
3:2:22:PRO:HG2	3:2:25:VAL:HG23	1.86	0.58
12:F:111:ILE:O	12:F:115:VAL:HG23	2.03	0.58
21:O:78:ALA:C	21:O:98:LEU:HD13	2.29	0.58
28:V:39:ALA:N	28:V:40:PRO:CD	2.66	0.58
1:0:2064:U:H5'	1:0:2652:U:H4'	1.86	0.58
1:0:2815:G:OP2	16:J:99:GLU:HG2	2.04	0.58
7:A:39:ALA:HB3	7:A:61:GLU:OE2	2.03	0.58
7:A:99:ILE:O	7:A:131:HIS:HE1	1.87	0.58
8:B:278:PRO:HD3	8:B:294:TYR:CE2	2.39	0.58
20:N:78:MET:HB2	20:N:79:PRO:HD3	1.86	0.58
1:0:1118:A:C8	1:0:1119:G:H5''	2.38	0.58
9:C:1:MET:HG2	9:C:2:GLN:N	2.14	0.58
10:D:25:MET:HE1	10:D:37:ALA:HB1	1.86	0.58
10:D:25:MET:CE	10:D:37:ALA:HB1	2.33	0.58
18:L:149:ARG:O	18:L:150:GLN:HB3	2.04	0.58
30:X:31:ILE:O	30:X:35:GLU:HG3	2.03	0.58
1:0:1244:U:OP1	16:J:18:ILE:HD13	2.04	0.58
1:0:1278:A:H4'	1:0:1279:U:C4	2.39	0.58
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.58
10:D:23:VAL:HG23	10:D:23:VAL:O	2.03	0.58
20:N:97:VAL:HG12	20:N:127:LEU:HD11	1.85	0.58
1:0:21:G:H4'	24:R:2:ILE:HG22	1.85	0.58
1:0:2676:C:H4'	16:J:70:PHE:CE1	2.39	0.58
3:2:36:ASN:HB3	3:2:39:ARG:NE	2.17	0.58
17:K:4:LEU:HD22	17:K:116:GLU:HB3	1.86	0.58
1:0:583:C:H2'	1:0:584:U:C6	2.39	0.58
1:0:588:G:O6	29:W:154:ARG:NH1	2.37	0.58
1:0:968:G:H1'	14:H:35:LYS:HD2	1.85	0.58
1:0:1687:C:O2	2:1:9:GLY:HA2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:233:THR:HG22	9:C:234:VAL:H	1.69	0.58
25:S:33:SER:O	25:S:37:VAL:HG23	2.04	0.58
26:T:50:VAL:HG12	26:T:56:ALA:HA	1.85	0.58
8:B:205:VAL:O	8:B:307:ARG:NE	2.37	0.57
13:G:23:ILE:HG22	13:G:27:ILE:HD11	1.86	0.57
16:J:52:GLN:HG3	16:J:53:ILE:N	2.19	0.57
16:J:131:THR:HG22	16:J:133:GLY:N	2.19	0.57
18:L:145:LEU:O	18:L:148:GLU:HG3	2.04	0.57
31:Y:97:LEU:HD21	31:Y:235:GLU:OE2	2.04	0.57
1:0:635:A:H2'	1:0:636:G:H5''	1.86	0.57
1:0:1527:A:H1'	1:0:1528:A:C8	2.39	0.57
9:C:77:ALA:O	9:C:78:ARG:HG3	2.04	0.57
32:Z:72:GLU:OE1	32:Z:77:LYS:HE2	2.05	0.57
1:0:945:U:H2'	1:0:946:C:C6	2.40	0.57
1:0:1120:U:H5''	1:0:1120:U:C6	2.39	0.57
1:0:2824:C:H5''	1:0:2825:C:H5'	1.87	0.57
28:V:49:LEU:O	28:V:53:ILE:HG13	2.04	0.57
1:0:1060:C:H6	1:0:1060:C:H5'	1.69	0.57
1:0:1555:G:H4'	1:0:1630:A:H2	1.69	0.57
1:0:1771:U:H5'	32:Z:20:ARG:HH21	1.67	0.57
8:B:162:MET:HE2	8:B:310:ARG:HD3	1.86	0.57
20:N:110:THR:HB	20:N:113:SER:OG	2.04	0.57
1:0:2721:U:H4'	17:K:87:ARG:HG3	1.86	0.57
6:9:54:A:O2'	6:9:55:U:H5'	2.03	0.57
7:A:94:LEU:HG	7:A:99:ILE:HD11	1.87	0.57
8:B:41:PHE:HB3	8:B:190:MET:CE	2.34	0.57
24:R:111:ILE:HG23	24:R:145:LEU:CD1	2.35	0.57
25:S:53:ASN:HD22	25:S:53:ASN:N	2.02	0.57
1:0:1162:G:H1'	15:I:112:LEU:HD11	1.87	0.57
1:0:2036:C:C1'	17:K:44:LEU:HG	2.34	0.57
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.57
10:D:23:VAL:HG21	10:D:45:THR:HG21	1.87	0.57
29:W:122:ARG:HG3	29:W:122:ARG:HH11	1.69	0.57
6:9:6:C:OP1	20:N:37:ARG:NH1	2.38	0.57
8:B:55:ASN:CB	8:B:63:GLU:HA	2.33	0.57
17:K:113:ILE:HD12	17:K:128:ALA:HB2	1.87	0.57
29:W:21:LEU:HB3	29:W:26:ILE:HG12	1.87	0.57
29:W:65:VAL:HG12	29:W:116:LEU:HD13	1.86	0.57
29:W:88:THR:HG22	29:W:89:ASP:N	2.19	0.57
1:0:558:C:H2'	1:0:559:U:H5'	1.87	0.57
1:0:1162:G:H1'	15:I:112:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2649:A:H5'	1:0:2649:A:C8	2.40	0.57
14:H:49:GLN:HG3	14:H:140:TYR:CD2	2.40	0.57
15:I:71:ALA:O	15:I:75:LYS:HG3	2.04	0.57
15:I:118:ASN:HA	15:I:121:LYS:HD2	1.86	0.57
22:P:59:ARG:O	22:P:63:ARG:HG3	2.04	0.57
27:U:33:SER:O	27:U:37:GLU:HG3	2.04	0.57
1:0:1132:A:N6	1:0:1229:C:H2'	2.20	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.04	0.57
12:F:53:ASP:OD1	12:F:80:GLN:HB2	2.05	0.57
29:W:126:ASP:HB3	29:W:135:GLY:O	2.04	0.57
7:A:194:MET:HE3	7:A:199:HIS:HB2	1.86	0.56
15:I:108:HIS:N	15:I:109:PRO:HD2	2.20	0.56
8:B:62:ARG:HA	8:B:65:MET:CE	2.33	0.56
22:P:115:SER:C	22:P:117:SER:H	2.12	0.56
1:0:544:G:C2'	1:0:545:G:H5''	2.35	0.56
1:0:870:G:OP2	7:A:3:ARG:HD3	2.05	0.56
1:0:1393:A:H2'	1:0:1394:C:C6	2.41	0.56
1:0:1972:U:H2'	1:0:1973:A:H5'	1.88	0.56
1:0:2668:G:H2'	1:0:2669:U:C6	2.40	0.56
1:0:2840:A:OP1	8:B:211:THR:HG23	2.05	0.56
7:A:217:ARG:HH11	7:A:217:ARG:HG3	1.67	0.56
8:B:217:ARG:HG3	8:B:257:THR:CG2	2.35	0.56
9:C:151:GLN:HA	9:C:151:GLN:HE21	1.70	0.56
29:W:151:GLU:O	29:W:154:ARG:HB2	2.06	0.56
31:Y:126:PRO:HG2	31:Y:128:PHE:CE1	2.40	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.56
7:A:33:GLU:O	7:A:34:ASP:HB2	2.04	0.56
8:B:7:ARG:HG2	8:B:7:ARG:HH11	1.70	0.56
8:B:145:HIS:HD2	8:B:146:THR:O	1.86	0.56
21:O:73:ASP:HA	21:O:92:VAL:O	2.04	0.56
22:P:104:LYS:HE2	22:P:138:GLU:OE1	2.04	0.56
29:W:4:LEU:HD22	29:W:52:VAL:HG21	1.87	0.56
1:0:2271:G:OP1	7:A:223:ARG:NH2	2.38	0.56
9:C:200:PRO:HB3	9:C:212:VAL:HG23	1.88	0.56
28:V:1:THR:O	28:V:4:HIS:CE1	2.59	0.56
1:0:282:C:O2'	1:0:283:U:H5'	2.06	0.56
1:0:1446:U:H2'	25:S:55:GLN:NE2	2.20	0.56
1:0:2419:U:H5''	1:0:2420:G:H5'	1.88	0.56
1:0:2601:A:N1	17:K:38:SER:HB2	2.20	0.56
6:9:42:C:O2	10:D:76:ARG:HD2	2.04	0.56
11:E:126:ILE:HB	11:E:131:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:61:ARG:HH11	14:H:61:ARG:HG3	1.71	0.56
21:O:32:ARG:O	21:O:32:ARG:HD3	2.04	0.56
29:W:147:ASP:O	29:W:151:GLU:HB2	2.06	0.56
1:O:538:C:OP2	31:Y:134:HIS:HE1	1.87	0.56
1:O:694:A:H2'	1:O:695:C:H5'	1.87	0.56
1:O:797:A:H4'	32:Z:10:ARG:N	2.21	0.56
1:O:952:G:N3	1:O:2302:A:H2'	2.21	0.56
1:O:1666:C:H2'	1:O:1667:A:C5'	2.35	0.56
1:O:1735:C:OP2	8:B:234:ARG:HG3	2.06	0.56
7:A:64:ASP:OD1	7:A:66:ARG:HD2	2.04	0.56
10:D:146:LYS:HZ3	20:N:107:ASN:HD21	1.53	0.56
11:E:154:ILE:HD11	11:E:157:LYS:HB2	1.88	0.56
17:K:109:LEU:HD13	17:K:113:ILE:HD11	1.87	0.56
18:L:72:ASN:OD1	18:L:75:LEU:HD12	2.06	0.56
1:O:447:A:O2'	1:O:448:G:H5'	2.06	0.56
1:O:1241:G:N3	16:J:86:MET:HE2	2.21	0.56
9:C:168:ARG:NH2	9:C:190:ALA:O	2.39	0.56
11:E:154:ILE:HD11	11:E:157:LYS:HE2	1.87	0.56
14:H:43:ALA:HB1	14:H:140:TYR:CE2	2.41	0.56
15:I:101:LYS:O	15:I:105:GLU:HG3	2.05	0.56
20:N:43:VAL:HG13	20:N:118:ILE:HD11	1.88	0.56
20:N:86:LEU:HD12	20:N:125:ALA:HB2	1.88	0.56
27:U:17:THR:HG22	27:U:18:GLY:N	2.21	0.56
1:O:92:G:H4'	28:V:44:GLY:HA3	1.87	0.56
1:O:447:A:OP2	26:T:1:SER:HB2	2.05	0.56
1:O:737:A:H2'	1:O:738:G:O4'	2.06	0.56
17:K:32:ILE:HD11	17:K:56:SER:HB3	1.87	0.56
22:P:13:VAL:HG21	22:P:41:ARG:HG2	1.87	0.56
1:O:1189:A:H1'	1:O:1209:C:O4'	2.06	0.56
9:C:127:ARG:HG2	9:C:127:ARG:HH11	1.71	0.56
17:K:14:LYS:CB	17:K:45:PRO:HG2	2.36	0.56
20:N:94:GLU:HG3	20:N:186:LEU:HD12	1.88	0.56
1:O:316:A:H5'	26:T:54:ASP:OD2	2.06	0.55
1:O:638:C:H2'	1:O:639:A:C8	2.41	0.55
8:B:141:ARG:HD2	8:B:163:GLU:OE2	2.06	0.55
8:B:307:ARG:HH11	8:B:307:ARG:HB2	1.70	0.55
8:B:314:ALA:CB	8:B:317:PRO:HG3	2.36	0.55
27:U:9:CYS:CA	27:U:52:THR:HG23	2.36	0.55
27:U:46:ALA:HB1	27:U:52:THR:HG21	1.88	0.55
29:W:59:GLN:HE22	29:W:97:ALA:HB3	1.70	0.55
30:X:78:GLU:HG2	30:X:79:GLU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:90:A:H2'	1:0:91:G:O4'	2.06	0.55
1:0:558:C:O2'	1:0:559:U:H5''	2.07	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.88	0.55
1:0:2300:A:H4'	1:0:2301:A:O5'	2.06	0.55
11:E:21:THR:HG23	11:E:30:THR:OG1	2.06	0.55
12:F:21:GLU:O	12:F:24:ARG:HG3	2.05	0.55
15:I:118:ASN:HA	15:I:121:LYS:CD	2.37	0.55
1:0:1236:A:H2'	1:0:1237:U:O4'	2.06	0.55
1:0:1632:A:C2'	1:0:1633:C:H5'	2.36	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.41	0.55
8:B:329:TYR:CE2	27:U:15:PRO:HG2	2.42	0.55
10:D:154:LYS:H	10:D:154:LYS:CD	2.05	0.55
11:E:84:MET:HG2	11:E:168:ILE:HD13	1.88	0.55
12:F:26:THR:HG21	12:F:102:GLY:C	2.32	0.55
12:F:46:GLU:O	12:F:73:PRO:HD2	2.06	0.55
20:N:38:LYS:HE2	20:N:107:ASN:HD21	1.71	0.55
20:N:49:THR:HG22	20:N:50:LEU:N	2.21	0.55
29:W:88:THR:HG23	29:W:110:GLN:HE21	1.70	0.55
32:Z:32:GLU:HA	32:Z:35:GLU:HG3	1.87	0.55
1:0:282:C:H2'	1:0:283:U:O4'	2.07	0.55
1:0:2081:A:H4'	16:J:69:TYR:CE1	2.41	0.55
15:I:113:SER:HB2	15:I:118:ASN:HB2	1.88	0.55
19:M:164:THR:CG2	19:M:165:GLY:N	2.69	0.55
1:0:20:G:H21	24:R:117:HIS:HD2	1.54	0.55
1:0:470:U:O2'	2:1:16:HIS:CD2	2.59	0.55
1:0:1847:A:OP1	7:A:175:LYS:HG3	2.07	0.55
2:1:25:LYS:HD2	3:2:49:GLU:N	2.19	0.55
3:2:36:ASN:HB3	3:2:39:ARG:HG3	1.88	0.55
7:A:66:ARG:HH11	7:A:66:ARG:HB2	1.71	0.55
27:U:11:THR:HG22	27:U:53:ASP:OD2	2.07	0.55
1:0:1159:G:H21	1:0:1189:A:H8	1.54	0.55
1:0:2807:U:P	8:B:27:ASN:HD21	2.30	0.55
10:D:86:THR:C	10:D:89:PRO:HD2	2.31	0.55
20:N:77:ASN:OD1	20:N:79:PRO:HD2	2.07	0.55
1:0:644:G:H5'	1:0:644:G:N3	2.22	0.55
1:0:820:G:H5'	1:0:821:U:H5'	1.89	0.55
1:0:2365:G:H4'	23:Q:45:PRO:O	2.07	0.55
8:B:162:MET:HG3	8:B:310:ARG:CD	2.36	0.55
21:O:14:LEU:CD2	21:O:102:ILE:HD11	2.34	0.55
25:S:25:GLN:HG2	25:S:65:VAL:HG22	1.89	0.55
28:V:64:GLY:O	28:V:65:ASP:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:6:GLN:CB	29:W:26:ILE:HD12	2.35	0.55
30:X:43:VAL:HG12	30:X:44:ASP:H	1.72	0.55
11:E:23:GLU:HG2	11:E:28:SER:HB2	1.89	0.55
17:K:132:VAL:HG11	27:U:22:VAL:HG22	1.88	0.55
24:R:18:LEU:HB2	24:R:143:VAL:CG1	2.33	0.55
28:V:12:THR:H	28:V:15:GLU:HB2	1.71	0.55
29:W:59:GLN:NE2	29:W:97:ALA:HB3	2.22	0.55
1:0:485:A:N3	1:0:487:G:H5''	2.22	0.55
1:0:2252:A:C5	1:0:2253:G:H1'	2.41	0.55
6:9:55:U:H4'	6:9:56:A:C8	2.42	0.55
8:B:217:ARG:HE	8:B:257:THR:HG22	1.71	0.55
29:W:76:ASP:O	29:W:77:ALA:C	2.49	0.55
1:0:1666:C:C2'	1:0:1667:A:C5'	2.85	0.55
4:3:11:CYS:HB2	4:3:20:HIS:CE1	2.42	0.55
8:B:74:ILE:HD13	8:B:309:VAL:HG21	1.88	0.55
8:B:98:THR:HG22	8:B:99:GLU:N	2.22	0.55
10:D:25:MET:HE2	10:D:41:LEU:CG	2.35	0.55
14:H:79:GLU:C	14:H:80:LEU:HD23	2.32	0.55
19:M:72:ALA:HB2	19:M:93:ARG:HG2	1.89	0.55
22:P:98:ILE:HD12	22:P:102:ARG:NE	2.22	0.55
1:0:1167:G:H4'	15:I:130:LEU:HD22	1.89	0.54
1:0:1972:U:H2'	1:0:1973:A:C5'	2.37	0.54
2:1:21:ARG:HD2	2:1:39:PHE:HB2	1.89	0.54
10:D:41:LEU:HA	10:D:44:ILE:HG22	1.88	0.54
10:D:58:VAL:CG1	10:D:60:GLU:HG2	2.37	0.54
19:M:184:ARG:HG3	19:M:185:PRO:HA	1.89	0.54
23:Q:94:GLN:O	23:Q:95:GLU:HB2	2.07	0.54
27:U:14:GLU:OE1	27:U:15:PRO:HD2	2.07	0.54
29:W:110:GLN:NE2	29:W:110:GLN:HA	2.22	0.54
1:0:1007:A:H2'	14:H:22:TYR:CZ	2.42	0.54
1:0:1120:U:H5''	1:0:1120:U:H6	1.73	0.54
1:0:1657:A:H2'	1:0:1658:A:C8	2.42	0.54
1:0:2737:C:OP2	22:P:61:ARG:NH2	2.37	0.54
6:9:44:A:O4'	10:D:76:ARG:NE	2.40	0.54
14:H:87:LYS:HB2	14:H:87:LYS:HZ2	1.73	0.54
32:Z:22:SER:O	32:Z:26:VAL:HG23	2.08	0.54
14:H:86:TYR:C	14:H:86:TYR:CD1	2.85	0.54
18:L:149:ARG:O	18:L:150:GLN:CB	2.55	0.54
27:U:52:THR:CG2	27:U:54:THR:HB	2.36	0.54
1:0:793:A:H5''	22:P:83:LYS:HG2	1.89	0.54
1:0:794:U:H3	1:0:819:A:H61	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1441:G:O2'	1:0:1442:A:H5'	2.07	0.54
8:B:62:ARG:HG2	8:B:65:MET:HE3	1.90	0.54
10:D:134:LEU:HD11	10:D:166:ILE:HD11	1.88	0.54
1:0:1164:U:OP1	15:I:69:PRO:HA	2.08	0.54
1:0:1741:U:HO2'	1:0:2723:G:H4'	1.72	0.54
8:B:36:PRO:HG3	8:B:169:GLY:H	1.71	0.54
12:F:58:GLU:OE1	19:M:27:ARG:NH2	2.34	0.54
23:Q:53:HIS:CE1	23:Q:55:ARG:HG3	2.42	0.54
25:S:52:VAL:C	25:S:53:ASN:HD22	2.16	0.54
1:0:119:A:H2'	1:0:120:A:H5''	1.90	0.54
6:9:39:U:H1'	6:9:44:A:N6	2.22	0.54
7:A:132:ASP:OD1	7:A:133:ARG:N	2.40	0.54
14:H:87:LYS:HB2	14:H:87:LYS:NZ	2.22	0.54
16:J:42:GLU:O	16:J:131:THR:HG23	2.08	0.54
22:P:20:ARG:NH1	22:P:54:LYS:HD3	2.22	0.54
26:T:92:ASP:OD1	26:T:94:SER:HB3	2.08	0.54
1:0:2256:G:O2'	1:0:2257:G:H5'	2.07	0.54
1:0:2524:G:H21	1:0:2526:C:N4	2.05	0.54
18:L:125:PHE:CZ	18:L:140:VAL:HG13	2.42	0.54
19:M:134:ILE:CG2	19:M:141:ILE:HD13	2.38	0.54
20:N:33:ARG:NH1	20:N:103:ASP:OD2	2.33	0.54
26:T:38:ARG:HG3	26:T:38:ARG:HH11	1.71	0.54
1:0:1535:G:H2'	1:0:1536:C:C6	2.43	0.54
6:9:20:G:O2'	6:9:21:G:H5'	2.07	0.54
7:A:194:MET:HE3	7:A:199:HIS:CB	2.38	0.54
10:D:63:ILE:O	10:D:64:ARG:C	2.50	0.54
22:P:7:LYS:HD3	22:P:21:VAL:HG21	1.89	0.54
1:0:1773:G:C8	32:Z:16:ALA:HA	2.43	0.54
1:0:2526:C:O2'	1:0:2527:U:H5'	2.08	0.54
1:0:2831:C:H2'	1:0:2832:C:H5'	1.90	0.54
2:1:28:HIS:CD2	2:1:31:LYS:HG3	2.43	0.54
6:9:55:U:H4'	6:9:56:A:H8	1.72	0.54
9:C:79:ARG:O	9:C:87:ARG:HG2	2.07	0.54
12:F:50:VAL:CG1	12:F:60:VAL:HG11	2.37	0.54
28:V:1:THR:HG23	28:V:2:VAL:N	2.23	0.54
29:W:4:LEU:HD22	29:W:52:VAL:CG2	2.38	0.54
1:0:475:G:H5'	9:C:73:LEU:HD23	1.88	0.54
1:0:1071:G:H4'	31:Y:154:ARG:NH2	2.23	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.54
6:9:42:C:H5'	6:9:43:G:OP2	2.08	0.54
22:P:80:ARG:HG2	22:P:87:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:145:LEU:HD12	24:R:146:ILE:H	1.73	0.54
31:Y:112:GLU:CD	31:Y:115:ARG:NH1	2.66	0.54
32:Z:46:ARG:O	32:Z:57:CYS:HA	2.08	0.54
10:D:18:ILE:HD13	10:D:84:LEU:HD12	1.89	0.53
1:O:1786:C:OP1	22:P:74:GLN:HG2	2.08	0.53
1:O:2251:G:H2'	1:O:2252:A:C8	2.43	0.53
1:O:2878:U:H2'	1:O:2879:A:O4'	2.07	0.53
7:A:36:ASP:HB2	7:A:83:GLY:CA	2.38	0.53
8:B:202:VAL:HG11	8:B:301:VAL:HG13	1.90	0.53
20:N:43:VAL:CG1	20:N:118:ILE:HD11	2.38	0.53
20:N:143:ARG:HA	20:N:172:PHE:CD2	2.43	0.53
24:R:104:PHE:CB	24:R:109:MET:HE2	2.37	0.53
27:U:9:CYS:HA	27:U:52:THR:CG2	2.38	0.53
1:O:1528:A:H2'	1:O:1529:G:O4'	2.08	0.53
1:O:1589:G:H22	1:O:1605:G:H1'	1.72	0.53
1:O:2433:A:H2'	1:O:2434:A:C8	2.42	0.53
6:9:1:U:H4'	6:9:3:A:OP1	2.08	0.53
15:I:88:GLN:HA	15:I:91:PHE:CE2	2.44	0.53
19:M:69:LYS:HG3	19:M:126:GLN:CA	2.38	0.53
20:N:72:GLU:H	20:N:171:HIS:CE1	2.27	0.53
24:R:23:MET:HE3	24:R:28:SER:OG	2.09	0.53
1:O:189:A:OP1	19:M:171:ARG:NH2	2.40	0.53
8:B:217:ARG:NE	8:B:257:THR:HG22	2.22	0.53
20:N:170:GLU:O	20:N:174:GLU:HG3	2.09	0.53
24:R:39:THR:HB	24:R:42:GLU:CG	2.37	0.53
31:Y:112:GLU:HA	31:Y:112:GLU:OE1	2.07	0.53
1:O:136:C:H2'	1:O:137:U:O4'	2.09	0.53
1:O:1798:C:H4'	22:P:66:GLN:HG2	1.91	0.53
1:O:2521:A:OP2	14:H:6:ALA:HB3	2.08	0.53
1:O:2769:C:H2'	1:O:2770:G:O4'	2.08	0.53
8:B:17:LYS:O	8:B:260:HIS:HD2	1.92	0.53
17:K:81:ARG:HD3	17:K:87:ARG:CZ	2.38	0.53
21:O:88:LYS:O	21:O:91:GLN:HB2	2.08	0.53
26:T:49:GLU:OE2	26:T:97:ARG:NH1	2.39	0.53
31:Y:107:PRO:HB3	31:Y:182:PHE:CD2	2.44	0.53
1:O:1596:U:H2'	1:O:1598:A:OP2	2.09	0.53
1:O:2756:U:N3	1:O:2896:A:H2	2.02	0.53
10:D:35:ALA:C	10:D:37:ALA:H	2.15	0.53
24:R:40:ALA:O	24:R:44:VAL:HG23	2.07	0.53
27:U:6:CYS:HA	27:U:13:ILE:HD11	1.91	0.53
28:V:55:ARG:O	28:V:59:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1768:C:H2'	1:0:1769:C:O4'	2.09	0.53
10:D:25:MET:SD	10:D:40:ILE:HD11	2.48	0.53
10:D:49:PRO:HA	10:D:73:VAL:HG22	1.90	0.53
14:H:6:ALA:HA	14:H:61:ARG:NH1	2.24	0.53
15:I:88:GLN:HA	15:I:91:PHE:HE2	1.74	0.53
25:S:14:ALA:HA	25:S:25:GLN:NE2	2.23	0.53
1:0:1496:A:H5'	1:0:1572:A:H1'	1.90	0.53
1:0:2578:G:H5'	1:0:2578:G:C8	2.40	0.53
8:B:52:VAL:O	8:B:53:LEU:HD12	2.09	0.53
20:N:42:HIS:CG	20:N:62:HIS:HE1	2.26	0.53
1:0:282:C:H1'	1:0:368:C:H42	1.74	0.53
1:0:289:G:O2'	1:0:290:C:H5'	2.09	0.53
4:3:3:MET:O	4:3:90:PHE:HA	2.09	0.53
9:C:162:VAL:HG22	9:C:232:LEU:HD21	1.89	0.53
12:F:36:THR:HG23	12:F:97:ALA:HB2	1.90	0.53
15:I:68:PRO:HB2	15:I:69:PRO:HD2	1.91	0.53
20:N:73:ALA:HB1	20:N:74:PRO:CD	2.39	0.53
23:Q:66:LYS:HB2	23:Q:70:ALA:O	2.09	0.53
24:R:113:HIS:O	24:R:145:LEU:HD12	2.09	0.53
1:0:1477:C:H5'	1:0:1868:G:H5''	1.91	0.53
11:E:80:TRP:O	11:E:134:SER:HA	2.09	0.53
12:F:56:PRO:HG2	19:M:43:PRO:O	2.09	0.53
12:F:107:ASP:O	12:F:111:ILE:HG13	2.09	0.53
27:U:6:CYS:HB2	27:U:32:CYS:HB3	1.90	0.53
1:0:396:U:O2'	1:0:418:C:H4'	2.09	0.52
14:H:157:TYR:CD1	14:H:157:TYR:C	2.87	0.52
17:K:62:PRO:HG3	17:K:65:ARG:HH22	1.72	0.52
17:K:103:ASP:HA	17:K:123:SER:OG	2.09	0.52
18:L:121:ILE:HG12	18:L:141:GLU:HB2	1.90	0.52
19:M:34:GLU:HB3	19:M:38:GLU:HG3	1.91	0.52
1:0:1086:A:N6	29:W:11:VAL:HG11	2.25	0.52
1:0:1213:C:O2'	1:0:1214:G:H5'	2.09	0.52
1:0:2344:G:H2'	1:0:2344:G:N3	2.24	0.52
7:A:51:ARG:NH1	7:A:120:ARG:O	2.42	0.52
8:B:75:GLU:C	8:B:77:PRO:HD3	2.35	0.52
9:C:145:GLU:OE1	9:C:198:ASP:HB2	2.09	0.52
10:D:159:PRO:O	10:D:163:VAL:HG23	2.09	0.52
19:M:81:ARG:HG3	19:M:85:ARG:HB2	1.90	0.52
19:M:102:GLU:CD	19:M:164:THR:HG21	2.34	0.52
20:N:163:PHE:O	20:N:164:ASP:O	2.26	0.52
26:T:35:TYR:CG	26:T:112:LEU:HD22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:39:ASN:ND2	27:U:44:ARG:HH11	2.07	0.52
30:X:41:PHE:O	30:X:43:VAL:HG23	2.10	0.52
31:Y:105:LYS:HE2	31:Y:198:GLY:O	2.10	0.52
1:0:317:A:OP1	26:T:52:ARG:O	2.27	0.52
1:0:383:A:H2'	1:0:384:G:O4'	2.09	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.09	0.52
1:0:1242:A:H5'	16:J:82:THR:CG2	2.26	0.52
1:0:1874:U:H2'	7:A:120:ARG:HG3	1.90	0.52
3:2:25:VAL:O	3:2:29:THR:HG23	2.09	0.52
3:2:48:ASP:O	3:2:49:GLU:HB2	2.09	0.52
8:B:63:GLU:HG3	8:B:63:GLU:O	2.08	0.52
9:C:22:PHE:HA	9:C:116:ALA:HA	1.91	0.52
11:E:69:ILE:HA	11:E:72:MET:CE	2.39	0.52
16:J:77:GLY:O	16:J:78:ILE:C	2.52	0.52
31:Y:203:VAL:HG12	31:Y:228:VAL:HG22	1.91	0.52
1:0:1342:C:O2'	1:0:1343:C:H5'	2.09	0.52
1:0:2002:C:H2'	1:0:2003:U:H5'	1.91	0.52
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.91	0.52
7:A:76:VAL:CG2	32:Z:63:LYS:HB3	2.39	0.52
10:D:39:ASP:O	10:D:43:GLU:HG3	2.09	0.52
15:I:97:VAL:CG1	15:I:101:LYS:HE3	2.40	0.52
17:K:81:ARG:HB2	17:K:87:ARG:NH1	2.24	0.52
27:U:20:MET:HE2	27:U:30:HIS:CE1	2.44	0.52
1:0:1086:A:C6	29:W:11:VAL:HG11	2.44	0.52
1:0:2694:A:H4'	11:E:91:PHE:CE1	2.44	0.52
1:0:2821:C:H4'	8:B:116:PRO:HB3	1.90	0.52
6:9:64:C:H2'	6:9:65:A:H5'	1.91	0.52
7:A:153:ARG:HB2	7:A:153:ARG:NH1	2.19	0.52
10:D:10:PHE:CG	10:D:11:HIS:N	2.77	0.52
16:J:93:ARG:HH11	16:J:93:ARG:CB	2.16	0.52
1:0:775:G:OP1	2:1:16:HIS:HE1	1.92	0.52
1:0:1834:C:H2'	1:0:1840:A:H62	1.74	0.52
1:0:2728:C:H4'	1:0:2894:C:HO2'	1.75	0.52
6:9:1:U:O3'	6:9:3:A:H5'	2.10	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
1:0:1266:U:H4'	31:Y:115:ARG:HH21	1.74	0.52
1:0:1825:U:O2'	1:0:1826:C:H5'	2.09	0.52
7:A:74:VAL:O	32:Z:65:THR:HG23	2.10	0.52
18:L:82:ALA:O	18:L:83:GLU:C	2.53	0.52
21:O:18:ALA:HA	21:O:23:GLY:O	2.10	0.52
24:R:39:THR:O	24:R:40:ALA:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:C2'	1:0:1667:A:H5''	2.39	0.52
9:C:1:MET:HG2	9:C:2:GLN:NE2	2.25	0.52
9:C:127:ARG:HG2	9:C:127:ARG:NH1	2.24	0.52
9:C:151:GLN:HA	9:C:151:GLN:NE2	2.25	0.52
11:E:105:GLU:HG2	11:E:113:PRO:HB3	1.91	0.52
1:0:371:U:H2'	1:0:372:A:H8	1.75	0.52
1:0:1268:C:H2'	1:0:1269:G:H8	1.75	0.52
1:0:1333:U:H2'	1:0:1334:C:C6	2.45	0.52
6:9:39:U:H3'	6:9:40:C:H5''	1.92	0.52
6:9:49:G:O2'	6:9:50:G:H5'	2.10	0.52
17:K:20:CYS:HB2	17:K:29:LEU:HG	1.91	0.52
20:N:61:ALA:CB	20:N:88:ALA:HB2	2.40	0.52
1:0:1010:C:H4'	20:N:4:PRO:HB2	1.91	0.52
1:0:1926:G:H2'	1:0:1927:A:H8	1.75	0.52
1:0:2073:G:OP2	1:0:2490:A:H5'	2.10	0.52
6:9:2:U:P	6:9:3:A:H5'	2.49	0.52
6:9:28:U:H5''	20:N:40:ASN:HD21	1.72	0.52
7:A:94:LEU:HG	7:A:99:ILE:CD1	2.40	0.52
7:A:134:ASN:O	7:A:150:PRO:HD3	2.10	0.52
9:C:39:GLN:O	9:C:43:LYS:HD3	2.09	0.52
10:D:23:VAL:HG21	10:D:45:THR:CG2	2.39	0.52
15:I:69:PRO:HG2	15:I:72:GLU:HB2	1.92	0.52
17:K:7:ASP:OD2	17:K:81:ARG:NH2	2.43	0.52
20:N:164:ASP:OD2	20:N:168:LEU:HG	2.09	0.52
1:0:797:A:H5'	32:Z:10:ARG:N	2.25	0.51
1:0:926:A:O2'	18:L:41:HIS:CD2	2.63	0.51
1:0:2135:A:O2'	1:0:2136:G:H5'	2.10	0.51
9:C:138:VAL:O	9:C:234:VAL:HA	2.10	0.51
10:D:135:VAL:HG22	10:D:136:ARG:N	2.24	0.51
11:E:69:ILE:HA	11:E:72:MET:HE2	1.91	0.51
18:L:65:ASP:CG	18:L:111:ALA:HB3	2.35	0.51
18:L:104:ASP:O	18:L:105:TYR:HB3	2.10	0.51
19:M:31:TRP:HA	19:M:34:GLU:HG3	1.91	0.51
19:M:65:VAL:HG21	19:M:105:ALA:HB2	1.91	0.51
20:N:73:ALA:HB1	20:N:74:PRO:HD2	1.91	0.51
31:Y:219:GLU:HG3	31:Y:220:GLU:N	2.25	0.51
1:0:474:C:O3'	9:C:73:LEU:HD21	2.10	0.51
1:0:1008:C:H5''	14:H:19:ARG:HH12	1.75	0.51
1:0:1422:U:H2'	1:0:1423:C:C6	2.45	0.51
1:0:2834:G:OP1	30:X:39:LYS:HE2	2.10	0.51
1:0:2900:G:H2'	1:0:2901:C:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:65:ARG:C	7:A:66:ARG:HG3	2.35	0.51
7:A:99:ILE:O	7:A:131:HIS:CE1	2.64	0.51
9:C:98:ARG:HG2	9:C:98:ARG:NH1	2.22	0.51
9:C:136:VAL:HG22	9:C:137:PRO:HA	1.92	0.51
19:M:59:GLY:HA3	19:M:141:ILE:CD1	2.40	0.51
32:Z:25:ARG:O	32:Z:29:ILE:HG13	2.10	0.51
1:O:1160:G:O2'	1:O:1190:G:H1'	2.10	0.51
1:O:2421:G:H3'	1:O:2422:U:H5''	1.91	0.51
1:O:2862:G:H4'	8:B:336:GLN:O	2.10	0.51
11:E:84:MET:HE1	11:E:148:ILE:HD12	1.91	0.51
13:G:64:ASN:ND2	13:G:64:ASN:H	2.08	0.51
8:B:238:ASN:ND2	8:B:240:GLY:H	2.07	0.51
10:D:88:LEU:HB2	10:D:89:PRO:HD3	1.92	0.51
15:I:111:LEU:HD22	15:I:122:GLU:OE1	2.10	0.51
17:K:41:LYS:O	17:K:42:ASN:HB2	2.10	0.51
22:P:94:TRP:CZ2	22:P:98:ILE:HG13	2.45	0.51
26:T:43:ASN:HD22	26:T:108:ARG:NH2	2.08	0.51
31:Y:184:GLU:OE1	31:Y:204:ARG:NH1	2.43	0.51
31:Y:189:ASN:ND2	31:Y:192:ASP:H	2.09	0.51
1:O:24:G:N2	1:O:518:G:H1'	2.25	0.51
1:O:474:C:O3'	9:C:73:LEU:CD2	2.59	0.51
1:O:947:U:H2'	1:O:948:G:C8	2.45	0.51
1:O:1205:U:H2'	1:O:1206:U:H5'	1.92	0.51
1:O:2256:G:C2'	1:O:2257:G:H5'	2.41	0.51
1:O:2435:U:OP1	4:3:28:GLY:HA3	2.11	0.51
1:O:2597:U:H2'	1:O:2598:U:H5'	1.91	0.51
6:9:73:A:H61	6:9:108:C:N4	2.07	0.51
19:M:99:ARG:CD	19:M:167:GLY:HA2	2.39	0.51
20:N:15:GLU:HB3	20:N:17:ARG:HD2	1.93	0.51
6:9:114:G:H2'	6:9:115:C:C6	2.46	0.51
7:A:217:ARG:HH11	7:A:217:ARG:CG	2.24	0.51
8:B:195:ARG:HG2	8:B:323:LEU:HD22	1.93	0.51
9:C:16:VAL:HG12	9:C:17:ASP:H	1.76	0.51
9:C:47:GLY:HA2	9:C:92:PRO:HB2	1.92	0.51
11:E:101:GLU:HB3	11:E:117:THR:HA	1.92	0.51
13:G:71:LEU:C	13:G:73:ASP:H	2.19	0.51
20:N:154:LEU:C	20:N:156:GLU:N	2.68	0.51
20:N:179:LEU:HD23	20:N:184:ILE:CD1	2.41	0.51
26:T:71:VAL:HG13	26:T:91:LEU:O	2.11	0.51
28:V:64:GLY:O	28:V:65:ASP:CB	2.58	0.51
1:O:776:A:OP1	2:1:28:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2105:C:H2'	1:0:2106:C:C6	2.45	0.51
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.51
8:B:13:PHE:O	8:B:16:ARG:HD2	2.10	0.51
8:B:41:PHE:HB3	8:B:190:MET:HE1	1.91	0.51
8:B:217:ARG:HG3	8:B:257:THR:HG22	1.91	0.51
12:F:39:SER:HB3	12:F:45:ALA:HB2	1.93	0.51
24:R:47:LEU:O	24:R:51:ILE:HG13	2.11	0.51
26:T:9:LYS:CE	26:T:13:ARG:NH1	2.68	0.51
29:W:107:LEU:O	29:W:112:LEU:HB2	2.11	0.51
32:Z:36:ASP:HB3	32:Z:45:ASP:HB3	1.92	0.51
1:0:669:G:O2'	1:0:670:G:H5'	2.11	0.51
1:0:2104:C:O2	1:0:2485:A:N1	2.43	0.51
1:0:2769:C:H2'	1:0:2770:G:H5'	1.93	0.51
7:A:66:ARG:HH11	7:A:66:ARG:CB	2.24	0.51
7:A:129:LEU:CD1	7:A:145:MET:HE1	2.41	0.51
1:0:621:C:H5'	31:Y:132:ASP:OD2	2.11	0.51
4:3:3:MET:HG3	4:3:4:PRO:HD2	1.92	0.51
7:A:70:ALA:HB1	32:Z:65:THR:HG21	1.92	0.51
9:C:151:GLN:HE21	9:C:151:GLN:CA	2.24	0.51
10:D:64:ARG:HB3	10:D:67:ASP:OD2	2.11	0.51
19:M:165:GLY:O	19:M:169:ARG:HG3	2.11	0.51
31:Y:126:PRO:HG2	31:Y:128:PHE:CZ	2.46	0.51
1:0:1165:G:H4'	1:0:1174:A:O2'	2.11	0.51
1:0:1644:C:H2'	1:0:1645:U:H6	1.75	0.51
1:0:2445:U:H2'	1:0:2446:G:C8	2.46	0.51
1:0:2717:C:O2'	1:0:2718:C:H5''	2.10	0.51
6:9:73:A:N6	6:9:108:C:H42	2.07	0.51
25:S:17:ASP:HB3	25:S:23:LYS:HB2	1.93	0.51
30:X:47:ALA:O	30:X:82:GLU:HB2	2.10	0.51
1:0:157:G:H4'	19:M:95:LYS:HE2	1.93	0.50
1:0:559:U:H2'	1:0:560:U:O4'	2.11	0.50
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.50
1:0:960:G:H3'	1:0:960:G:N3	2.26	0.50
1:0:1293:U:H5'	31:Y:154:ARG:HH21	1.76	0.50
6:9:64:C:C2'	6:9:65:A:H5'	2.41	0.50
7:A:125:ASN:HB3	7:A:158:VAL:HG12	1.93	0.50
7:A:179:MET:HG2	7:A:186:TRP:CB	2.41	0.50
24:R:53:GLY:HA2	24:R:80:TYR:CD2	2.47	0.50
1:0:656:G:OP2	21:O:37:ARG:HD2	2.11	0.50
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
10:D:55:LYS:HA	10:D:65:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:47:ARG:HG3	21:O:47:ARG:NH1	2.26	0.50
30:X:43:VAL:HG11	30:X:82:GLU:HA	1.93	0.50
1:O:371:U:H2'	1:O:372:A:C8	2.46	0.50
1:O:1853:C:O2'	7:A:217:ARG:NH2	2.44	0.50
1:O:2507:G:H2'	1:O:2510:C:H42	1.77	0.50
7:A:36:ASP:CB	7:A:83:GLY:HA3	2.41	0.50
12:F:56:PRO:CG	19:M:44:THR:HA	2.40	0.50
13:G:71:LEU:C	13:G:73:ASP:N	2.69	0.50
15:I:133:THR:HG22	15:I:134:ILE:N	2.27	0.50
16:J:107:ASN:HD22	16:J:109:TYR:H	1.57	0.50
16:J:130:VAL:CG1	16:J:131:THR:N	2.74	0.50
20:N:154:LEU:HD12	20:N:156:GLU:O	2.11	0.50
1:O:128:A:O2'	1:O:129:A:H5'	2.10	0.50
1:O:1211:G:H5''	13:G:64:ASN:OD1	2.11	0.50
1:O:2533:C:H6	1:O:2533:C:C5'	2.18	0.50
1:O:2613:G:O2'	1:O:2614:C:H5'	2.11	0.50
12:F:46:GLU:OE1	12:F:100:ASP:HA	2.11	0.50
17:K:125:ALA:C	17:K:127:ALA:H	2.19	0.50
20:N:86:LEU:O	20:N:90:LEU:HG	2.12	0.50
1:O:138:U:OP2	1:O:139:C:H5	1.94	0.50
1:O:1120:U:H5'	1:O:1121:G:OP2	2.11	0.50
8:B:14:GLY:HA2	8:B:15:PRO:C	2.36	0.50
9:C:165:ASP:O	9:C:168:ARG:HB3	2.11	0.50
10:D:13:MET:HA	10:D:137:PRO:HG2	1.93	0.50
10:D:64:ARG:CD	10:D:67:ASP:HB3	2.41	0.50
10:D:172:VAL:HG12	10:D:173:GLU:N	2.26	0.50
17:K:66:ARG:HG2	17:K:66:ARG:HH11	1.77	0.50
21:O:21:SER:OG	21:O:106:PRO:HB2	2.11	0.50
25:S:37:VAL:O	25:S:41:VAL:HG23	2.12	0.50
28:V:42:ASN:N	28:V:43:PRO:HD3	2.27	0.50
1:O:65:C:O2'	1:O:66:G:H5'	2.11	0.50
1:O:1595:G:O2'	1:O:1596:U:H5'	2.11	0.50
20:N:15:GLU:HB3	20:N:17:ARG:HG3	1.92	0.50
1:O:449:A:N7	9:C:43:LYS:HG2	2.26	0.50
1:O:2443:C:H1'	18:L:56:LYS:HE3	1.94	0.50
6:9:52:A:H2'	6:9:53:G:O4'	2.12	0.50
7:A:55:VAL:HG23	7:A:68:ILE:O	2.11	0.50
22:P:83:LYS:O	22:P:86:ALA:HB3	2.12	0.50
31:Y:99:ALA:HB2	31:Y:233:TYR:CZ	2.46	0.50
1:O:661:G:C5	1:O:686:A:C2	3.00	0.50
1:O:1377:C:H5'	1:O:1377:C:C6	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1636:G:O2'	1:0:1637:A:H5'	2.12	0.50
1:0:1790:C:H2'	1:0:1791:U:H6	1.76	0.50
8:B:315:VAL:HG23	8:B:316:ARG:HG2	1.94	0.50
1:0:1667:A:H2'	1:0:1668:U:C6	2.47	0.50
1:0:1942:A:O2'	1:0:1943:C:H5'	2.12	0.50
6:9:76:G:C3'	6:9:77:A:H5''	2.31	0.50
7:A:132:ASP:HB3	7:A:135:VAL:O	2.12	0.50
8:B:320:GLN:NE2	8:B:321:PRO:CD	2.73	0.50
9:C:219:ASN:O	9:C:222:ASP:HB2	2.10	0.50
26:T:9:LYS:HE3	26:T:13:ARG:CZ	2.41	0.50
28:V:16:ARG:NH2	28:V:63:GLU:HG3	2.27	0.50
1:0:671:A:O2'	1:0:672:G:H2'	2.12	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
7:A:192:VAL:O	7:A:192:VAL:HG12	2.12	0.49
10:D:18:ILE:HD13	10:D:84:LEU:CD1	2.41	0.49
18:L:143:THR:CG2	18:L:144:ASP:N	2.75	0.49
29:W:130:HIS:O	29:W:136:GLY:HA3	2.12	0.49
1:0:646:G:H5''	9:C:96:LYS:HD2	1.93	0.49
1:0:1515:A:H2'	1:0:1516:U:C6	2.47	0.49
1:0:2421:G:H3'	1:0:2422:U:C5'	2.43	0.49
7:A:192:VAL:HG12	7:A:207:GLN:HB3	1.93	0.49
8:B:51:VAL:CG2	8:B:327:VAL:HG13	2.42	0.49
9:C:130:GLU:OE1	9:C:130:GLU:HA	2.11	0.49
16:J:127:ILE:O	16:J:127:ILE:HG12	2.12	0.49
20:N:151:ASP:OD1	20:N:154:LEU:HD13	2.12	0.49
24:R:39:THR:HB	24:R:42:GLU:CD	2.36	0.49
26:T:64:ASN:HB3	26:T:73:HIS:HB2	1.93	0.49
26:T:69:LYS:O	26:T:71:VAL:HG23	2.12	0.49
1:0:944:G:C8	29:W:23:MET:HE1	2.47	0.49
1:0:1641:A:C2'	1:0:1642:A:H5'	2.42	0.49
9:C:7:ASP:C	9:C:9:ASP:H	2.20	0.49
11:E:24:GLY:HA3	11:E:76:VAL:HB	1.94	0.49
12:F:117:GLU:C	12:F:119:ARG:H	2.18	0.49
13:G:20:VAL:O	13:G:24:VAL:HG23	2.12	0.49
18:L:145:LEU:HD23	18:L:145:LEU:C	2.37	0.49
26:T:38:ARG:HG3	26:T:38:ARG:NH1	2.26	0.49
27:U:6:CYS:C	27:U:8:TYR:H	2.19	0.49
1:0:894:A:C2	9:C:87:ARG:NH2	2.81	0.49
1:0:1116:U:O2'	1:0:1118:A:C2	2.54	0.49
1:0:1352:A:N1	9:C:48:SER:HB3	2.28	0.49
1:0:2453:G:H4'	18:L:50:GLY:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2899:A:H2'	1:0:2900:G:C8	2.48	0.49
6:9:91:C:H2'	6:9:92:G:O4'	2.12	0.49
8:B:7:ARG:NH1	8:B:11:LEU:HD21	2.27	0.49
8:B:62:ARG:CA	8:B:65:MET:HE3	2.37	0.49
20:N:67:ALA:HA	20:N:71:TRP:HB3	1.94	0.49
27:U:13:ILE:HG12	27:U:32:CYS:HB3	1.93	0.49
1:0:945:U:O2'	29:W:43:GLY:HA3	2.13	0.49
1:0:1015:C:H2'	1:0:1016:U:C6	2.47	0.49
1:0:1450:C:O2'	1:0:1494:A:H5'	2.11	0.49
1:0:1845:A:OP2	7:A:190:ARG:NH1	2.45	0.49
6:9:24:U:H3'	6:9:25:G:H5'	1.95	0.49
7:A:88:ILE:HD13	7:A:100:PRO:CD	2.36	0.49
7:A:186:TRP:CG	7:A:187:PRO:HA	2.47	0.49
8:B:255:GLY:O	8:B:257:THR:HG23	2.12	0.49
16:J:39:VAL:HG11	16:J:107:ASN:HB2	1.94	0.49
16:J:45:VAL:HG22	16:J:130:VAL:O	2.12	0.49
18:L:57:VAL:O	18:L:57:VAL:HG12	2.13	0.49
20:N:38:LYS:HE2	20:N:107:ASN:ND2	2.26	0.49
29:W:142:ASP:HB3	29:W:145:GLY:H	1.77	0.49
1:0:88:G:H8	1:0:88:G:H5'	1.77	0.49
6:9:56:A:O2'	10:D:14:ARG:HD3	2.12	0.49
20:N:152:GLU:OE1	20:N:152:GLU:HA	2.12	0.49
26:T:28:SER:O	26:T:32:ARG:HG3	2.12	0.49
26:T:43:ASN:ND2	26:T:108:ARG:CZ	2.76	0.49
29:W:72:PRO:CG	29:W:77:ALA:HB3	2.30	0.49
1:0:1167:G:H2'	1:0:1168:C:O4'	2.13	0.49
1:0:1717:A:H5''	22:P:54:LYS:HB2	1.93	0.49
1:0:2511:A:H2'	1:0:2512:U:O4'	2.13	0.49
7:A:35:GLY:O	7:A:36:ASP:CB	2.50	0.49
8:B:180:ASP:O	8:B:181:ILE:C	2.56	0.49
8:B:304:PRO:HD2	8:B:307:ARG:CD	2.38	0.49
10:D:101:THR:O	10:D:101:THR:HG22	2.12	0.49
14:H:41:LYS:HD3	14:H:46:TYR:CZ	2.48	0.49
16:J:133:GLY:O	16:J:137:GLU:HG3	2.13	0.49
17:K:74:VAL:HG13	17:K:113:ILE:HG12	1.94	0.49
19:M:59:GLY:HA3	19:M:141:ILE:HD11	1.95	0.49
1:0:318:U:O2'	1:0:338:C:H2'	2.13	0.49
1:0:1594:C:OP2	22:P:120:ARG:HD2	2.12	0.49
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.49
9:C:236:THR:O	9:C:237:GLU:C	2.54	0.49
20:N:83:LEU:HD13	20:N:175:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:76:ARG:O	30:X:77:PHE:HB3	2.12	0.49
31:Y:106:THR:CG2	31:Y:107:PRO:HD2	2.43	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.13	0.49
1:0:1236:A:C8	16:J:63:ILE:HD11	2.48	0.49
1:0:1450:C:C4'	1:0:1451:C:OP2	2.55	0.49
9:C:5:ILE:HD11	9:C:16:VAL:CG2	2.43	0.49
9:C:118:THR:CG2	9:C:137:PRO:HB3	2.42	0.49
16:J:6:PHE:O	16:J:8:ALA:N	2.45	0.49
1:0:920:C:H5'	1:0:921:G:C4	2.48	0.49
1:0:944:G:H21	29:W:44:MET:HE2	1.78	0.49
1:0:2314:G:C2'	1:0:2315:C:H5'	2.43	0.49
8:B:195:ARG:N	8:B:198:GLU:OE1	2.46	0.49
9:C:7:ASP:OD1	9:C:11:ASN:HB2	2.12	0.49
11:E:5:LEU:HD21	11:E:66:GLN:HG3	1.94	0.49
29:W:80:ASP:O	29:W:84:VAL:HG23	2.12	0.49
1:0:12:U:H2'	1:0:13:G:H5'	1.95	0.48
1:0:166:A:N7	18:L:25:GLY:HA2	2.28	0.48
1:0:969:G:H1	1:0:999:C:H42	1.60	0.48
1:0:1594:C:O2'	1:0:1607:A:H4'	2.13	0.48
1:0:1973:A:H2'	1:0:1974:G:O4'	2.13	0.48
1:0:2509:A:H2'	1:0:2510:C:O4'	2.13	0.48
1:0:2825:C:H4'	1:0:2826:G:O5'	2.13	0.48
1:0:2904:U:H4'	30:X:8:ARG:NH1	2.27	0.48
8:B:243:ASN:HA	8:B:244:PRO:C	2.37	0.48
10:D:94:ALA:HA	10:D:174:VAL:O	2.13	0.48
14:H:46:TYR:HE2	14:H:85:ASP:O	1.96	0.48
14:H:69:ARG:HH21	14:H:70:LEU:HD12	1.78	0.48
16:J:131:THR:HB	16:J:134:GLU:HG3	1.94	0.48
24:R:80:TYR:O	24:R:82:GLU:N	2.45	0.48
26:T:43:ASN:HD22	26:T:108:ARG:CZ	2.26	0.48
29:W:65:VAL:CA	29:W:68:THR:HG22	2.41	0.48
32:Z:11:SER:HB3	32:Z:23:ARG:HB2	1.95	0.48
1:0:816:G:H5'	1:0:1598:A:H4'	1.95	0.48
1:0:926:A:O2'	18:L:41:HIS:HD2	1.96	0.48
1:0:968:G:O2'	1:0:969:G:H5'	2.13	0.48
1:0:1183:C:H42	1:0:1184:C:H41	1.59	0.48
1:0:2716:G:C5'	8:B:206:THR:HG21	2.41	0.48
1:0:2758:G:H2'	1:0:2759:C:C6	2.49	0.48
6:9:61:C:H2'	6:9:62:A:H8	1.77	0.48
9:C:127:ARG:HH21	9:C:225:PRO:HG2	1.73	0.48
11:E:23:GLU:HG2	11:E:28:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:12:THR:CG2	28:V:15:GLU:H	2.26	0.48
28:V:27:LEU:HA	28:V:49:LEU:HD13	1.94	0.48
30:X:10:VAL:HG11	30:X:36:HIS:CE1	2.47	0.48
31:Y:99:ALA:HB2	31:Y:233:TYR:CE2	2.48	0.48
1:0:319:A:H4'	1:0:338:C:C4	2.49	0.48
1:0:960:G:N3	1:0:960:G:C2'	2.76	0.48
3:2:29:THR:C	3:2:31:ARG:N	2.70	0.48
9:C:27:ARG:HH11	9:C:27:ARG:HG3	1.78	0.48
9:C:173:LYS:HB3	9:C:187:ARG:HG3	1.94	0.48
10:D:28:GLY:CA	10:D:69:ILE:HG23	2.38	0.48
16:J:75:PRO:HB3	16:J:132:LEU:HB3	1.95	0.48
20:N:183:ASP:O	20:N:184:ILE:O	2.31	0.48
24:R:114:VAL:HG13	24:R:114:VAL:O	2.13	0.48
1:0:1654:U:H2'	7:A:47:HIS:HD2	1.77	0.48
1:0:2055:A:H4'	24:R:132:ARG:NH2	2.29	0.48
8:B:36:PRO:HA	8:B:168:GLY:HA3	1.95	0.48
10:D:37:ALA:O	10:D:40:ILE:HG12	2.13	0.48
16:J:54:VAL:HG11	16:J:138:THR:HG21	1.94	0.48
17:K:28:GLU:HG2	17:K:58:THR:HB	1.96	0.48
22:P:10:ALA:HA	22:P:13:VAL:HG12	1.94	0.48
30:X:30:MET:HE3	30:X:55:ASN:OD1	2.14	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.14	0.48
1:0:2361:A:H5'	1:0:2361:A:H8	1.79	0.48
6:9:56:A:C3'	6:9:57:A:H5''	2.44	0.48
7:A:36:ASP:HB2	7:A:83:GLY:C	2.38	0.48
8:B:279:THR:HG22	8:B:280:VAL:N	2.28	0.48
10:D:128:LEU:C	10:D:128:LEU:HD23	2.38	0.48
20:N:12:ARG:HD3	20:N:18:THR:OG1	2.13	0.48
22:P:38:GLU:HA	22:P:41:ARG:NH1	2.29	0.48
26:T:71:VAL:HG12	26:T:72:ILE:N	2.28	0.48
1:0:23:G:H1'	1:0:520:A:N6	2.29	0.48
1:0:812:A:H2'	1:0:813:C:O4'	2.13	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.48
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.48
1:0:2502:C:H2'	1:0:2503:A:C5'	2.42	0.48
7:A:109:GLU:HG2	7:A:116:GLY:H	1.78	0.48
9:C:118:THR:HG22	9:C:137:PRO:HB3	1.94	0.48
10:D:27:ILE:HB	10:D:69:ILE:O	2.13	0.48
10:D:140:ARG:HH11	10:D:140:ARG:HG3	1.78	0.48
16:J:15:ARG:NH1	16:J:43:ARG:NH1	2.62	0.48
22:P:10:ALA:HA	22:P:13:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:64:GLU:OE1	23:Q:64:GLU:HA	2.13	0.48
26:T:40:VAL:HG23	26:T:119:ALA:C	2.37	0.48
29:W:108:ARG:HG3	29:W:114:PRO:HG3	1.94	0.48
1:0:952:G:OP1	23:Q:42:LYS:HE2	2.14	0.48
1:0:1321:A:H2'	1:0:1322:G:C8	2.49	0.48
1:0:1845:A:O3'	7:A:187:PRO:HB2	2.14	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
1:0:2064:U:H4'	1:0:2653:A:OP1	2.14	0.48
1:0:2329:C:O2'	1:0:2330:U:H5'	2.13	0.48
1:0:2506:A:O2'	1:0:2507:G:O5'	2.31	0.48
7:A:43:VAL:CG2	7:A:59:GLU:HG3	2.44	0.48
7:A:97:ALA:HB2	7:A:150:PRO:HB2	1.94	0.48
7:A:179:MET:HG2	7:A:186:TRP:CG	2.48	0.48
10:D:95:THR:OG1	10:D:174:VAL:HG13	2.13	0.48
14:H:12:ILE:HG12	14:H:59:GLN:HG2	1.96	0.48
15:I:73:LEU:HD12	15:I:107:LYS:NZ	2.28	0.48
15:I:94:ASP:HA	15:I:133:THR:O	2.13	0.48
18:L:72:ASN:O	18:L:76:LEU:HG	2.14	0.48
25:S:8:PRO:HD2	28:V:32:ALA:HA	1.95	0.48
26:T:19:ARG:NH1	26:T:68:ASP:O	2.46	0.48
1:0:204:A:H2'	1:0:205:U:H5'	1.95	0.48
1:0:539:G:H2'	1:0:540:A:C8	2.48	0.48
1:0:1151:G:OP1	13:G:63:ARG:NH1	2.46	0.48
1:0:1471:A:H2'	1:0:1472:C:C6	2.48	0.48
6:9:51:A:H5'	20:N:160:SER:HB3	1.95	0.48
8:B:207:LYS:HG2	8:B:304:PRO:HB3	1.94	0.48
10:D:136:ARG:HD2	10:D:155:HIS:O	2.14	0.48
11:E:84:MET:HB2	11:E:131:LEU:HB2	1.96	0.48
14:H:122:LYS:O	14:H:124:VAL:HG13	2.13	0.48
19:M:47:ASP:CG	19:M:48:LYS:N	2.72	0.48
20:N:42:HIS:HB3	20:N:62:HIS:CE1	2.49	0.48
22:P:9:LEU:O	22:P:13:VAL:HG12	2.14	0.48
29:W:64:THR:O	29:W:68:THR:HG22	2.13	0.48
30:X:74:ALA:CB	30:X:85:VAL:HG22	2.44	0.48
1:0:558:C:H2'	1:0:559:U:H5''	1.95	0.48
1:0:625:U:H5''	1:0:1044:C:N4	2.29	0.48
1:0:1289:C:O2'	1:0:1290:G:H5'	2.14	0.48
1:0:1753:C:O2	8:B:229:ARG:NH2	2.46	0.48
1:0:1839:A:H5'	1:0:2643:G:H4'	1.96	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2897:C:H2'	1:0:2898:G:H8	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.48
1:0:316:A:N3	1:0:336:G:O2'	2.45	0.48
1:0:1163:G:H5'	15:I:110:ASP:O	2.14	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.96	0.48
1:0:2044:G:OP1	30:X:23:HIS:HE1	1.97	0.48
16:J:107:ASN:C	16:J:107:ASN:ND2	2.71	0.48
19:M:157:ASP:HB3	19:M:160:PHE:HD1	1.78	0.48
20:N:139:TRP:HA	20:N:139:TRP:CE3	2.49	0.48
24:R:119:VAL:HG12	24:R:119:VAL:O	2.14	0.48
1:0:285:A:C2	1:0:368:C:H4'	2.49	0.47
1:0:2781:U:H1'	11:E:139:GLU:OE2	2.13	0.47
7:A:36:ASP:HA	7:A:83:GLY:HA3	1.95	0.47
15:I:94:ASP:OD1	15:I:133:THR:HB	2.15	0.47
20:N:114:LYS:O	20:N:117:ALA:HB3	2.14	0.47
24:R:9:ASP:O	24:R:13:THR:HB	2.14	0.47
29:W:1:MET:N	29:W:103:GLU:OE2	2.47	0.47
32:Z:19:GLY:O	32:Z:23:ARG:HG2	2.14	0.47
1:0:17:G:H2'	1:0:18:C:C6	2.49	0.47
1:0:1184:C:O2'	1:0:1185:U:OP2	2.29	0.47
7:A:32:VAL:O	7:A:33:GLU:C	2.57	0.47
8:B:162:MET:HG3	8:B:310:ARG:CZ	2.44	0.47
21:O:80:ASP:OD1	21:O:81:PHE:N	2.46	0.47
21:O:105:ASN:HD21	21:O:109:SER:N	2.13	0.47
26:T:37:GLN:OE1	26:T:118:SER:HA	2.15	0.47
29:W:26:ILE:O	29:W:26:ILE:CG1	2.61	0.47
31:Y:154:ARG:NH1	31:Y:155:ARG:HG3	2.29	0.47
32:Z:72:GLU:HB2	32:Z:77:LYS:HE3	1.95	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
1:0:926:A:H5'	18:L:39:GLU:OE2	2.14	0.47
1:0:1790:C:H2'	1:0:1791:U:C6	2.48	0.47
1:0:2072:G:C6	1:0:2533:C:H1'	2.50	0.47
9:C:136:VAL:HA	9:C:137:PRO:C	2.39	0.47
10:D:104:PHE:CE2	10:D:166:ILE:HD13	2.49	0.47
16:J:108:PRO:HG2	16:J:109:TYR:CD1	2.50	0.47
19:M:54:TYR:CG	19:M:55:LYS:N	2.82	0.47
19:M:99:ARG:HE	19:M:170:ASN:HD22	1.61	0.47
24:R:99:ALA:CB	24:R:109:MET:HE3	2.43	0.47
24:R:119:VAL:CG2	24:R:142:ASP:HB2	2.44	0.47
28:V:20:LEU:HD11	28:V:53:ILE:HG23	1.96	0.47
29:W:7:LEU:HD12	29:W:53:ALA:HB2	1.96	0.47
29:W:13:MET:HE1	29:W:21:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:308:U:H5'	1:0:309:C:OP1	2.14	0.47
1:0:820:G:C6	7:A:171:LYS:HB2	2.49	0.47
1:0:958:G:H2'	1:0:959:C:C6	2.49	0.47
1:0:1055:G:OP2	14:H:99:ARG:NH1	2.48	0.47
1:0:1925:G:H5'	4:3:29:ARG:NH1	2.26	0.47
14:H:29:SER:HA	14:H:62:HIS:HD2	1.78	0.47
15:I:108:HIS:N	15:I:109:PRO:CD	2.77	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
8:B:41:PHE:CZ	8:B:79:MET:HG3	2.49	0.47
8:B:313:PRO:O	8:B:314:ALA:C	2.57	0.47
9:C:107:ARG:HB3	9:C:107:ARG:CZ	2.45	0.47
12:F:43:GLY:C	12:F:45:ALA:H	2.22	0.47
17:K:28:GLU:OE2	17:K:58:THR:HG21	2.15	0.47
31:Y:186:ARG:HG2	31:Y:186:ARG:HH11	1.78	0.47
1:0:657:G:H2'	1:0:658:C:C6	2.50	0.47
1:0:1166:A:H1'	1:0:1192:A:C2	2.50	0.47
1:0:2781:U:H2'	1:0:2782:G:H5'	1.96	0.47
4:3:69:TYR:CZ	4:3:80:ARG:HD2	2.50	0.47
4:3:69:TYR:HB2	4:3:78:HIS:CE1	2.49	0.47
8:B:171:VAL:O	8:B:175:LEU:HB2	2.14	0.47
12:F:56:PRO:HG2	19:M:44:THR:HA	1.95	0.47
17:K:34:VAL:HG22	17:K:47:ALA:HB2	1.95	0.47
17:K:113:ILE:HG22	17:K:114:ALA:O	2.15	0.47
20:N:49:THR:CG2	20:N:50:LEU:N	2.77	0.47
20:N:58:LEU:N	20:N:58:LEU:HD12	2.30	0.47
20:N:82:TYR:C	20:N:82:TYR:CD2	2.93	0.47
21:O:53:GLN:HG2	21:O:56:GLU:OE1	2.14	0.47
23:Q:32:GLU:HA	23:Q:71:TYR:OH	2.15	0.47
24:R:18:LEU:HG	24:R:91:LEU:HD13	1.97	0.47
25:S:51:GLN:HB3	25:S:67:ARG:NH1	2.29	0.47
1:0:475:G:OP1	9:C:73:LEU:HD22	2.15	0.47
1:0:969:G:H1	1:0:999:C:N4	2.12	0.47
1:0:1205:U:C2'	1:0:1206:U:H5''	2.41	0.47
1:0:1279:U:O2	1:0:1279:U:H2'	2.13	0.47
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.47
1:0:2780:C:C1'	11:E:143:GLN:HE21	2.27	0.47
8:B:34:GLY:O	8:B:35:GLN:C	2.58	0.47
9:C:104:ASP:O	9:C:108:GLN:HG3	2.15	0.47
9:C:115:LEU:HD13	9:C:223:LEU:CD2	2.42	0.47
9:C:233:THR:HG22	9:C:234:VAL:N	2.28	0.47
12:F:15:ASP:O	12:F:18:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:26:THR:HG21	12:F:103:GLU:HB2	1.97	0.47
14:H:88:MET:HA	14:H:139:ALA:HA	1.97	0.47
15:I:87:PRO:HB3	15:I:129:SER:C	2.40	0.47
19:M:49:ALA:HB1	19:M:54:TYR:HB2	1.97	0.47
19:M:164:THR:HG22	19:M:166:ALA:H	1.79	0.47
20:N:43:VAL:O	20:N:84:THR:HG21	2.13	0.47
28:V:39:ALA:C	28:V:41:GLU:N	2.73	0.47
29:W:1:MET:N	29:W:37:GLU:HG3	2.30	0.47
32:Z:10:ARG:HG3	32:Z:11:SER:N	2.29	0.47
32:Z:10:ARG:HB2	32:Z:27:ALA:CB	2.45	0.47
1:O:809:G:H2'	1:O:810:G:H8	1.79	0.47
1:O:2785:C:H4'	1:O:2786:G:OP2	2.15	0.47
2:1:8:GLN:HE22	2:1:11:LYS:HZ1	1.57	0.47
8:B:80:ARG:HA	8:B:186:GLY:O	2.15	0.47
9:C:20:ASP:O	9:C:23:GLU:HB2	2.15	0.47
15:I:72:GLU:C	15:I:74:ILE:N	2.71	0.47
18:L:98:GLU:C	18:L:99:GLU:HG3	2.38	0.47
20:N:72:GLU:O	20:N:72:GLU:HG2	2.14	0.47
27:U:31:PHE:CG	27:U:37:GLU:HG2	2.50	0.47
29:W:21:LEU:HD21	29:W:48:VAL:HG13	1.97	0.47
1:O:308:U:C4	1:O:342:C:H1'	2.50	0.47
1:O:960:G:N3	1:O:960:G:H2'	2.30	0.47
1:O:1206:U:H2'	1:O:1207:A:O4'	2.15	0.47
1:O:1506:U:H6	1:O:1506:U:H5'	1.79	0.47
1:O:2256:G:H2'	1:O:2257:G:C5'	2.45	0.47
1:O:2724:U:H2'	1:O:2725:G:O4'	2.15	0.47
4:3:91:GLN:O	4:3:92:GLU:HB2	2.14	0.47
8:B:5:ARG:HD2	8:B:8:LYS:HZ1	1.78	0.47
9:C:49:ASP:HB3	9:C:52:ALA:HB2	1.96	0.47
10:D:10:PHE:CD1	10:D:11:HIS:N	2.83	0.47
10:D:60:GLU:O	10:D:61:PHE:C	2.57	0.47
15:I:87:PRO:C	15:I:89:GLU:H	2.23	0.47
1:O:1328:A:OP1	31:Y:169:ARG:CD	2.63	0.47
1:O:1576:G:H2'	1:O:1577:U:O4'	2.15	0.47
1:O:1787:C:OP1	22:P:68:LYS:HE2	2.15	0.47
1:O:1973:A:H5'	1:O:1973:A:C8	2.47	0.47
1:O:2846:C:H4'	8:B:156:LYS:HB3	1.95	0.47
6:9:49:G:H2'	6:9:50:G:O4'	2.15	0.47
8:B:5:ARG:NH1	8:B:8:LYS:HE2	2.30	0.47
8:B:23:THR:CG2	8:B:162:MET:HE3	2.44	0.47
10:D:146:LYS:HZ1	20:N:107:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:87:PRO:HB3	15:I:129:SER:O	2.15	0.47
18:L:53:ARG:NH2	18:L:57:VAL:HG12	2.30	0.47
21:O:105:ASN:HD21	21:O:109:SER:H	1.63	0.47
22:P:141:ILE:O	22:P:143:ALA:N	2.38	0.47
29:W:122:ARG:HG3	29:W:152:ALA:O	2.15	0.47
29:W:139:GLY:O	29:W:141:HIS:HD2	1.97	0.47
31:Y:205:ILE:HB	31:Y:230:ASN:HD21	1.79	0.47
1:O:441:A:H1'	1:O:442:A:N7	2.30	0.46
1:O:506:G:N2	1:O:508:A:H3'	2.30	0.46
1:O:745:G:H5''	1:O:746:A:OP1	2.15	0.46
1:O:1298:U:H2'	1:O:1299:G:C8	2.50	0.46
1:O:1845:A:P	7:A:190:ARG:HH11	2.38	0.46
7:A:59:GLU:HG2	7:A:65:ARG:HD3	1.97	0.46
8:B:34:GLY:O	8:B:35:GLN:O	2.33	0.46
9:C:46:TYR:CE2	9:C:98:ARG:NH1	2.82	0.46
10:D:54:ALA:CB	10:D:69:ILE:HD12	2.45	0.46
29:W:4:LEU:O	29:W:32:CYS:HA	2.15	0.46
30:X:66:THR:HG23	30:X:67:PRO:HD2	1.97	0.46
1:O:503:G:H2'	1:O:504:G:H8	1.80	0.46
1:O:711:G:C2	1:O:718:C:C2	3.03	0.46
1:O:1314:U:H5''	1:O:1316:G:O4'	2.14	0.46
1:O:2670:G:O2'	1:O:2671:U:H5'	2.14	0.46
1:O:2717:C:H5'	8:B:302:PRO:HA	1.96	0.46
1:O:2793:A:H2'	1:O:2794:G:H5'	1.97	0.46
10:D:27:ILE:HG22	10:D:28:GLY:N	2.30	0.46
16:J:42:GLU:HG2	16:J:43:ARG:N	2.29	0.46
19:M:59:GLY:C	19:M:141:ILE:HD11	2.40	0.46
19:M:80:GLY:O	19:M:81:ARG:HD2	2.16	0.46
30:X:43:VAL:HG12	30:X:47:ALA:HB3	1.95	0.46
1:O:398:U:H2'	1:O:399:C:C6	2.50	0.46
1:O:820:G:C5	7:A:171:LYS:HB2	2.50	0.46
1:O:1375:A:C2'	1:O:1376:G:H5'	2.45	0.46
1:O:2768:A:O2'	1:O:2769:C:H5'	2.15	0.46
26:T:40:VAL:HG22	26:T:41:ARG:N	2.30	0.46
1:O:222:A:H2'	1:O:223:G:O4'	2.15	0.46
1:O:440:C:H2'	1:O:441:A:C8	2.50	0.46
1:O:1041:U:H4'	1:O:1295:G:H5'	1.98	0.46
1:O:1398:G:H2'	1:O:1399:A:C8	2.51	0.46
1:O:2839:C:H2'	1:O:2840:A:H5''	1.96	0.46
1:O:2894:C:O2'	1:O:2895:C:H5'	2.15	0.46
7:A:55:VAL:HG21	7:A:67:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:49:GLN:NE2	14:H:140:TYR:HE2	2.10	0.46
16:J:19:MET:CE	16:J:132:LEU:HD21	2.45	0.46
27:U:17:THR:CG2	27:U:18:GLY:N	2.79	0.46
32:Z:50:GLN:HB2	32:Z:54:ILE:HG22	1.96	0.46
1:O:35:U:H5'	9:C:47:GLY:O	2.16	0.46
1:O:106:A:H2'	1:O:107:U:O4'	2.16	0.46
1:O:285:A:H2'	1:O:286:U:O4'	2.15	0.46
1:O:1181:A:O4'	15:I:87:PRO:HG2	2.16	0.46
1:O:1185:U:OP1	15:I:121:LYS:HD3	2.15	0.46
1:O:2582:G:O3'	17:K:41:LYS:HA	2.16	0.46
16:J:97:ALA:O	16:J:101:VAL:HG23	2.16	0.46
26:T:52:ARG:O	26:T:53:GLY:O	2.34	0.46
29:W:139:GLY:O	29:W:141:HIS:CD2	2.68	0.46
1:O:263:U:O4'	12:F:59:ILE:HD13	2.15	0.46
1:O:524:A:H5'	24:R:29:LYS:HE2	1.97	0.46
1:O:542:A:H2'	1:O:543:G:O4'	2.16	0.46
1:O:1029:U:O2'	1:O:1273:C:OP1	2.31	0.46
7:A:125:ASN:CB	7:A:158:VAL:HG12	2.46	0.46
12:F:16:ALA:HA	12:F:111:ILE:HD13	1.96	0.46
12:F:100:ASP:O	12:F:101:ALA:O	2.33	0.46
14:H:60:LEU:O	14:H:65:LEU:HD21	2.16	0.46
14:H:100:GLU:HB3	14:H:124:VAL:HG11	1.97	0.46
18:L:90:ARG:HH11	18:L:90:ARG:HG3	1.81	0.46
19:M:122:GLN:OE1	19:M:127:LYS:HE2	2.16	0.46
24:R:44:VAL:O	24:R:48:GLU:HG3	2.16	0.46
26:T:18:GLU:O	26:T:21:LYS:HG2	2.16	0.46
30:X:70:ILE:HG23	30:X:70:ILE:O	2.15	0.46
1:O:569:A:H5''	1:O:587:A:N1	2.31	0.46
1:O:603:A:H4'	1:O:604:G:O5'	2.16	0.46
1:O:945:U:H2'	1:O:946:C:H6	1.79	0.46
1:O:1268:C:H2'	1:O:1269:G:C8	2.50	0.46
1:O:2676:C:H4'	16:J:70:PHE:CD1	2.51	0.46
10:D:18:ILE:HA	10:D:134:LEU:HD23	1.96	0.46
10:D:78:GLU:O	10:D:82:GLU:HG3	2.16	0.46
17:K:29:LEU:HB3	17:K:55:VAL:CG1	2.39	0.46
19:M:9:ARG:HB2	19:M:47:ASP:OD2	2.16	0.46
20:N:47:LEU:HD12	20:N:92:ALA:HB1	1.96	0.46
27:U:52:THR:HG21	27:U:54:THR:HB	1.98	0.46
30:X:37:LEU:CD1	30:X:85:VAL:HG21	2.35	0.46
1:O:107:U:H2'	1:O:108:U:H5'	1.98	0.46
1:O:553:G:O4'	1:O:1325:G:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1579:C:H4'	1:0:1580:A:OP1	2.15	0.46
1:0:1805:G:H2'	1:0:1806:G:H8	1.80	0.46
1:0:2708:G:H2'	1:0:2709:G:O4'	2.16	0.46
1:0:2850:C:H5'	1:0:2850:C:C6	2.48	0.46
7:A:109:GLU:HG2	7:A:116:GLY:N	2.31	0.46
27:U:52:THR:HG22	27:U:54:THR:HB	1.96	0.46
28:V:42:ASN:O	28:V:44:GLY:N	2.49	0.46
29:W:19:ASP:O	29:W:23:MET:HG3	2.15	0.46
1:0:553:G:P	31:Y:204:ARG:NH2	2.87	0.46
1:0:907:A:H4'	1:0:1328:A:C2	2.51	0.46
1:0:1384:C:H5'	30:X:30:MET:HG2	1.96	0.46
7:A:42:VAL:HG21	7:A:74:VAL:CG1	2.46	0.46
7:A:105:VAL:HG12	7:A:106:CYS:N	2.30	0.46
14:H:123:ILE:HD12	14:H:123:ILE:N	2.31	0.46
16:J:46:ILE:O	16:J:46:ILE:HG12	2.15	0.46
16:J:131:THR:HG22	16:J:133:GLY:H	1.80	0.46
26:T:24:ARG:HH21	26:T:39:ASN:HD22	1.63	0.46
29:W:73:LEU:HD12	29:W:73:LEU:HA	1.78	0.46
1:0:266:G:OP2	19:M:55:LYS:HE2	2.16	0.46
1:0:542:A:H5'	1:0:542:A:C8	2.40	0.46
1:0:1182:C:H1'	1:0:1192:A:H8	1.80	0.46
1:0:2443:C:H5'	18:L:57:VAL:HG21	1.98	0.46
1:0:2521:A:P	14:H:6:ALA:HB3	2.56	0.46
9:C:54:LEU:HD23	9:C:79:ARG:HG3	1.97	0.46
9:C:133:ARG:NE	9:C:135:GLU:O	2.49	0.46
9:C:170:ASP:O	9:C:171:GLU:HG3	2.16	0.46
9:C:235:PHE:CE2	9:C:243:VAL:HG21	2.45	0.46
11:E:16:ASP:O	11:E:17:HIS:HB2	2.16	0.46
11:E:68:HIS:O	11:E:72:MET:HG3	2.16	0.46
17:K:115:ARG:HG3	17:K:116:GLU:N	2.31	0.46
21:O:39:THR:O	21:O:115:ARG:NH2	2.49	0.46
28:V:26:GLU:OE2	28:V:45:ARG:NH1	2.49	0.46
1:0:821:U:H2'	1:0:822:C:H6	1.81	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.51	0.45
1:0:911:G:H5'	1:0:932:U:OP1	2.16	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.16	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
1:0:2028:U:H2'	1:0:2029:C:C6	2.50	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
1:0:2815:G:N7	16:J:80:LYS:NZ	2.64	0.45
25:S:32:ALA:HA	25:S:36:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:23:VAL:C	26:T:93:THR:HG21	2.42	0.45
30:X:27:ASP:OD2	30:X:27:ASP:N	2.46	0.45
1:0:137:U:OP1	1:0:259:G:O2'	2.34	0.45
1:0:366:U:H2'	1:0:367:G:O4'	2.16	0.45
1:0:2379:G:N7	1:0:2408:A:N1	2.64	0.45
1:0:2781:U:C2'	1:0:2782:G:H5'	2.46	0.45
4:3:42:ARG:HH11	4:3:42:ARG:HG3	1.82	0.45
6:9:8:G:O6	20:N:11:ARG:NH1	2.49	0.45
7:A:61:GLU:C	7:A:63:GLY:H	2.24	0.45
8:B:81:ALA:O	8:B:186:GLY:HA3	2.17	0.45
8:B:238:ASN:HD22	8:B:240:GLY:N	2.08	0.45
9:C:98:ARG:HH11	9:C:98:ARG:CG	2.23	0.45
14:H:30:LYS:N	14:H:62:HIS:HD2	2.13	0.45
14:H:157:TYR:C	14:H:157:TYR:HD1	2.24	0.45
25:S:57:THR:C	25:S:59:ASP:H	2.24	0.45
30:X:34:ARG:NH1	30:X:48:VAL:O	2.46	0.45
1:0:204:A:C2'	1:0:205:U:H5'	2.45	0.45
1:0:682:A:H2'	1:0:683:G:O4'	2.16	0.45
1:0:815:U:O2'	1:0:1598:A:H4'	2.16	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.51	0.45
1:0:2090:G:H2'	1:0:2091:G:C8	2.51	0.45
1:0:2504:A:H4'	14:H:74:ARG:HH11	1.81	0.45
6:9:95:C:O2'	6:9:96:C:H5'	2.16	0.45
7:A:55:VAL:CG2	7:A:67:LEU:HB3	2.47	0.45
7:A:88:ILE:CD1	7:A:100:PRO:HD3	2.39	0.45
7:A:105:VAL:HG11	7:A:154:ALA:CB	2.46	0.45
10:D:91:ALA:HB2	10:D:106:PHE:CE2	2.51	0.45
12:F:57:GLU:O	12:F:61:MET:HG3	2.16	0.45
13:G:71:LEU:O	13:G:73:ASP:N	2.49	0.45
16:J:6:PHE:HB3	16:J:109:TYR:HH	1.81	0.45
16:J:127:ILE:HG22	36:J:8801:CL:CL	2.53	0.45
18:L:145:LEU:C	18:L:147:GLU:N	2.75	0.45
22:P:55:LYS:CG	22:P:56:GLY:N	2.79	0.45
26:T:73:HIS:CD2	26:T:88:PRO:HG3	2.51	0.45
30:X:73:ARG:NH2	30:X:88:GLU:OE2	2.50	0.45
32:Z:72:GLU:CB	32:Z:77:LYS:HE3	2.46	0.45
1:0:215:A:OP1	18:L:52:LYS:NZ	2.47	0.45
1:0:363:C:O2'	1:0:364:U:H5'	2.17	0.45
1:0:1058:A:H2'	1:0:1060:C:C5'	2.44	0.45
1:0:1557:G:O2'	1:0:1558:C:H5'	2.16	0.45
1:0:1783:A:O2'	1:0:1784:U:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1829:A:H2'	1:0:1830:C:H5'	1.99	0.45
1:0:1878:G:O2'	1:0:1879:U:C6	2.67	0.45
1:0:2506:A:N6	1:0:2511:A:O2'	2.49	0.45
1:0:2880:A:H2'	1:0:2881:C:H5'	1.99	0.45
10:D:169:THR:O	10:D:169:THR:HG22	2.17	0.45
18:L:54:PRO:HG2	18:L:57:VAL:CG2	2.46	0.45
24:R:124:GLY:HA3	24:R:136:TRP:O	2.16	0.45
29:W:3:ALA:O	29:W:54:PHE:HA	2.16	0.45
30:X:7:GLU:HG2	30:X:8:ARG:N	2.31	0.45
1:0:188:C:H5''	19:M:163:LEU:HD21	1.99	0.45
1:0:1209:C:H2'	1:0:1210:G:H8	1.81	0.45
1:0:2276:U:H2'	1:0:2277:U:C6	2.51	0.45
1:0:2564:G:OP2	1:0:2565:C:H5''	2.15	0.45
1:0:2667:G:H1'	1:0:2914:A:N3	2.31	0.45
6:9:22:G:H5'	6:9:23:U:OP1	2.16	0.45
8:B:215:VAL:HA	8:B:220:VAL:HG22	1.97	0.45
8:B:280:VAL:HG12	8:B:334:SER:HA	1.97	0.45
14:H:41:LYS:HE2	14:H:45:ASP:CB	2.40	0.45
14:H:53:ILE:HA	14:H:134:GLU:O	2.17	0.45
14:H:154:ARG:HA	14:H:157:TYR:CE2	2.51	0.45
15:I:87:PRO:HB2	15:I:129:SER:HA	1.99	0.45
17:K:113:ILE:CG2	17:K:114:ALA:N	2.79	0.45
19:M:166:ALA:HA	19:M:169:ARG:NH1	2.32	0.45
20:N:79:PRO:HB3	20:N:172:PHE:CD1	2.52	0.45
20:N:178:THR:O	20:N:181:ASP:HB3	2.17	0.45
28:V:39:ALA:O	28:V:41:GLU:N	2.50	0.45
28:V:44:GLY:O	28:V:48:GLU:HG2	2.16	0.45
29:W:48:VAL:HG12	29:W:48:VAL:O	2.17	0.45
30:X:20:GLU:OE1	30:X:21:PRO:HD2	2.17	0.45
1:0:105:G:O2'	1:0:106:A:H5'	2.16	0.45
1:0:113:A:OP2	1:0:114:A:H2'	2.16	0.45
1:0:152:A:O2'	1:0:153:C:H5'	2.15	0.45
1:0:638:C:H2'	1:0:639:A:H8	1.80	0.45
1:0:2089:A:O2'	1:0:2090:G:H5'	2.17	0.45
1:0:2265:U:H2'	1:0:2266:A:H8	1.78	0.45
3:2:36:ASN:HB3	3:2:39:ARG:CG	2.46	0.45
8:B:41:PHE:CD2	8:B:190:MET:HE3	2.52	0.45
8:B:109:LEU:HD11	8:B:113:LEU:HD12	1.99	0.45
16:J:36:VAL:HG12	16:J:37:ALA:N	2.32	0.45
21:O:25:VAL:O	21:O:29:VAL:HG23	2.16	0.45
22:P:115:SER:C	22:P:117:SER:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1483:C:O2'	1:0:1484:G:H5'	2.17	0.45
1:0:2005:G:H3'	1:0:2005:G:OP2	2.17	0.45
1:0:2387:U:H2'	1:0:2388:C:C6	2.51	0.45
4:3:65:THR:CG2	4:3:67:LEU:HG	2.46	0.45
9:C:85:LYS:HA	9:C:85:LYS:HD2	1.86	0.45
10:D:35:ALA:C	10:D:37:ALA:N	2.74	0.45
10:D:55:LYS:O	10:D:56:ARG:HB2	2.17	0.45
25:S:57:THR:CG2	25:S:58:MET:N	2.80	0.45
26:T:96:VAL:HG13	26:T:97:ARG:N	2.30	0.45
29:W:90:TYR:CE2	29:W:99:ALA:HB2	2.52	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.45
1:0:1071:G:H4'	31:Y:154:ARG:HH22	1.80	0.45
8:B:82:VAL:HG12	8:B:101:TRP:CE3	2.51	0.45
8:B:150:ALA:O	8:B:152:PRO:HD3	2.17	0.45
8:B:162:MET:HE2	8:B:310:ARG:CD	2.46	0.45
8:B:264:GLU:HG2	8:B:267:LYS:CE	2.42	0.45
11:E:72:MET:O	11:E:76:VAL:HG22	2.16	0.45
16:J:14:ALA:O	16:J:17:CYS:HB2	2.17	0.45
17:K:24:THR:HG21	17:K:105:ARG:HB3	1.98	0.45
22:P:94:TRP:CH2	22:P:98:ILE:HG13	2.52	0.45
28:V:12:THR:HG23	28:V:15:GLU:H	1.82	0.45
30:X:30:MET:CE	30:X:55:ASN:HA	2.47	0.45
1:0:816:G:C6	1:0:817:G:N1	2.85	0.45
1:0:1097:A:H5''	29:W:125:HIS:NE2	2.32	0.45
1:0:1925:G:O2'	1:0:1926:G:H5'	2.17	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.81	0.45
1:0:2594:C:O2'	1:0:2595:U:H5'	2.17	0.45
1:0:2768:A:C2'	1:0:2769:C:O4'	2.61	0.45
12:F:13:GLU:OE2	12:F:78:GLU:HG2	2.17	0.45
14:H:102:LYS:HD3	14:H:122:LYS:CD	2.40	0.45
19:M:164:THR:HG23	19:M:165:GLY:N	2.32	0.45
26:T:49:GLU:OE2	26:T:97:ARG:HD2	2.17	0.45
27:U:6:CYS:C	27:U:8:TYR:N	2.75	0.45
29:W:26:ILE:O	29:W:26:ILE:HG13	2.16	0.45
1:0:380:A:OP2	19:M:9:ARG:HD2	2.17	0.45
1:0:2001:G:O2'	1:0:2002:C:H5'	2.16	0.45
1:0:2314:G:H2'	1:0:2315:C:H5'	1.99	0.45
1:0:2708:G:N2	17:K:1:MET:O	2.47	0.45
13:G:24:VAL:HA	13:G:27:ILE:HD12	1.99	0.45
14:H:72:ALA:HB2	14:H:156:ALA:HB2	1.99	0.45
18:L:130:ARG:O	18:L:131:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:145:LEU:O	18:L:147:GLU:N	2.50	0.45
20:N:47:LEU:HD23	20:N:47:LEU:HA	1.78	0.45
22:P:114:LEU:HA	22:P:118:GLN:NE2	2.32	0.45
1:O:11:A:H5'	1:O:12:U:OP2	2.17	0.44
1:O:195:C:H2'	1:O:196:G:H5'	2.00	0.44
1:O:941:G:C5	1:O:942:U:C4	3.05	0.44
1:O:1119:G:N2	1:O:1246:A:H2	2.10	0.44
1:O:1909:A:H2'	1:O:1910:A:C8	2.52	0.44
1:O:2301:A:H5''	1:O:2302:A:H5'	1.99	0.44
1:O:2719:A:C2	8:B:70:PRO:HG3	2.52	0.44
6:9:39:U:HO2'	6:9:42:C:H5	1.64	0.44
9:C:140:VAL:HG12	9:C:141:SER:N	2.32	0.44
14:H:50:ILE:HD12	14:H:149:VAL:CG1	2.47	0.44
14:H:91:ARG:NH1	14:H:138:THR:OG1	2.43	0.44
28:V:23:LEU:HD22	28:V:49:LEU:HD23	1.98	0.44
32:Z:20:ARG:O	32:Z:21:VAL:C	2.60	0.44
1:O:497:A:H2'	1:O:498:A:C5'	2.46	0.44
1:O:1641:A:H2'	1:O:1642:A:C5'	2.45	0.44
1:O:1762:C:H2'	1:O:1763:C:H6	1.82	0.44
1:O:2099:G:H21	5:8:5:MEA:CE1	2.31	0.44
1:O:2498:C:O2'	1:O:2499:U:H5'	2.17	0.44
1:O:2598:U:O2	1:O:2600:A:H8	2.00	0.44
1:O:2729:C:H4'	1:O:2893:C:O2	2.17	0.44
7:A:30:ARG:HE	7:A:30:ARG:HB3	1.62	0.44
8:B:56:ASP:HB3	8:B:322:ARG:HE	1.82	0.44
8:B:162:MET:CG	8:B:310:ARG:HD3	2.44	0.44
8:B:183:GLU:O	8:B:184:ASP:C	2.60	0.44
10:D:76:ARG:O	10:D:77:ASP:HB2	2.17	0.44
14:H:12:ILE:HD12	14:H:57:THR:HG22	2.00	0.44
15:I:97:VAL:O	15:I:101:LYS:HG3	2.18	0.44
16:J:45:VAL:HG11	16:J:121:LEU:HD22	1.99	0.44
17:K:109:LEU:CD1	17:K:113:ILE:HD11	2.47	0.44
18:L:67:ARG:HB2	18:L:112:GLY:HA3	1.99	0.44
20:N:86:LEU:HD21	20:N:180:LEU:HD11	1.99	0.44
20:N:139:TRP:HA	20:N:139:TRP:HE3	1.82	0.44
29:W:90:TYR:CD1	29:W:90:TYR:N	2.85	0.44
1:O:1398:G:O2'	1:O:1399:A:H5'	2.17	0.44
8:B:83:ALA:HB2	8:B:101:TRP:CD2	2.53	0.44
10:D:60:GLU:O	10:D:60:GLU:HG3	2.17	0.44
10:D:89:PRO:C	10:D:91:ALA:H	2.25	0.44
11:E:77:THR:OG1	11:E:78:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:95:LEU:O	15:I:134:ILE:HG23	2.17	0.44
22:P:142:ASP:O	22:P:143:ALA:O	2.36	0.44
30:X:21:PRO:HG2	30:X:24:LYS:HD3	1.99	0.44
32:Z:60:CYS:O	32:Z:61:ASP:HB2	2.17	0.44
1:O:21:G:H5''	24:R:1:GLY:O	2.18	0.44
1:O:920:C:H4'	1:O:921:G:C2	2.52	0.44
1:O:1168:C:H5'	15:I:83:GLY:CA	2.46	0.44
1:O:1205:U:C2'	1:O:1206:U:C5'	2.93	0.44
1:O:1262:C:H1'	29:W:120:PRO:HG3	1.99	0.44
1:O:1307:A:H2'	1:O:1308:A:C8	2.52	0.44
1:O:1947:G:N2	1:O:1966:U:C2	2.85	0.44
1:O:2869:G:H2'	1:O:2870:C:C6	2.52	0.44
4:3:69:TYR:O	4:3:77:ALA:HA	2.17	0.44
6:9:57:A:H8	10:D:141:VAL:HG21	1.82	0.44
7:A:27:LEU:HD12	7:A:69:LEU:HD22	1.99	0.44
8:B:140:LEU:HD13	8:B:175:LEU:HA	1.99	0.44
13:G:23:ILE:HD13	13:G:67:LEU:HD23	1.99	0.44
14:H:167:LYS:HE2	14:H:169:GLU:OE1	2.16	0.44
26:T:113:GLU:O	26:T:114:SER:C	2.60	0.44
29:W:35:VAL:HG22	29:W:36:PRO:O	2.18	0.44
32:Z:10:ARG:CG	32:Z:11:SER:H	2.27	0.44
1:O:64:G:H2'	1:O:65:C:O4'	2.17	0.44
1:O:236:A:H8	1:O:236:A:OP1	2.00	0.44
1:O:241:A:C2	1:O:378:A:H4'	2.52	0.44
1:O:308:U:H5'	26:T:97:ARG:NH2	2.33	0.44
1:O:512:G:O3'	1:O:513:A:H8	2.01	0.44
1:O:705:C:H2'	1:O:706:G:O4'	2.17	0.44
1:O:947:U:H2'	1:O:948:G:H8	1.81	0.44
1:O:1175:G:H1'	1:O:1193:A:H2'	2.00	0.44
1:O:1587:U:H2'	1:O:1588:G:O4'	2.18	0.44
7:A:36:ASP:CG	7:A:85:SER:HB2	2.42	0.44
7:A:129:LEU:HD12	7:A:145:MET:HE1	2.00	0.44
7:A:192:VAL:CG1	7:A:207:GLN:HB3	2.48	0.44
7:A:214:SER:HA	7:A:227:ASP:O	2.17	0.44
8:B:62:ARG:NH2	8:B:66:GLU:O	2.50	0.44
8:B:294:TYR:CD1	8:B:294:TYR:C	2.94	0.44
14:H:139:ALA:HB3	14:H:149:VAL:HG21	2.00	0.44
24:R:114:VAL:HA	24:R:144:GLU:O	2.18	0.44
32:Z:57:CYS:O	32:Z:61:ASP:HA	2.17	0.44
1:O:47:G:N3	1:O:114:A:C2	2.86	0.44
1:O:553:G:H2'	1:O:554:G:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:853:C:H2'	1:0:854:G:O4'	2.17	0.44
1:0:1652:C:OP2	32:Z:49:ARG:NH2	2.50	0.44
1:0:1872:C:H5	7:A:20:SER:HB3	1.82	0.44
6:9:3:A:H2	6:9:21:G:N3	2.15	0.44
12:F:48:VAL:CG2	12:F:74:PHE:HB3	2.47	0.44
16:J:39:VAL:CG1	16:J:107:ASN:HB2	2.47	0.44
24:R:17:MET:CE	24:R:19:ARG:CZ	2.94	0.44
30:X:22:ASN:C	30:X:24:LYS:H	2.26	0.44
1:0:67:A:H5''	1:0:69:A:C8	2.53	0.44
1:0:283:U:C5	1:0:284:C:N3	2.85	0.44
1:0:474:C:O2'	9:C:73:LEU:HD21	2.18	0.44
1:0:1287:A:O4'	29:W:117:ARG:HD3	2.17	0.44
1:0:2002:C:C2'	1:0:2003:U:H5'	2.47	0.44
1:0:2032:U:H2'	1:0:2033:G:C5'	2.48	0.44
1:0:2064:U:H5'	1:0:2652:U:O3'	2.18	0.44
1:0:2717:C:H2'	1:0:2718:C:C5'	2.34	0.44
1:0:2897:C:O2'	1:0:2898:G:H5'	2.18	0.44
3:2:40:ARG:HG3	3:2:45:ASN:CB	2.48	0.44
9:C:133:ARG:HG2	9:C:134:ASP:N	2.33	0.44
10:D:173:GLU:O	10:D:174:VAL:C	2.60	0.44
11:E:125:GLU:HB2	11:E:132:THR:CG2	2.47	0.44
15:I:70:THR:HA	15:I:107:LYS:NZ	2.32	0.44
15:I:80:PHE:CD2	15:I:92:VAL:HG12	2.53	0.44
15:I:95:LEU:HD23	15:I:99:GLN:OE1	2.17	0.44
17:K:113:ILE:HG22	17:K:114:ALA:N	2.31	0.44
20:N:154:LEU:HG	20:N:155:GLU:N	2.33	0.44
26:T:89:ARG:HG3	26:T:89:ARG:O	2.17	0.44
29:W:63:GLU:HG2	29:W:93:ILE:HG22	1.99	0.44
31:Y:205:ILE:O	31:Y:206:ALA:C	2.61	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.18	0.44
1:0:877:G:C5'	1:0:878:G:OP1	2.63	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.17	0.44
1:0:2600:A:H2'	1:0:2601:A:O4'	2.18	0.44
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.53	0.44
1:0:2780:C:H2'	1:0:2781:U:C6	2.53	0.44
8:B:195:ARG:HD2	8:B:324:ASP:OD1	2.17	0.44
14:H:53:ILE:HD11	14:H:167:LYS:HD3	2.00	0.44
14:H:117:ARG:O	14:H:118:ALA:C	2.61	0.44
20:N:144:GLY:O	20:N:147:ILE:CG2	2.65	0.44
21:O:25:VAL:HG23	21:O:26:TRP:N	2.33	0.44
21:O:32:ARG:HE	21:O:35:LYS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:35:TYR:CD2	26:T:112:LEU:HD22	2.53	0.44
28:V:12:THR:OG1	28:V:13:PRO:HD2	2.18	0.44
29:W:142:ASP:CB	29:W:145:GLY:H	2.30	0.44
1:0:1168:C:H5''	15:I:83:GLY:H	1.82	0.44
1:0:1316:G:H1'	1:0:1340:G:N2	2.33	0.44
1:0:1855:G:H4'	1:0:1856:C:O5'	2.17	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.53	0.44
1:0:2424:U:H1'	23:Q:7:LEU:HD12	2.00	0.44
1:0:2599:A:C2	1:0:2684:A:H4'	2.52	0.44
1:0:2866:U:C4	27:U:50:GLU:HB3	2.52	0.44
2:1:26:SER:HB3	2:1:35:SER:OG	2.18	0.44
9:C:14:GLY:O	9:C:15:GLU:HB3	2.18	0.44
11:E:119:HIS:HE1	11:E:147:ASP:OD2	2.01	0.44
12:F:110:ASP:O	12:F:114:LYS:HG3	2.17	0.44
17:K:13:GLU:OE2	17:K:44:LEU:HB2	2.17	0.44
17:K:55:VAL:CG1	17:K:56:SER:N	2.81	0.44
19:M:164:THR:CG2	19:M:166:ALA:H	2.31	0.44
1:0:613:C:H2'	1:0:614:U:H6	1.82	0.43
1:0:668:C:H2'	1:0:669:G:H8	1.83	0.43
1:0:820:G:OP2	7:A:171:LYS:NZ	2.43	0.43
1:0:1385:G:O3'	30:X:49:ARG:NH1	2.51	0.43
1:0:1593:C:OP1	22:P:117:SER:HB3	2.16	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
1:0:2676:C:H4'	16:J:70:PHE:HE1	1.81	0.43
1:0:2761:A:C4	1:0:2763:G:C8	3.06	0.43
6:9:11:A:P	23:Q:19:ARG:HH21	2.41	0.43
8:B:55:ASN:HB3	8:B:63:GLU:CA	2.41	0.43
17:K:131:ILE:O	17:K:131:ILE:HG22	2.17	0.43
18:L:35:ARG:O	18:L:40:PHE:HA	2.18	0.43
24:R:145:LEU:HD12	24:R:146:ILE:N	2.32	0.43
29:W:119:HIS:HD2	29:W:120:PRO:O	2.00	0.43
32:Z:13:ARG:HH22	32:Z:30:GLU:CD	2.26	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
1:0:485:A:O2'	1:0:487:G:H5'	2.18	0.43
1:0:1855:G:O6	7:A:142:SER:HB3	2.18	0.43
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.54	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
1:0:2619:UR3:O2	1:0:2619:UR3:O4'	2.35	0.43
7:A:94:LEU:N	7:A:94:LEU:CD2	2.81	0.43
7:A:192:VAL:O	7:A:192:VAL:CG1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:36:PRO:HB3	8:B:174:ARG:HA	1.99	0.43
8:B:44:TYR:OH	8:B:148:PRO:HG3	2.18	0.43
10:D:136:ARG:H	10:D:136:ARG:HG2	1.59	0.43
11:E:11:VAL:HG13	11:E:23:GLU:O	2.19	0.43
11:E:20:ILE:CD1	11:E:40:VAL:HG11	2.48	0.43
17:K:72:VAL:HG11	17:K:121:PHE:CD1	2.53	0.43
22:P:55:LYS:HG2	22:P:56:GLY:N	2.33	0.43
24:R:46:TYR:O	24:R:50:VAL:HG23	2.18	0.43
28:V:12:THR:HG23	28:V:14:ALA:H	1.83	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.52	0.43
1:0:559:U:H6	1:0:559:U:C5'	2.23	0.43
1:0:790:A:H1'	1:0:1710:A:H2'	2.00	0.43
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.43
1:0:1925:G:H5''	4:3:29:ARG:HH22	1.82	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.48	0.43
1:0:2740:G:H2'	1:0:2741:A:O4'	2.17	0.43
6:9:28:U:H2'	6:9:29:C:C6	2.54	0.43
7:A:86:ALA:HB1	7:A:92:ASN:HD22	1.83	0.43
8:B:17:LYS:O	8:B:260:HIS:CD2	2.72	0.43
11:E:86:VAL:CG1	11:E:129:GLU:HA	2.48	0.43
16:J:52:GLN:HG3	16:J:53:ILE:H	1.83	0.43
1:0:876:A:H2'	1:0:876:A:N3	2.33	0.43
1:0:932:U:H2'	1:0:933:C:C6	2.53	0.43
1:0:1345:A:H2'	1:0:1346:U:C6	2.53	0.43
1:0:1407:A:O2'	1:0:1408:U:H3'	2.18	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2769:C:C2'	1:0:2770:G:C5'	2.96	0.43
2:1:28:HIS:CD2	2:1:30:LYS:HB2	2.53	0.43
6:9:34:A:O5'	6:9:34:A:H8	2.02	0.43
8:B:217:ARG:CD	8:B:257:THR:HG22	2.49	0.43
9:C:7:ASP:O	9:C:9:ASP:N	2.51	0.43
10:D:21:VAL:HA	10:D:131:THR:O	2.18	0.43
11:E:81:GLU:HA	11:E:133:VAL:O	2.18	0.43
17:K:81:ARG:HD3	17:K:87:ARG:NH2	2.32	0.43
28:V:29:ASN:O	28:V:33:VAL:HG23	2.18	0.43
1:0:1003:U:H4'	14:H:91:ARG:O	2.19	0.43
1:0:1940:C:H5''	7:A:234:GLY:HA3	2.00	0.43
6:9:13:A:N3	20:N:14:ARG:NH2	2.66	0.43
9:C:57:PRO:HG2	9:C:73:LEU:HD13	2.00	0.43
24:R:80:TYR:CD1	24:R:80:TYR:N	2.86	0.43
26:T:71:VAL:CG1	26:T:72:ILE:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:42:ASN:N	28:V:43:PRO:CD	2.81	0.43
29:W:38:THR:CG2	29:W:39:ASP:N	2.81	0.43
29:W:42:ARG:HA	29:W:45:VAL:CG2	2.49	0.43
31:Y:112:GLU:OE2	31:Y:115:ARG:NH1	2.51	0.43
32:Z:56:GLN:HA	32:Z:62:TYR:O	2.17	0.43
1:0:243:A:H61	1:0:269:G:H1'	1.83	0.43
1:0:777:U:O2'	2:1:11:LYS:HG2	2.18	0.43
1:0:1375:A:O2'	1:0:1376:G:H5'	2.18	0.43
1:0:1617:C:C4	1:0:1643:C:H4'	2.53	0.43
1:0:2728:C:H4'	1:0:2894:C:O2'	2.19	0.43
2:1:2:GLY:O	2:1:6:PRO:HG2	2.18	0.43
6:9:107:C:O2'	6:9:108:C:H5'	2.19	0.43
7:A:211:LYS:CB	7:A:212:PRO:HD2	2.33	0.43
8:B:162:MET:HE2	8:B:310:ARG:CG	2.47	0.43
8:B:280:VAL:CG1	8:B:334:SER:HA	2.49	0.43
9:C:132:ASP:O	9:C:161:ASP:HB2	2.19	0.43
12:F:9:PRO:O	12:F:10:ALA:C	2.61	0.43
25:S:19:ASP:O	25:S:20:PHE:HD2	2.01	0.43
1:0:100:C:H4'	26:T:16:LEU:HB2	2.01	0.43
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.43
1:0:1165:G:C4'	1:0:1174:A:O2'	2.66	0.43
1:0:2420:G:H2'	1:0:2421:G:C8	2.54	0.43
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.19	0.43
4:3:34:LYS:HD2	4:3:34:LYS:N	2.33	0.43
8:B:55:ASN:HB3	8:B:64:GLY:H	1.83	0.43
8:B:57:GLU:O	8:B:63:GLU:HB3	2.19	0.43
9:C:78:ARG:NH1	9:C:78:ARG:CG	2.73	0.43
9:C:98:ARG:NH1	9:C:98:ARG:CG	2.81	0.43
10:D:99:ASP:N	10:D:103:ASN:O	2.39	0.43
19:M:49:ALA:C	19:M:54:TYR:HB3	2.44	0.43
20:N:168:LEU:C	20:N:170:GLU:N	2.77	0.43
24:R:39:THR:HG22	24:R:42:GLU:H	1.84	0.43
29:W:122:ARG:HG3	29:W:122:ARG:NH1	2.33	0.43
1:0:110:C:H2'	1:0:111:C:C6	2.54	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:482:G:H4'	1:0:508:A:N1	2.34	0.43
1:0:694:A:C2'	1:0:695:C:H5'	2.48	0.43
1:0:1025:C:H5'	29:W:23:MET:O	2.19	0.43
3:2:29:THR:C	3:2:31:ARG:H	2.27	0.43
8:B:195:ARG:CZ	8:B:323:LEU:HD13	2.49	0.43
9:C:127:ARG:HD2	9:C:229:PRO:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:200:PRO:HB3	9:C:212:VAL:CG2	2.49	0.43
20:N:143:ARG:HG2	20:N:172:PHE:CD2	2.53	0.43
23:Q:93:ARG:HG3	23:Q:93:ARG:NH1	2.33	0.43
24:R:91:LEU:CD2	24:R:143:VAL:HG22	2.48	0.43
29:W:4:LEU:HD23	29:W:4:LEU:HA	1.77	0.43
29:W:88:THR:HG23	29:W:110:GLN:CB	2.47	0.43
1:O:758:A:H2'	1:O:759:C:O4'	2.19	0.43
1:O:1544:U:H2'	1:O:1545:C:H6	1.84	0.43
1:O:1819:G:H2'	1:O:1820:G:C4'	2.45	0.43
1:O:2270:G:C4'	7:A:223:ARG:HH12	2.31	0.43
1:O:2831:C:C2'	1:O:2832:C:H5'	2.49	0.43
7:A:100:PRO:O	7:A:103:VAL:HG23	2.19	0.43
10:D:96:SER:C	10:D:98:PHE:H	2.27	0.43
11:E:6:GLU:HG2	11:E:46:THR:HG22	2.01	0.43
11:E:84:MET:HG2	11:E:168:ILE:HA	2.01	0.43
11:E:93:MET:HE1	11:E:165:GLY:N	2.34	0.43
12:F:106:ALA:O	12:F:109:GLU:HB3	2.18	0.43
15:I:70:THR:C	15:I:72:GLU:N	2.75	0.43
20:N:170:GLU:HA	20:N:173:ASP:OD2	2.19	0.43
31:Y:187:VAL:CG2	31:Y:192:ASP:HB2	2.30	0.43
31:Y:234:VAL:HG12	31:Y:235:GLU:N	2.34	0.43
32:Z:10:ARG:HB2	32:Z:27:ALA:HB1	2.01	0.43
1:O:466:A:H2'	1:O:467:G:O4'	2.18	0.43
1:O:1597:A:O4'	22:P:95:GLU:HG2	2.19	0.43
1:O:1681:G:H5''	1:O:1682:A:H5'	2.00	0.43
1:O:2133:U:H4'	1:O:2134:G:C5'	2.49	0.43
1:O:2281:C:H2'	1:O:2282:U:H5'	2.01	0.43
1:O:2866:U:H4'	1:O:2867:G:H5'	2.01	0.43
6:9:14:G:O2'	20:N:1:ALA:HB2	2.19	0.43
7:A:57:ALA:HA	7:A:67:LEU:HD23	2.00	0.43
8:B:307:ARG:HH11	8:B:307:ARG:CB	2.31	0.43
9:C:140:VAL:CG1	9:C:141:SER:N	2.82	0.43
10:D:156:ARG:HG3	10:D:156:ARG:HH11	1.84	0.43
14:H:64:SER:O	14:H:65:LEU:C	2.61	0.43
29:W:42:ARG:HA	29:W:45:VAL:HG22	2.00	0.43
29:W:125:HIS:CD2	29:W:127:GLY:H	2.37	0.43
1:O:121:U:OP2	3:2:10:ARG:NH2	2.41	0.42
1:O:581:G:O2'	1:O:582:U:H5'	2.19	0.42
1:O:1168:C:C5'	15:I:83:GLY:H	2.32	0.42
1:O:2715:G:N2	8:B:264:GLU:OE1	2.41	0.42
3:2:28:LYS:O	3:2:28:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:217:ARG:CG	7:A:217:ARG:NH1	2.80	0.42
9:C:4:THR:HB	9:C:135:GLU:OE2	2.19	0.42
14:H:80:LEU:HD11	14:H:145:ASP:HB3	2.01	0.42
24:R:25:PHE:CE2	24:R:29:LYS:HE2	2.54	0.42
27:U:20:MET:CG	27:U:28:THR:HG23	2.49	0.42
28:V:11:MET:HE1	28:V:19:GLU:HG2	2.01	0.42
29:W:10:GLU:HG3	29:W:11:VAL:N	2.33	0.42
30:X:43:VAL:HG22	30:X:76:ARG:NH1	2.34	0.42
1:O:940:G:C5	1:O:1027:G:C2	3.07	0.42
1:O:1249:U:H2'	1:O:1250:C:C6	2.54	0.42
1:O:1250:C:O2'	1:O:1251:C:H5'	2.20	0.42
1:O:1787:C:O2'	1:O:1788:U:H5'	2.19	0.42
1:O:1852:A:H4'	7:A:230:SER:HB2	2.01	0.42
1:O:2112:A:H2'	1:O:2113:G:C8	2.54	0.42
1:O:2269:C:C2'	1:O:2270:G:H5'	2.48	0.42
1:O:2515:C:H2'	1:O:2516:G:O4'	2.18	0.42
1:O:2781:U:H2'	1:O:2782:G:C5'	2.49	0.42
9:C:19:PRO:HD2	9:C:240:LEU:CD2	2.50	0.42
10:D:103:ASN:ND2	10:D:134:LEU:H	2.17	0.42
12:F:118:LEU:O	12:F:119:ARG:OXT	2.37	0.42
18:L:81:VAL:O	18:L:81:VAL:HG12	2.19	0.42
18:L:145:LEU:C	18:L:147:GLU:H	2.27	0.42
19:M:42:ARG:HA	19:M:43:PRO:HD3	1.87	0.42
26:T:41:ARG:NH1	26:T:42:VAL:O	2.51	0.42
29:W:48:VAL:CG1	29:W:52:VAL:HB	2.46	0.42
31:Y:145:LYS:O	31:Y:147:ARG:HG2	2.18	0.42
1:O:629:A:H2'	1:O:630:A:O4'	2.20	0.42
1:O:704:C:H2'	1:O:705:C:H6	1.84	0.42
1:O:1180:U:H2'	1:O:1181:A:O4'	2.19	0.42
1:O:1524:U:OP1	1:O:1524:U:H4'	2.19	0.42
1:O:1943:C:O4'	7:A:212:PRO:HA	2.18	0.42
1:O:2345:A:H3'	1:O:2346:C:C6	2.54	0.42
1:O:2644:C:O2'	1:O:2645:U:H5'	2.18	0.42
1:O:2906:A:H5'	1:O:2907:C:O4'	2.19	0.42
8:B:109:LEU:HD11	8:B:113:LEU:CD1	2.50	0.42
9:C:27:ARG:HH11	9:C:27:ARG:CG	2.32	0.42
9:C:84:VAL:O	9:C:85:LYS:HB2	2.19	0.42
11:E:91:PHE:CD2	11:E:109:GLY:HA2	2.54	0.42
15:I:115:ASP:C	15:I:117:THR:N	2.76	0.42
17:K:34:VAL:CG2	17:K:47:ALA:HB2	2.49	0.42
17:K:64:MET:HA	17:K:67:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:75:ARG:O	17:K:93:ASN:HA	2.19	0.42
20:N:50:LEU:HD12	20:N:50:LEU:HA	1.93	0.42
26:T:73:HIS:CD2	26:T:88:PRO:CB	3.02	0.42
26:T:79:LEU:O	26:T:87:VAL:HG22	2.19	0.42
1:O:875:A:C2	7:A:194:MET:SD	3.12	0.42
1:O:1391:G:H2'	1:O:1392:A:H5'	2.01	0.42
1:O:1500:U:P	22:P:41:ARG:HH22	2.42	0.42
1:O:2379:G:H5'	1:O:2381:C:O4'	2.20	0.42
1:O:2720:C:O2	17:K:87:ARG:NH2	2.52	0.42
7:A:41:THR:HG23	7:A:77:GLY:O	2.19	0.42
8:B:181:ILE:HG22	8:B:186:GLY:HA2	2.01	0.42
8:B:275:GLY:C	8:B:291:ASP:HA	2.45	0.42
10:D:20:LYS:HA	10:D:75:LEU:O	2.20	0.42
11:E:102:VAL:HG11	11:E:148:ILE:HG12	2.01	0.42
16:J:84:ARG:HB2	16:J:98:PHE:CE1	2.55	0.42
29:W:73:LEU:O	29:W:74:GLU:HG3	2.19	0.42
1:O:484:A:N1	1:O:506:G:H4'	2.34	0.42
1:O:1104:C:H4'	16:J:88:PRO:HD3	2.01	0.42
1:O:1503:U:H2'	1:O:1504:A:O4'	2.19	0.42
1:O:1811:A:H2'	1:O:1812:G:H5'	2.01	0.42
1:O:1842:A:C4	1:O:1979:G:C6	3.08	0.42
1:O:2269:C:H2'	1:O:2270:G:H5'	2.00	0.42
1:O:2547:C:OP2	8:B:5:ARG:NH1	2.53	0.42
1:O:2634:G:OP2	7:A:204:GLY:N	2.50	0.42
1:O:2656:G:C2'	1:O:2657:G:H5'	2.50	0.42
6:9:47:A:C2	6:9:48:C:C2	3.07	0.42
11:E:7:ILE:HA	11:E:8:PRO:HD3	1.95	0.42
11:E:11:VAL:HG12	11:E:12:ASP:H	1.81	0.42
11:E:18:LEU:HD13	11:E:34:TRP:CG	2.55	0.42
12:F:28:ALA:CB	12:F:99:THR:HG23	2.50	0.42
18:L:73:VAL:HG21	18:L:116:HIS:CE1	2.55	0.42
20:N:32:PRO:HD2	20:N:99:GLU:O	2.19	0.42
21:O:77:ALA:HA	21:O:96:VAL:O	2.19	0.42
26:T:3:GLN:HA	26:T:4:PRO:HD3	1.94	0.42
28:V:12:THR:O	28:V:13:PRO:C	2.61	0.42
1:O:292:G:H2'	1:O:358:G:N2	2.33	0.42
1:O:533:U:H2'	1:O:2814:A:C6	2.54	0.42
1:O:799:C:O2'	1:O:800:G:H5'	2.18	0.42
1:O:1754:A:H2'	1:O:1755:A:O4'	2.20	0.42
1:O:1878:G:O2'	1:O:1879:U:OP2	2.37	0.42
1:O:2684:A:H2'	1:O:2685:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:119:HIS:O	8:B:121:PRO:HD3	2.20	0.42
17:K:74:VAL:HG21	17:K:96:VAL:HG23	2.01	0.42
20:N:64:SER:C	20:N:66:LEU:H	2.27	0.42
25:S:12:GLU:OE1	25:S:12:GLU:N	2.50	0.42
29:W:108:ARG:C	29:W:110:GLN:N	2.77	0.42
30:X:22:ASN:HA	30:X:25:ARG:HG3	2.00	0.42
30:X:26:ALA:HB2	30:X:63:ARG:HA	2.01	0.42
30:X:43:VAL:CG1	30:X:44:ASP:N	2.81	0.42
1:O:51:G:O2'	1:O:52:A:H5'	2.20	0.42
1:O:134:U:C2	1:O:145:A:C2	3.08	0.42
1:O:1160:G:H5'	1:O:1161:A:O4'	2.20	0.42
1:O:2270:G:H4'	7:A:223:ARG:NH1	2.32	0.42
1:O:2326:C:H4'	1:O:2412:G:H4'	2.02	0.42
1:O:2338:G:O3'	10:D:107:GLY:O	2.36	0.42
1:O:2419:U:H5''	1:O:2420:G:C5'	2.48	0.42
1:O:2727:A:H2'	1:O:2728:C:H5'	2.02	0.42
2:1:37:CYS:SG	2:1:39:PHE:HB2	2.60	0.42
6:9:80:A:H2'	6:9:81:C:O4'	2.19	0.42
7:A:45:ILE:HG22	32:Z:54:ILE:HG12	2.02	0.42
8:B:153:SER:HB2	8:B:287:TYR:CZ	2.54	0.42
9:C:1:MET:HG2	9:C:2:GLN:HE21	1.83	0.42
10:D:170:TYR:CD1	10:D:170:TYR:N	2.88	0.42
12:F:21:GLU:HA	12:F:24:ARG:HE	1.83	0.42
15:I:114:TYR:CD1	15:I:114:TYR:N	2.88	0.42
16:J:131:THR:CG2	16:J:133:GLY:H	2.32	0.42
18:L:90:ARG:HG3	18:L:90:ARG:NH1	2.34	0.42
20:N:11:ARG:HA	20:N:14:ARG:CZ	2.49	0.42
22:P:16:VAL:HG12	22:P:17:GLY:N	2.35	0.42
23:Q:21:ARG:HG2	23:Q:22:GLY:H	1.85	0.42
25:S:57:THR:HG22	25:S:58:MET:N	2.34	0.42
31:Y:184:GLU:CD	31:Y:204:ARG:HH11	2.27	0.42
1:O:216:A:O2'	1:O:217:C:H5'	2.19	0.42
1:O:626:U:C4	1:O:627:G:C6	3.07	0.42
1:O:809:G:H2'	1:O:810:G:C8	2.54	0.42
1:O:827:A:H2'	1:O:828:G:O4'	2.18	0.42
1:O:1098:A:H2'	1:O:1099:G:O4'	2.19	0.42
1:O:2039:A:OP2	8:B:234:ARG:NH2	2.53	0.42
1:O:2241:C:H2'	1:O:2242:U:C6	2.55	0.42
1:O:2325:U:O2'	1:O:2411:C:H1'	2.20	0.42
1:O:2831:C:H2'	1:O:2832:C:C5'	2.49	0.42
3:2:9:LYS:O	3:2:12:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:29:C:C2'	6:9:30:C:H5'	2.46	0.42
8:B:7:ARG:HH11	8:B:7:ARG:CG	2.32	0.42
11:E:116:THR:CG2	11:E:151:LEU:HD22	2.49	0.42
11:E:145:ALA:HB1	11:E:168:ILE:HD11	2.01	0.42
12:F:28:ALA:C	12:F:99:THR:HG23	2.44	0.42
14:H:50:ILE:HD12	14:H:149:VAL:HG11	2.01	0.42
15:I:117:THR:O	15:I:121:LYS:HG3	2.19	0.42
17:K:9:THR:O	17:K:10:GLN:C	2.63	0.42
19:M:67:VAL:HB	19:M:97:ILE:HG23	2.02	0.42
20:N:79:PRO:HG3	20:N:143:ARG:C	2.44	0.42
23:Q:32:GLU:O	23:Q:93:ARG:NH2	2.53	0.42
1:0:80:A:H5''	26:T:41:ARG:CZ	2.50	0.42
1:0:685:C:O2	1:0:748:C:H4'	2.20	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.19	0.42
1:0:1181:A:N1	1:0:1192:A:O2'	2.52	0.42
1:0:1477:C:H5'	1:0:1868:G:H5'	2.01	0.42
1:0:1600:G:OP2	1:0:1600:G:H8	2.03	0.42
1:0:1675:C:H5''	3:2:5:LYS:HD2	2.02	0.42
1:0:2050:G:OP1	24:R:79:ARG:HB3	2.20	0.42
1:0:2237:G:O2'	1:0:2238:A:C8	2.73	0.42
3:2:20:ARG:HG2	3:2:21:VAL:N	2.35	0.42
6:9:31:C:H2'	6:9:32:G:O4'	2.20	0.42
9:C:129:HIS:CE1	9:C:231:ARG:HA	2.55	0.42
10:D:44:ILE:HG23	10:D:45:THR:HG23	2.02	0.42
10:D:60:GLU:O	10:D:62:ASP:N	2.53	0.42
20:N:116:PHE:HB3	20:N:136:LEU:HD23	2.01	0.42
20:N:151:ASP:O	20:N:154:LEU:HB2	2.20	0.42
20:N:166:ALA:O	20:N:167:ASP:HB2	2.20	0.42
29:W:67:ALA:HB2	29:W:93:ILE:HD13	2.02	0.42
1:0:255:A:H2'	1:0:256:C:O4'	2.19	0.42
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.42
1:0:1544:U:H2'	1:0:1545:C:C6	2.55	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.49	0.42
4:3:6:ARG:NH1	4:3:21:GLU:HG3	2.35	0.42
8:B:51:VAL:HG23	8:B:330:VAL:HG22	2.01	0.42
8:B:69:VAL:HA	8:B:70:PRO:HD3	1.88	0.42
8:B:165:ARG:CG	8:B:166:VAL:N	2.83	0.42
8:B:266:ASN:OD1	8:B:317:PRO:HA	2.20	0.42
11:E:126:ILE:HB	11:E:131:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:55:VAL:O	17:K:68:VAL:HA	2.20	0.42
18:L:89:PHE:N	18:L:117:GLU:O	2.53	0.42
22:P:14:LEU:O	22:P:16:VAL:HG23	2.19	0.42
23:Q:93:ARG:HG3	23:Q:93:ARG:HH11	1.85	0.42
29:W:41:TYR:O	29:W:45:VAL:HG22	2.20	0.42
29:W:149:LEU:CG	29:W:153:MET:HE2	2.37	0.42
1:0:37:A:H2'	1:0:38:G:H8	1.85	0.41
1:0:74:G:H2'	1:0:75:U:C6	2.54	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.36	0.41
1:0:886:A:OP2	1:0:2113:G:H5'	2.20	0.41
1:0:949:U:H4'	23:Q:95:GLU:HA	2.02	0.41
1:0:1308:A:O4'	9:C:226:GLY:HA3	2.20	0.41
1:0:1677:U:OP2	3:2:8:LYS:NZ	2.53	0.41
1:0:1853:C:OP1	7:A:231:LYS:HG3	2.19	0.41
1:0:1903:U:O2'	1:0:1904:A:C8	2.72	0.41
1:0:2614:C:O2'	1:0:2615:U:H5'	2.20	0.41
4:3:24:LYS:HE3	4:3:90:PHE:HE1	1.84	0.41
8:B:82:VAL:HG12	8:B:82:VAL:O	2.19	0.41
8:B:233:ARG:HG2	8:B:233:ARG:HH11	1.84	0.41
11:E:88:TYR:CD1	11:E:88:TYR:C	2.98	0.41
12:F:68:ASP:C	12:F:70:LYS:H	2.28	0.41
13:G:15:TRP:CE2	13:G:16:LYS:HG3	2.55	0.41
29:W:88:THR:CG2	29:W:110:GLN:NE2	2.82	0.41
30:X:76:ARG:NH1	30:X:76:ARG:CG	2.81	0.41
1:0:107:U:C2'	1:0:108:U:H5'	2.50	0.41
1:0:182:G:O3'	19:M:157:ASP:OD2	2.38	0.41
1:0:602:A:O2'	1:0:605:C:H4'	2.19	0.41
1:0:958:G:O2'	1:0:959:C:H5'	2.20	0.41
1:0:1304:U:H2'	1:0:1305:C:C6	2.55	0.41
1:0:1855:G:H8	7:A:144:GLU:OE2	2.04	0.41
1:0:1890:U:H4'	1:0:2010:A:C6	2.56	0.41
6:9:52:A:O2'	6:9:53:G:H5'	2.20	0.41
6:9:57:A:C8	10:D:141:VAL:HG21	2.56	0.41
10:D:173:GLU:OE1	10:D:174:VAL:HG23	2.20	0.41
11:E:15:GLN:HB3	11:E:42:VAL:CG2	2.50	0.41
11:E:24:GLY:CA	11:E:76:VAL:HB	2.51	0.41
14:H:92:LYS:HG3	14:H:130:VAL:HG22	2.01	0.41
15:I:130:LEU:HB2	15:I:132:VAL:HG23	2.02	0.41
24:R:31:ILE:O	24:R:32:ALA:C	2.62	0.41
28:V:64:GLY:O	28:V:65:ASP:OD1	2.38	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:N7	18:L:6:ARG:NH1	2.67	0.41
1:0:1461:U:H2'	1:0:1462:C:C6	2.55	0.41
1:0:1883:U:O2'	1:0:1884:G:H5'	2.19	0.41
1:0:2821:C:H4'	8:B:116:PRO:CB	2.50	0.41
7:A:34:ASP:OD1	7:A:35:GLY:N	2.47	0.41
8:B:175:LEU:C	8:B:175:LEU:CD2	2.94	0.41
9:C:191:SER:OG	9:C:192:ILE:N	2.53	0.41
11:E:158:ASP:C	11:E:158:ASP:OD1	2.64	0.41
15:I:67:VAL:HG13	15:I:68:PRO:HD2	2.02	0.41
16:J:95:ARG:O	16:J:99:GLU:HB2	2.21	0.41
18:L:24:ALA:HB2	18:L:30:ARG:HD2	2.02	0.41
20:N:11:ARG:HG3	20:N:14:ARG:CZ	2.50	0.41
20:N:42:HIS:CB	20:N:62:HIS:HE1	2.34	0.41
20:N:86:LEU:HD21	20:N:180:LEU:CD1	2.50	0.41
20:N:124:ASP:C	20:N:126:GLY:H	2.28	0.41
21:O:44:ASN:CG	21:O:67:SER:HB2	2.45	0.41
22:P:13:VAL:HG11	22:P:40:VAL:HG11	2.03	0.41
28:V:8:ILE:HG21	28:V:59:ILE:HG13	2.02	0.41
29:W:54:PHE:CZ	29:W:140:LYS:HB2	2.55	0.41
29:W:73:LEU:HD13	29:W:112:LEU:C	2.45	0.41
1:0:926:A:H1'	18:L:38:HIS:O	2.20	0.41
1:0:1820:G:C6	1:0:2030:A:C2	3.08	0.41
1:0:2088:C:H1'	1:0:2841:A:N1	2.35	0.41
1:0:2507:G:H2'	1:0:2510:C:N4	2.35	0.41
1:0:2714:U:H4'	8:B:10:SER:HB2	2.02	0.41
3:2:16:ASN:C	3:2:18:ASN:N	2.77	0.41
8:B:232:TRP:CD1	8:B:235:ARG:HD2	2.55	0.41
9:C:27:ARG:HG3	9:C:29:ASP:OD1	2.19	0.41
10:D:139:TYR:CE2	10:D:143:LYS:HE2	2.56	0.41
11:E:107:PHE:O	11:E:108:LEU:C	2.62	0.41
14:H:69:ARG:NH2	14:H:70:LEU:HD12	2.36	0.41
16:J:80:LYS:HE2	16:J:98:PHE:CZ	2.54	0.41
19:M:68:ARG:O	19:M:68:ARG:HD3	2.20	0.41
26:T:79:LEU:HG	26:T:89:ARG:HB2	2.01	0.41
26:T:81:LYS:HD2	26:T:87:VAL:HG11	2.02	0.41
28:V:12:THR:HG23	28:V:14:ALA:N	2.35	0.41
29:W:7:LEU:CD1	29:W:53:ALA:HB2	2.50	0.41
31:Y:184:GLU:OE2	31:Y:204:ARG:HD2	2.21	0.41
32:Z:37:HIS:O	32:Z:45:ASP:HA	2.21	0.41
1:0:111:C:H2'	1:0:112:G:O4'	2.21	0.41
1:0:517:U:H2'	1:0:518:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:545:G:H2'	1:0:546:C:O4'	2.19	0.41
1:0:790:A:H2'	1:0:791:A:O4'	2.21	0.41
1:0:2520:G:H5'	14:H:64:SER:OG	2.20	0.41
1:0:2719:A:H2'	1:0:2720:C:H5'	2.01	0.41
2:1:28:HIS:O	2:1:32:LYS:N	2.47	0.41
7:A:75:GLY:HA2	32:Z:64:PHE:HA	2.02	0.41
7:A:88:ILE:HG21	7:A:100:PRO:HG3	2.01	0.41
8:B:53:LEU:HD21	8:B:270:ILE:HD12	2.02	0.41
8:B:102:THR:HG22	8:B:182:VAL:HG12	2.03	0.41
10:D:167:GLU:C	10:D:169:THR:H	2.29	0.41
17:K:78:LYS:HA	17:K:79:PRO:HD3	1.91	0.41
18:L:73:VAL:CG1	18:L:118:LEU:HD21	2.50	0.41
19:M:50:ARG:N	19:M:54:TYR:HB3	2.36	0.41
19:M:133:LEU:HD12	19:M:133:LEU:N	2.34	0.41
20:N:152:GLU:C	20:N:154:LEU:N	2.74	0.41
29:W:38:THR:HG22	29:W:39:ASP:H	1.82	0.41
30:X:47:ALA:HB1	30:X:82:GLU:CB	2.47	0.41
32:Z:53:GLY:HA2	32:Z:67:GLY:O	2.20	0.41
1:0:445:U:H2'	1:0:446:G:H8	1.84	0.41
1:0:560:U:H2'	1:0:561:G:H8	1.85	0.41
1:0:949:U:O2'	23:Q:40:HIS:HE1	2.03	0.41
1:0:1421:C:O2'	1:0:1422:U:H5'	2.20	0.41
1:0:1746:A:O2'	1:0:1752:G:N7	2.50	0.41
1:0:2672:C:H2'	1:0:2673:U:H6	1.85	0.41
1:0:2842:G:H5'	24:R:68:HIS:O	2.20	0.41
8:B:119:HIS:C	8:B:121:PRO:HD3	2.46	0.41
9:C:21:VAL:C	9:C:23:GLU:H	2.27	0.41
14:H:5:PRO:HB2	14:H:7:SER:OG	2.20	0.41
14:H:46:TYR:HA	14:H:47:PRO:HD3	1.80	0.41
20:N:72:GLU:HB3	20:N:171:HIS:HE1	1.86	0.41
22:P:84:ALA:C	22:P:86:ALA:H	2.28	0.41
24:R:75:TRP:CG	24:R:76:ASP:H	2.39	0.41
29:W:11:VAL:O	29:W:12:ASN:HB2	2.20	0.41
31:Y:154:ARG:NH1	31:Y:155:ARG:CG	2.84	0.41
1:0:249:G:H2'	1:0:250:C:C6	2.56	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:1160:G:H5''	1:0:1161:A:H5'	1.98	0.41
1:0:1514:C:O2'	1:0:1515:A:H5'	2.21	0.41
1:0:1821:A:O2'	1:0:1822:A:H5'	2.21	0.41
1:0:2864:U:C5	1:0:2865:G:C6	3.09	0.41
9:C:40:ALA:HB3	9:C:100:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:25:MET:HE2	10:D:41:LEU:CD1	2.50	0.41
14:H:41:LYS:HD3	14:H:46:TYR:CE1	2.55	0.41
14:H:79:GLU:O	14:H:80:LEU:HD23	2.20	0.41
21:O:106:PRO:HG2	21:O:107:GLU:OE1	2.20	0.41
1:O:10:U:O4	1:O:532:A:OP2	2.38	0.41
1:O:958:G:H2'	1:O:959:C:H6	1.84	0.41
1:O:1086:A:P	29:W:9:GLY:H	2.44	0.41
1:O:1762:C:H2'	1:O:1763:C:C6	2.56	0.41
1:O:1771:U:O2'	1:O:1773:G:N7	2.53	0.41
1:O:2270:G:O3'	7:A:223:ARG:NH1	2.54	0.41
1:O:2445:U:H2'	1:O:2446:G:H8	1.85	0.41
3:2:8:LYS:HE3	25:S:58:MET:SD	2.61	0.41
6:9:13:A:OP1	6:9:113:C:H5'	2.20	0.41
8:B:51:VAL:HG23	8:B:329:TYR:O	2.21	0.41
8:B:307:ARG:HH11	8:B:307:ARG:CG	2.33	0.41
10:D:48:MET:HE2	10:D:48:MET:HB3	1.95	0.41
14:H:61:ARG:HG3	14:H:61:ARG:NH1	2.36	0.41
17:K:4:LEU:HD23	17:K:4:LEU:HA	1.94	0.41
18:L:34:GLY:HA3	18:L:38:HIS:CE1	2.55	0.41
18:L:89:PHE:N	18:L:89:PHE:CD1	2.89	0.41
19:M:184:ARG:CZ	19:M:184:ARG:HB2	2.50	0.41
24:R:44:VAL:HG13	24:R:89:LEU:HD22	2.03	0.41
24:R:59:PHE:HZ	24:R:81:PRO:HG3	1.85	0.41
25:S:6:LYS:HB2	25:S:27:ALA:O	2.19	0.41
29:W:88:THR:HG22	29:W:90:TYR:HD1	1.84	0.41
1:O:111:C:O2'	1:O:112:G:H5'	2.21	0.41
1:O:164:G:O3'	18:L:30:ARG:HB2	2.21	0.41
1:O:424:C:H2'	1:O:425:U:C6	2.56	0.41
1:O:553:G:C2'	1:O:554:G:H5'	2.51	0.41
1:O:746:A:C6	21:O:65:LEU:HD13	2.56	0.41
1:O:820:G:H5'	1:O:821:U:C5'	2.51	0.41
1:O:1139:U:H2'	1:O:1140:C:C6	2.56	0.41
1:O:1242:A:OP2	16:J:60:ARG:NH2	2.50	0.41
1:O:1335:C:OP2	31:Y:207:SER:HB3	2.20	0.41
1:O:1706:G:H1'	1:O:1712:A:H61	1.86	0.41
1:O:1755:A:H2'	1:O:1756:G:O4'	2.20	0.41
1:O:1778:A:H2'	1:O:1779:A:H5'	2.03	0.41
1:O:1933:G:O2'	1:O:1934:A:H5'	2.21	0.41
1:O:1972:U:C2'	1:O:1973:A:C5'	2.99	0.41
1:O:2271:G:N3	1:O:2271:G:H2'	2.35	0.41
1:O:2714:U:H2'	1:O:2715:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:8:GLN:NE2	2:1:11:LYS:NZ	2.62	0.41
2:1:53:LYS:HB3	9:C:51:TYR:CE2	2.56	0.41
7:A:66:ARG:CB	7:A:66:ARG:NH1	2.83	0.41
7:A:105:VAL:CG1	7:A:106:CYS:N	2.83	0.41
8:B:24:PRO:HG2	8:B:204:GLY:HA2	2.03	0.41
8:B:87:TYR:HA	8:B:95:ARG:O	2.21	0.41
8:B:265:LEU:HD21	8:B:316:ARG:HD3	2.03	0.41
9:C:13:ASP:OD1	9:C:13:ASP:O	2.39	0.41
10:D:159:PRO:O	10:D:162:ALA:HB3	2.20	0.41
11:E:31:ARG:HE	11:E:31:ARG:HB3	1.76	0.41
12:F:60:VAL:O	12:F:61:MET:C	2.63	0.41
12:F:63:ILE:HB	12:F:64:PRO:CD	2.45	0.41
17:K:98:VAL:HG13	17:K:102:GLU:HA	1.98	0.41
20:N:24:LEU:HD13	23:Q:26:PRO:HB3	2.02	0.41
20:N:71:TRP:CE3	20:N:175:LEU:HD23	2.56	0.41
21:O:96:VAL:HG12	21:O:97:SER:N	2.36	0.41
22:P:38:GLU:HA	22:P:41:ARG:HH11	1.86	0.41
22:P:89:ASN:HB3	22:P:92:GLU:OE1	2.21	0.41
23:Q:24:SER:HB3	23:Q:28:ARG:HH21	1.86	0.41
32:Z:80:ARG:O	32:Z:81:ARG:C	2.64	0.41
1:0:1588:G:C6	1:0:1589:G:N1	2.89	0.41
8:B:285:VAL:O	8:B:286:ASN:HB2	2.20	0.41
9:C:46:TYR:HE2	9:C:98:ARG:HH12	1.68	0.41
9:C:115:LEU:HD12	9:C:115:LEU:HA	1.89	0.41
12:F:119:ARG:HD3	12:F:119:ARG:C	2.46	0.41
15:I:70:THR:C	15:I:72:GLU:H	2.28	0.41
29:W:29:VAL:O	29:W:30:ASN:HB2	2.21	0.41
29:W:131:PRO:HD2	29:W:134:GLU:OE1	2.21	0.41
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.40
1:0:1707:G:N2	1:0:1709:G:H3'	2.36	0.40
1:0:2438:G:H2'	1:0:2439:C:O4'	2.21	0.40
1:0:2630:G:O6	7:A:206:ARG:NH2	2.54	0.40
8:B:24:PRO:O	8:B:25:ARG:HD3	2.22	0.40
8:B:175:LEU:C	8:B:175:LEU:HD23	2.46	0.40
11:E:24:GLY:N	11:E:76:VAL:HB	2.36	0.40
15:I:95:LEU:HD12	15:I:132:VAL:CG1	2.51	0.40
17:K:101:ASN:O	17:K:102:GLU:HB2	2.21	0.40
29:W:13:MET:HE2	29:W:18:GLN:N	2.36	0.40
29:W:83:TRP:CE2	29:W:87:HIS:CD2	3.10	0.40
1:0:69:A:H2'	1:0:70:A:OP2	2.21	0.40
1:0:291:C:H2'	1:0:292:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:653:U:H2'	1:0:654:A:C8	2.56	0.40
1:0:724:G:O2'	1:0:725:C:H5'	2.21	0.40
1:0:858:U:H2'	1:0:859:C:C6	2.56	0.40
1:0:968:G:C1'	14:H:35:LYS:HD2	2.51	0.40
8:B:233:ARG:HG2	8:B:233:ARG:NH1	2.37	0.40
10:D:24:HIS:HB2	10:D:72:LYS:HB3	2.03	0.40
12:F:7:ASP:O	12:F:9:PRO:HD3	2.21	0.40
21:O:96:VAL:CG1	21:O:100:GLN:HB2	2.51	0.40
1:0:1051:C:H2'	1:0:1052:G:O4'	2.21	0.40
1:0:1311:G:O6	9:C:173:LYS:HE3	2.21	0.40
1:0:1463:U:H2'	1:0:1464:C:C6	2.56	0.40
1:0:1747:A:C8	17:K:44:LEU:HD13	2.57	0.40
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.40
1:0:2091:G:O3'	8:B:235:ARG:HD3	2.22	0.40
9:C:153:VAL:O	9:C:157:LEU:HG	2.21	0.40
11:E:83:GLY:HA3	11:E:170:ARG:HE	1.87	0.40
14:H:4:LYS:HE2	14:H:100:GLU:OE2	2.22	0.40
14:H:123:ILE:N	14:H:123:ILE:CD1	2.84	0.40
18:L:97:VAL:HG12	18:L:98:GLU:O	2.21	0.40
31:Y:130:ARG:HB2	31:Y:142:SER:O	2.21	0.40
1:0:271:C:H41	1:0:378:A:H2	1.65	0.40
1:0:401:C:O2'	19:M:92:THR:HB	2.21	0.40
1:0:461:C:N3	1:0:479:G:H5'	2.37	0.40
1:0:581:G:H4'	1:0:1254:C:O2'	2.20	0.40
1:0:1947:G:N2	1:0:1965:C:O2	2.55	0.40
1:0:2346:C:O3'	10:D:52:THR:CG2	2.69	0.40
4:3:22:VAL:HG11	4:3:67:LEU:HD13	2.02	0.40
8:B:79:MET:HE3	8:B:144:THR:HG21	2.04	0.40
9:C:151:GLN:O	9:C:154:VAL:HB	2.21	0.40
11:E:20:ILE:HD11	11:E:40:VAL:HG11	2.03	0.40
11:E:103:VAL:HG21	11:E:115:ARG:NH2	2.37	0.40
14:H:41:LYS:HD3	14:H:46:TYR:OH	2.21	0.40
22:P:13:VAL:HG11	22:P:40:VAL:CG1	2.52	0.40
22:P:16:VAL:HG12	22:P:20:ARG:HB2	2.04	0.40
26:T:43:ASN:C	26:T:45:GLY:H	2.29	0.40
32:Z:42:CYS:SG	32:Z:44:GLU:CB	3.09	0.40
1:0:792:G:O2'	1:0:793:A:H5'	2.21	0.40
1:0:907:A:H5''	31:Y:164:VAL:HG12	2.02	0.40
1:0:1080:C:H6	1:0:1080:C:O5'	2.05	0.40
1:0:1167:G:H2'	1:0:1168:C:C6	2.57	0.40
1:0:2385:G:H2'	1:0:2386:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2543:G:H2'	1:0:2544:G:O4'	2.22	0.40
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.40
1:0:2642:G:H2'	1:0:2643:G:O4'	2.21	0.40
7:A:32:VAL:HG12	7:A:34:ASP:O	2.21	0.40
7:A:81:GLN:HB2	7:A:92:ASN:HD22	1.83	0.40
10:D:23:VAL:HG12	10:D:130:VAL:HG22	2.04	0.40
12:F:57:GLU:HB2	19:M:23:LEU:HD11	2.03	0.40
12:F:107:ASP:O	12:F:108:VAL:C	2.65	0.40
14:H:31:ILE:HA	14:H:66:GLU:OE1	2.21	0.40
20:N:102:LEU:HG	20:N:104:ILE:HG23	2.04	0.40
22:P:131:PHE:CD1	22:P:137:LEU:HD13	2.56	0.40
25:S:11:THR:H	25:S:14:ALA:HB3	1.85	0.40
26:T:24:ARG:HH21	26:T:39:ASN:ND2	2.19	0.40
28:V:1:THR:HG23	28:V:3:LEU:H	1.86	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	
2	1	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
3	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
4	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	36
5	8	2/7 (29%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	202 (86%)	28 (12%)	5 (2%)	5	20
8	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	6	23
9	C	244/246 (99%)	216 (88%)	27 (11%)	1 (0%)	30	60
10	D	134/177 (76%)	97 (72%)	28 (21%)	9 (7%)	1	3
11	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	117/120 (98%)	101 (86%)	11 (9%)	5 (4%)	2	7
13	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
14	H	156/177 (88%)	142 (91%)	12 (8%)	2 (1%)	9	31
15	I	68/162 (42%)	43 (63%)	22 (32%)	3 (4%)	2	7
16	J	140/145 (97%)	127 (91%)	7 (5%)	6 (4%)	2	7
17	K	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
18	L	141/165 (86%)	115 (82%)	23 (16%)	3 (2%)	5	20
19	M	192/195 (98%)	176 (92%)	15 (8%)	1 (0%)	24	55
20	N	184/187 (98%)	161 (88%)	17 (9%)	6 (3%)	3	11
21	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	14	41
22	P	141/149 (95%)	131 (93%)	6 (4%)	4 (3%)	4	14
23	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
24	R	148/155 (96%)	134 (90%)	13 (9%)	1 (1%)	18	47
25	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
26	T	117/120 (98%)	103 (88%)	12 (10%)	2 (2%)	7	25
27	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
28	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	3	11
29	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	9	31
30	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	4	16
31	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	18	47
32	Z	71/83 (86%)	59 (83%)	9 (13%)	3 (4%)	2	7
All	All	3707/4444 (83%)	3293 (89%)	348 (9%)	66 (2%)	6	23

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
10	D	63	ILE
10	D	137	PRO
12	F	101	ALA
16	J	5	GLU
18	L	80	ASP
20	N	154	LEU
20	N	164	ASP
20	N	183	ASP

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Mol	Chain	Res	Type
20	N	184	ILE
28	V	43	PRO
30	X	87	ALA
32	Z	20	ARG
32	Z	81	ARG
8	B	206	THR
9	C	8	LEU
10	D	61	PHE
10	D	138	GLY
12	F	44	SER
14	H	19	ARG
14	H	143	VAL
16	J	7	ASP
21	O	20	SER
22	P	116	SER
26	T	53	GLY
7	A	36	ASP
8	B	35	GLN
8	B	184	ASP
10	D	27	ILE
10	D	64	ARG
16	J	143	LYS
20	N	139	TRP
22	P	132	ASP
29	W	77	ALA
30	X	70	ILE
8	B	2	GLN
8	B	185	GLY
10	D	173	GLU
12	F	100	ASP
15	I	95	LEU
16	J	76	ASP
18	L	105	TYR
22	P	97	ARG
22	P	142	ASP
24	R	81	PRO
26	T	46	ASP
29	W	49	ASN
32	Z	21	VAL
7	A	119	ALA
12	F	61	MET
4	3	58	GLY

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Mol	Chain	Res	Type
7	A	37	VAL
8	B	138	GLY
10	D	16	PRO
10	D	97	GLN
12	F	70	LYS
15	I	133	THR
16	J	65	ASN
16	J	89	HIS
31	Y	198	GLY
20	N	161	GLY
28	V	40	PRO
18	L	146	GLY
7	A	211	LYS
15	I	109	PRO
19	M	88	VAL

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	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	42 (100%)	0	100	100
4	3	79/79 (100%)	77 (98%)	2 (2%)	42	76
5	8	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	170 (95%)	9 (5%)	22	54
8	B	282/283 (100%)	263 (93%)	19 (7%)	15	42
9	C	193/193 (100%)	177 (92%)	16 (8%)	10	32
10	D	117/148 (79%)	111 (95%)	6 (5%)	21	54
11	E	152/156 (97%)	146 (96%)	6 (4%)	28	64
12	F	93/94 (99%)	91 (98%)	2 (2%)	45	78
13	G	27/283 (10%)	25 (93%)	2 (7%)	13	37
14	H	134/145 (92%)	129 (96%)	5 (4%)	30	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	I	58/130 (45%)	57 (98%)	1 (2%)	53	83
16	J	118/121 (98%)	109 (92%)	9 (8%)	12	36
17	K	106/106 (100%)	101 (95%)	5 (5%)	23	57
18	L	113/127 (89%)	109 (96%)	4 (4%)	32	67
19	M	158/159 (99%)	151 (96%)	7 (4%)	25	59
20	N	149/150 (99%)	143 (96%)	6 (4%)	28	63
21	O	93/94 (99%)	90 (97%)	3 (3%)	34	70
22	P	113/117 (97%)	108 (96%)	5 (4%)	25	59
23	Q	79/80 (99%)	76 (96%)	3 (4%)	29	64
24	R	117/122 (96%)	113 (97%)	4 (3%)	32	68
25	S	71/74 (96%)	68 (96%)	3 (4%)	26	61
26	T	105/106 (99%)	97 (92%)	8 (8%)	12	36
27	U	44/52 (85%)	43 (98%)	1 (2%)	44	78
28	V	51/57 (90%)	49 (96%)	2 (4%)	28	64
29	W	130/130 (100%)	122 (94%)	8 (6%)	16	45
30	X	66/74 (89%)	60 (91%)	6 (9%)	9	28
31	Y	120/196 (61%)	117 (98%)	3 (2%)	42	76
32	Z	60/68 (88%)	60 (100%)	0	100	100
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	23	57

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	15	ASN
4	3	42	ARG
7	A	33	GLU
7	A	36	ASP
7	A	69	LEU
7	A	94	LEU
7	A	131	HIS
7	A	153	ARG
7	A	175	LYS
7	A	179	MET
7	A	217	ARG
8	B	7	ARG
8	B	11	LEU

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Mol	Chain	Res	Type
8	B	27	ASN
8	B	49	THR
8	B	56	ASP
8	B	97	LEU
8	B	132	HIS
8	B	175	LEU
8	B	190	MET
8	B	195	ARG
8	B	234	ARG
8	B	251	VAL
8	B	254	GLN
8	B	256	GLN
8	B	264	GLU
8	B	277	GLU
8	B	304	PRO
8	B	307	ARG
8	B	312	ARG
9	C	2	GLN
9	C	16	VAL
9	C	76	ARG
9	C	78	ARG
9	C	101	ASP
9	C	115	LEU
9	C	162	VAL
9	C	187	ARG
9	C	199	GLU
9	C	214	THR
9	C	223	LEU
9	C	234	VAL
9	C	236	THR
9	C	237	GLU
9	C	240	LEU
9	C	243	VAL
10	D	24	HIS
10	D	133	ASN
10	D	136	ARG
10	D	137	PRO
10	D	149	ARG
10	D	153	THR
11	E	7	ILE
11	E	16	ASP
11	E	86	VAL

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Mol	Chain	Res	Type
11	E	102	VAL
11	E	126	ILE
11	E	156	ASP
12	F	46	GLU
12	F	99	THR
13	G	12	ILE
13	G	64	ASN
14	H	21	GLU
14	H	33	GLN
14	H	87	LYS
14	H	135	GLN
14	H	157	TYR
15	I	95	LEU
16	J	7	ASP
16	J	45	VAL
16	J	46	ILE
16	J	52	GLN
16	J	74	ARG
16	J	93	ARG
16	J	99	GLU
16	J	127	ILE
16	J	131	THR
17	K	10	GLN
17	K	63	GLU
17	K	107	THR
17	K	129	THR
17	K	132	VAL
18	L	35	ARG
18	L	90	ARG
18	L	99	GLU
18	L	101	ASP
19	M	46	LEU
19	M	57	LYS
19	M	93	ARG
19	M	99	ARG
19	M	116	ASN
19	M	130	GLU
19	M	164	THR
20	N	17	ARG
20	N	26	LEU
20	N	50	LEU
20	N	53	ASN

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Mol	Chain	Res	Type
20	N	56	ASP
20	N	94	GLU
21	O	3	THR
21	O	28	ASP
21	O	38	ARG
22	P	21	VAL
22	P	52	LYS
22	P	61	ARG
22	P	91	LYS
22	P	98	ILE
23	Q	16	ASN
23	Q	57	ASP
23	Q	95	GLU
24	R	13	THR
24	R	39	THR
24	R	82	GLU
24	R	143	VAL
25	S	10	VAL
25	S	12	GLU
25	S	53	ASN
26	T	19	ARG
26	T	23	VAL
26	T	26	THR
26	T	39	ASN
26	T	48	VAL
26	T	89	ARG
26	T	96	VAL
26	T	112	LEU
27	U	47	ARG
28	V	13	PRO
28	V	43	PRO
29	W	4	LEU
29	W	13	MET
29	W	26	ILE
29	W	52	VAL
29	W	73	LEU
29	W	142	ASP
29	W	146	ILE
29	W	151	GLU
30	X	15	ARG
30	X	27	ASP
30	X	49	ARG

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Mol	Chain	Res	Type
30	X	52	PRO
30	X	72	VAL
30	X	88	GLU
31	Y	163	THR
31	Y	189	ASN
31	Y	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	8	GLN
2	1	16	HIS
2	1	28	HIS
3	2	16	ASN
3	2	17	GLN
3	2	18	ASN
3	2	41	HIS
3	2	45	ASN
4	3	2	GLN
4	3	30	GLN
4	3	48	ASN
7	A	47	HIS
7	A	92	ASN
7	A	199	HIS
7	A	218	ASN
8	B	27	ASN
8	B	145	HIS
8	B	221	GLN
8	B	238	ASN
8	B	260	HIS
8	B	320	GLN
8	B	332	ASN
9	C	2	GLN
9	C	39	GLN
9	C	129	HIS
9	C	151	GLN
9	C	163	HIS
10	D	97	GLN
10	D	103	ASN
10	D	133	ASN
11	E	71	ASN
11	E	106	ASN

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Mol	Chain	Res	Type
11	E	119	HIS
11	E	143	GLN
13	G	64	ASN
14	H	40	GLN
14	H	59	GLN
14	H	62	HIS
14	H	148	HIS
15	I	88	GLN
16	J	25	GLN
16	J	52	GLN
16	J	107	ASN
17	K	10	GLN
17	K	67	GLN
18	L	18	HIS
18	L	41	HIS
18	L	42	ASN
18	L	58	GLN
18	L	116	HIS
19	M	24	GLN
19	M	58	GLN
19	M	170	ASN
20	N	22	GLN
20	N	40	ASN
20	N	62	HIS
20	N	107	ASN
20	N	140	GLN
20	N	153	GLN
22	P	28	GLN
22	P	50	GLN
22	P	66	GLN
22	P	89	ASN
22	P	118	GLN
23	Q	16	ASN
23	Q	27	GLN
23	Q	40	HIS
23	Q	94	GLN
24	R	22	GLN
24	R	61	GLN
24	R	98	ASN
24	R	113	HIS
24	R	117	HIS
24	R	140	GLN

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Mol	Chain	Res	Type
25	S	9	HIS
25	S	25	GLN
25	S	53	ASN
25	S	55	GLN
25	S	56	ASN
26	T	39	ASN
26	T	43	ASN
26	T	73	HIS
27	U	39	ASN
28	V	4	HIS
28	V	29	ASN
28	V	42	ASN
28	V	60	GLN
29	W	14	HIS
29	W	27	HIS
29	W	28	HIS
29	W	87	HIS
29	W	110	GLN
29	W	119	HIS
29	W	125	HIS
29	W	141	HIS
30	X	36	HIS
31	Y	119	GLN
31	Y	134	HIS
31	Y	149	GLN
31	Y	189	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	27 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	261 (9%)	28 (0%)

All (261) 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

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Mol	Chain	Res	Type
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	187	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	319	A
1	0	331	A
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	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A

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Mol	Chain	Res	Type
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	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	701	U
1	0	759	C
1	0	777	U
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
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	884	C
1	0	885	G
1	0	898	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

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Mol	Chain	Res	Type
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1205	U
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	1380	U
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A

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Mol	Chain	Res	Type
1	0	1528	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1857	A
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G

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Mol	Chain	Res	Type
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
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	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U

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Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2645	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	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2914	A
6	9	2	U
6	9	7	G
6	9	14	G
6	9	22	G
6	9	23	U
6	9	24	U
6	9	25	G
6	9	40	C
6	9	41	C
6	9	43	G
6	9	52	A

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Mol	Chain	Res	Type
6	9	57	A
6	9	66	G
6	9	77	A
6	9	114	G
6	9	122	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	318	U
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1685	A
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2644	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
6	9	65	A

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

10 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
5	MHV	8	6	5	7,9,10	1.16	1 (14%)	8,11,13	1.49	1 (12%)
5	004	8	7	5	9,10,11	2.02	2 (22%)	9,12,14	1.45	1 (11%)
5	MHW	8	1	33,5	9,9,10	1.94	3 (33%)	10,11,13	1.27	2 (20%)
5	MEA	8	5	5	11,12,13	1.87	5 (45%)	13,14,16	1.58	3 (23%)
1	OMU	0	2587	1	19,22,23	0.30	0	25,31,34	0.36	0
1	UR3	0	2619	1	19,22,23	0.53	0	26,32,35	0.85	1 (3%)
1	OMG	0	2588	1	23,26,27	0.28	0	32,38,41	0.34	0
5	DBB	8	3	5	4,5,6	0.75	0	1,5,7	0.02	0
1	1MA	0	628	1	21,25,26	0.73	1 (4%)	30,37,40	0.91	2 (6%)
1	PSU	0	2621	1	18,21,22	1.44	2 (11%)	21,30,33	1.27	3 (14%)

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
5	MHV	8	6	5	-	0/1/12/14	0/1/1/1
5	004	8	7	5	-	0/4/6/8	0/1/1/1
5	MHW	8	1	33,5	-	0/2/2/4	0/1/1/1
5	MEA	8	5	5	-	0/5/8/10	0/1/1/1
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	2/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
5	DBB	8	3	5	-	0/3/4/6	-
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	8	7	004	CB-CA	5.21	1.57	1.52
1	0	2621	PSU	C2-N1	4.74	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	8	5	MEA	CE2-CD2	3.17	1.44	1.38
5	8	1	MHW	CA-C	3.05	1.52	1.48
5	8	1	MHW	CA-N	3.00	1.39	1.35
5	8	1	MHW	CB-CA	2.82	1.44	1.40
1	0	2621	PSU	C6-C5	2.71	1.38	1.35
5	8	7	004	CD2-CG2	2.65	1.43	1.38
5	8	6	MHV	CB-CG	2.64	1.54	1.50
1	0	628	1MA	C6-N6	2.62	1.34	1.28
5	8	5	MEA	CD1-CG	2.53	1.43	1.38
5	8	5	MEA	CE2-CZ	2.32	1.43	1.38
5	8	5	MEA	CA-N	2.28	1.51	1.47
5	8	5	MEA	CB-CA	2.01	1.58	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	8	5	MEA	O-C-CA	-3.07	116.88	124.77
1	0	2619	UR3	C4-N3-C2	3.02	127.01	124.58
1	0	2621	PSU	C6-C5-C4	3.02	120.21	118.17
5	8	7	004	CG2-CB-CA	3.01	125.32	120.64
1	0	2621	PSU	C6-N1-C2	-2.85	120.05	122.69
1	0	628	1MA	N1-C2-N3	2.84	129.37	126.00
1	0	2621	PSU	O2-C2-N1	2.75	125.62	122.79
5	8	5	MEA	CB-CA-N	2.74	114.51	110.48
1	0	628	1MA	CM1-N1-C6	2.68	124.31	120.15
5	8	6	MHV	CB-CA-N	-2.62	107.09	112.50
5	8	1	MHW	CB-CA-C	2.30	121.80	120.09
5	8	1	MHW	O-C-CA	-2.22	121.59	124.37
5	8	5	MEA	C1-N-CA	2.12	120.03	113.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2619	UR3	O4'-C1'-N1-C6
1	0	2619	UR3	O4'-C1'-N1-C2
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
5	8	5	MEA	1	0
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	VIR	0	9000	-	38,40,40	2.56	18 (47%)	42,55,55	1.88	12 (28%)

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
37	VIR	0	9000	-	-	9/48/58/58	0/2/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9000	VIR	C28-C29	-6.78	1.17	1.32
37	0	9000	VIR	C4-N5	5.57	1.55	1.47
37	0	9000	VIR	C13-C10	-4.67	1.45	1.50
37	0	9000	VIR	C30-C32	3.91	1.63	1.54
37	0	9000	VIR	C28-C26	3.41	1.55	1.48
37	0	9000	VIR	C10-N9	-3.40	1.25	1.29
37	0	9000	VIR	C34-C33	3.26	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9000	VIR	C1-C37	-3.24	1.38	1.48
37	0	9000	VIR	C26-N25	3.04	1.40	1.34
37	0	9000	VIR	C21-C20	2.88	1.56	1.50
37	0	9000	VIR	C17-C19	-2.88	1.47	1.50
37	0	9000	VIR	C16-C17	-2.84	1.48	1.54
37	0	9000	VIR	O15-C14	2.77	1.26	1.21
37	0	9000	VIR	C6-N5	2.62	1.44	1.38
37	0	9000	VIR	C1-N5	2.16	1.42	1.39
37	0	9000	VIR	O36-C32	2.15	1.48	1.44
37	0	9000	VIR	O36-C37	2.13	1.39	1.34
37	0	9000	VIR	O38-C37	2.10	1.25	1.21

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9000	VIR	O27-C26-C28	5.37	135.33	122.95
37	0	9000	VIR	C28-C26-N25	-5.19	103.70	115.07
37	0	9000	VIR	C30-C29-C28	3.09	134.47	126.30
37	0	9000	VIR	O7-C6-C8	2.99	123.28	118.65
37	0	9000	VIR	O11-C10-C13	-2.91	115.02	117.70
37	0	9000	VIR	C12-C8-C6	-2.72	122.48	127.60
37	0	9000	VIR	C22-C20-C19	-2.59	111.89	118.82
37	0	9000	VIR	O7-C6-N5	2.54	125.51	120.69
37	0	9000	VIR	C31-C30-C32	2.47	115.45	111.11
37	0	9000	VIR	C6-C8-N9	2.43	127.96	123.70
37	0	9000	VIR	O36-C37-C1	2.28	114.00	110.77
37	0	9000	VIR	C21-C20-C22	2.10	121.30	118.09

There are no chirality outliers.

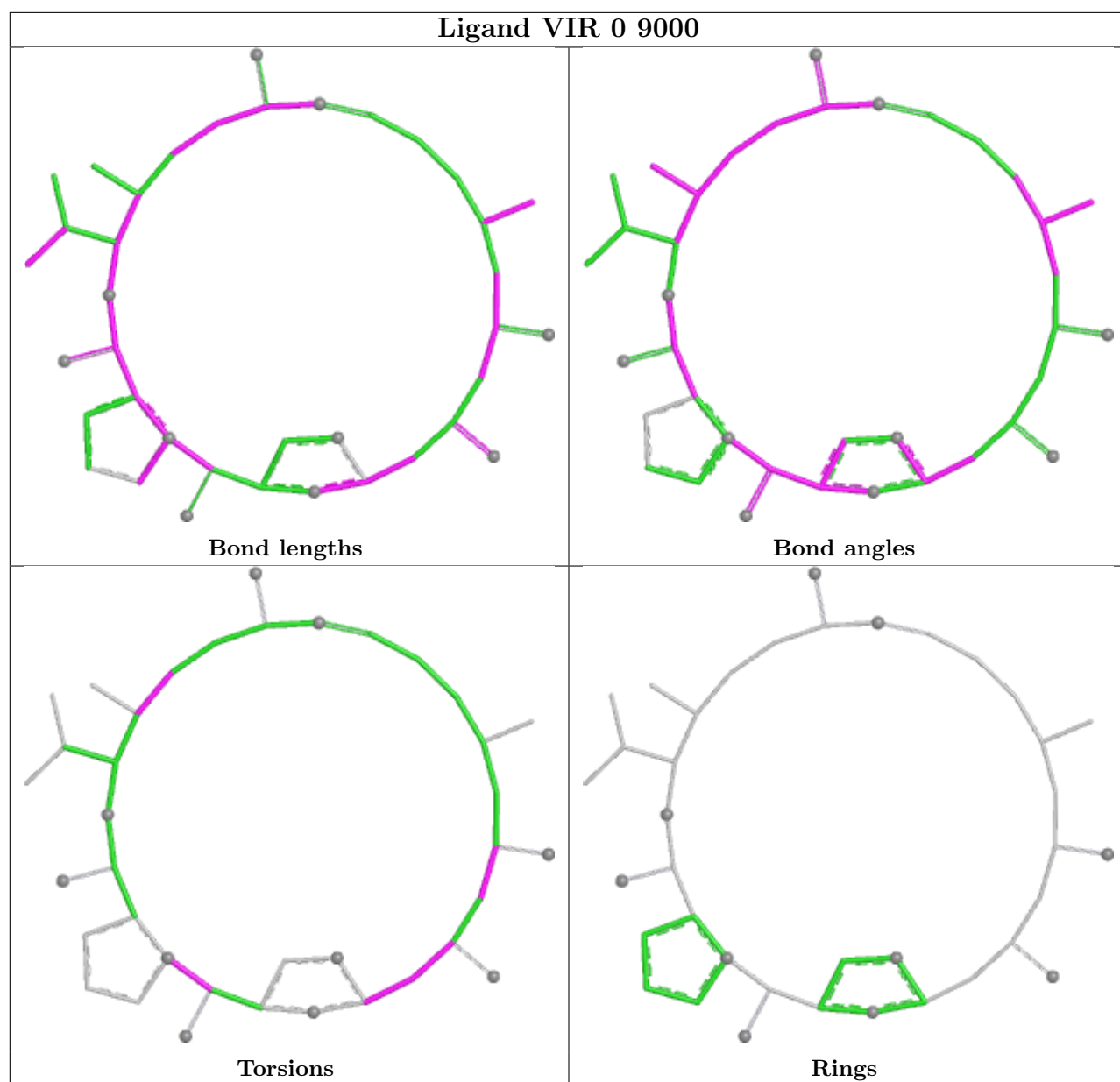
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	0	9000	VIR	O11-C10-C13-C14
37	0	9000	VIR	O7-C6-N5-C4
37	0	9000	VIR	C14-C16-C17-O18
37	0	9000	VIR	N9-C10-C13-C14
37	0	9000	VIR	C10-C13-C14-O15
37	0	9000	VIR	C14-C16-C17-C19
37	0	9000	VIR	C10-C13-C14-C16
37	0	9000	VIR	C8-C6-N5-C4
37	0	9000	VIR	C28-C29-C30-C31

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.14	80 (2%) 53 43	20, 45, 89, 150	0
2	1	56/57 (98%)	-0.33	0 100 100	25, 32, 36, 40	0
3	2	46/50 (92%)	1.08	14 (30%) 1 1	28, 59, 93, 108	0
4	3	92/92 (100%)	0.41	3 (3%) 49 39	42, 60, 72, 82	0
5	8	2/7 (28%)	0.22	0 100 100	40, 40, 40, 41	0
6	9	122/122 (100%)	0.39	6 (4%) 35 27	35, 62, 88, 150	0
7	A	237/240 (98%)	0.47	12 (5%) 33 25	26, 53, 88, 108	0
8	B	337/338 (99%)	0.31	7 (2%) 63 54	25, 51, 77, 89	0
9	C	246/246 (100%)	0.19	3 (1%) 76 68	21, 43, 68, 77	0
10	D	140/177 (79%)	1.95	58 (41%) 0 0	55, 98, 121, 131	0
11	E	172/178 (96%)	0.73	9 (5%) 33 25	42, 64, 86, 95	0
12	F	119/120 (99%)	0.85	9 (7%) 20 14	46, 69, 92, 107	0
13	G	29/348 (8%)	1.37	7 (24%) 2 1	70, 87, 93, 97	0
14	H	160/177 (90%)	0.52	15 (9%) 14 10	37, 56, 91, 103	0
15	I	70/162 (43%)	2.61	45 (64%) 0 0	105, 121, 139, 140	0
16	J	142/145 (97%)	0.22	4 (2%) 55 45	34, 48, 66, 85	0
17	K	132/132 (100%)	0.20	1 (0%) 82 75	28, 48, 68, 79	0
18	L	145/165 (87%)	0.89	24 (16%) 4 3	24, 64, 104, 118	0
19	M	194/195 (99%)	0.08	4 (2%) 63 54	28, 41, 57, 63	0
20	N	186/187 (99%)	0.88	25 (13%) 7 5	37, 63, 108, 116	0
21	O	115/116 (99%)	0.42	3 (2%) 57 47	35, 51, 70, 73	0
22	P	143/149 (95%)	0.38	4 (2%) 55 45	33, 53, 70, 75	0
23	Q	95/96 (98%)	0.02	1 (1%) 78 70	35, 42, 58, 75	0
24	R	150/155 (96%)	-0.14	1 (0%) 84 77	30, 42, 61, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	S	81/85 (95%)	0.36	2 (2%) 58 48	40, 59, 77, 84	0
26	T	119/120 (99%)	0.43	7 (5%) 28 21	36, 54, 82, 98	0
27	U	53/66 (80%)	0.35	2 (3%) 44 35	40, 53, 70, 80	0
28	V	65/71 (91%)	1.23	13 (20%) 3 2	51, 72, 112, 117	0
29	W	154/154 (100%)	0.07	0 100 100	32, 45, 62, 74	0
30	X	82/92 (89%)	0.48	8 (9%) 13 9	39, 54, 76, 93	0
31	Y	142/241 (58%)	0.13	4 (2%) 55 45	24, 42, 64, 87	0
32	Z	73/83 (87%)	1.36	14 (19%) 3 2	64, 78, 91, 99	0
All	All	6648/7488 (88%)	0.24	385 (5%) 29 22	20, 50, 97, 150	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	D	10	PHE	7.7
14	H	174	LEU	7.6
6	9	1	U	7.3
28	V	1	THR	7.3
7	A	37	VAL	6.9
15	I	128	THR	6.6
10	D	55	LYS	5.8
15	I	129	SER	5.8
10	D	62	ASP	5.3
1	0	1176	C	5.2
11	E	10	ASP	5.2
28	V	2	VAL	5.1
1	0	10	U	5.1
1	0	2345	A	5.0
14	H	171	GLY	5.0
6	9	2	U	5.0
15	I	113	SER	4.9
1	0	1173	A	4.9
1	0	1175	G	4.9
20	N	154	LEU	4.8
10	D	35	ALA	4.8
10	D	174	VAL	4.8
18	L	82	ALA	4.6
1	0	1171	A	4.5
10	D	63	ILE	4.5
1	0	1161	A	4.4

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Mol	Chain	Res	Type	RSRZ
10	D	44	ILE	4.4
15	I	74	ILE	4.4
10	D	26	GLY	4.3
15	I	130	LEU	4.3
15	I	112	LEU	4.3
11	E	45	ASP	4.3
22	P	143	ALA	4.3
15	I	126	THR	4.3
28	V	39	ALA	4.2
15	I	83	GLY	4.2
20	N	147	ILE	4.2
3	2	49	GLU	4.2
28	V	40	PRO	4.2
10	D	107	GLY	4.2
15	I	80	PHE	4.1
32	Z	82	SER	4.1
7	A	36	ASP	4.1
15	I	71	ALA	4.1
1	0	1192	A	4.0
15	I	85	GLY	4.0
18	L	102	ASP	3.9
10	D	69	ILE	3.9
10	D	53	LYS	3.9
20	N	169	PRO	3.9
30	X	87	ALA	3.9
18	L	99	GLU	3.9
20	N	165	ALA	3.9
10	D	56	ARG	3.8
13	G	12	ILE	3.8
20	N	168	LEU	3.8
15	I	88	GLN	3.8
1	0	2344	G	3.8
18	L	148	GLU	3.7
10	D	11	HIS	3.7
20	N	186	LEU	3.6
1	0	1177	A	3.6
1	0	1174	A	3.6
1	0	1172	G	3.6
6	9	24	U	3.6
18	L	78	ALA	3.6
15	I	91	PHE	3.6
10	D	172	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
7	A	211	LYS	3.5
10	D	59	GLY	3.5
3	2	35	ARG	3.5
32	Z	10	ARG	3.5
20	N	153	GLN	3.5
1	0	1169	U	3.5
11	E	156	ASP	3.5
6	9	23	U	3.5
28	V	43	PRO	3.5
15	I	101	LYS	3.4
12	F	101	ALA	3.4
15	I	66	GLY	3.4
14	H	169	GLU	3.4
1	0	283	U	3.4
15	I	109	PRO	3.4
1	0	284	C	3.4
28	V	44	GLY	3.4
20	N	164	ASP	3.4
15	I	116	LEU	3.3
15	I	108	HIS	3.3
15	I	124	VAL	3.3
15	I	132	VAL	3.3
7	A	237	GLY	3.3
3	2	38	LYS	3.3
32	Z	16	ALA	3.3
18	L	150	GLN	3.3
8	B	1	PRO	3.3
1	0	960	G	3.3
15	I	73	LEU	3.2
15	I	125	GLY	3.2
10	D	105	SER	3.2
15	I	135	GLU	3.2
12	F	28	ALA	3.2
10	D	36	ASN	3.2
15	I	107	LYS	3.2
1	0	1181	A	3.2
10	D	171	ASP	3.2
10	D	101	THR	3.2
30	X	88	GLU	3.2
26	T	118	SER	3.1
16	J	4	ALA	3.1
1	0	1183	C	3.1

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Mol	Chain	Res	Type	RSRZ
1	0	1525	G	3.1
1	0	1193	A	3.1
1	0	138	U	3.1
31	Y	216	ARG	3.1
1	0	1929	G	3.1
31	Y	236	VAL	3.1
11	E	154	ILE	3.1
10	D	170	TYR	3.1
1	0	1163	G	3.1
1	0	1166	A	3.1
18	L	83	GLU	3.1
12	F	98	VAL	3.0
10	D	68	PRO	3.0
14	H	173	GLU	3.0
20	N	149	GLU	3.0
1	0	1165	G	3.0
1	0	1167	G	3.0
10	D	54	ALA	3.0
1	0	1184	C	3.0
15	I	114	TYR	3.0
13	G	63	ARG	3.0
1	0	1561	U	3.0
3	2	41	HIS	3.0
13	G	73	ASP	3.0
14	H	170	ARG	3.0
10	D	75	LEU	3.0
16	J	92	GLN	3.0
20	N	161	GLY	3.0
1	0	1168	C	3.0
3	2	44	ARG	2.9
10	D	17	ARG	2.9
19	M	125	ARG	2.9
1	0	2637	A	2.9
10	D	90	LEU	2.9
1	0	1204	C	2.9
14	H	43	ALA	2.9
20	N	160	SER	2.9
15	I	97	VAL	2.9
30	X	85	VAL	2.9
3	2	37	HIS	2.9
18	L	149	ARG	2.9
1	0	2237	G	2.9

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Mol	Chain	Res	Type	RSRZ
10	D	128	LEU	2.9
1	0	1200	A	2.9
1	0	2664	A	2.9
1	0	1170	U	2.9
10	D	65	GLU	2.9
10	D	104	PHE	2.9
28	V	45	ARG	2.9
26	T	53	GLY	2.8
1	0	1198	U	2.8
8	B	57	GLU	2.8
15	I	78	ALA	2.8
15	I	104	ALA	2.8
32	Z	34	ASN	2.8
15	I	84	SER	2.8
11	E	126	ILE	2.8
31	Y	95	THR	2.8
15	I	77	GLU	2.8
20	N	150	TYR	2.8
21	O	24	ALA	2.8
18	L	75	LEU	2.8
1	0	1199	A	2.8
1	0	2346	C	2.8
20	N	157	PRO	2.8
20	N	21	HIS	2.8
18	L	81	VAL	2.7
1	0	1191	A	2.7
1	0	1524	U	2.7
1	0	1964	U	2.7
10	D	100	ASP	2.7
15	I	133	THR	2.7
10	D	12	GLU	2.7
1	0	2506	A	2.7
16	J	62	ASP	2.7
19	M	22	GLU	2.7
15	I	111	LEU	2.7
18	L	77	ALA	2.7
10	D	154	LYS	2.7
3	2	39	ARG	2.7
15	I	87	PRO	2.7
32	Z	23	ARG	2.7
1	0	1160	G	2.7
11	E	53	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
18	L	147	GLU	2.7
32	Z	11	SER	2.7
32	Z	35	GLU	2.7
13	G	71	LEU	2.7
15	I	127	CYS	2.7
20	N	151	ASP	2.7
30	X	79	GLU	2.7
10	D	27	ILE	2.6
15	I	119	ALA	2.6
3	2	46	ASP	2.6
10	D	99	ASP	2.6
28	V	41	GLU	2.6
20	N	184	ILE	2.6
10	D	13	MET	2.6
22	P	58	SER	2.6
32	Z	22	SER	2.6
32	Z	59	TYR	2.6
10	D	86	THR	2.6
1	0	1201	C	2.6
10	D	18	ILE	2.6
1	0	1203	G	2.6
12	F	99	THR	2.6
8	B	27	ASN	2.6
10	D	19	GLU	2.6
11	E	170	ARG	2.6
21	O	22	GLY	2.6
9	C	132	ASP	2.6
10	D	57	THR	2.5
12	F	106	ALA	2.5
4	3	8	ASN	2.5
3	2	48	ASP	2.5
9	C	101	ASP	2.5
26	T	114	SER	2.5
1	0	282	C	2.5
1	0	735	C	2.5
15	I	134	ILE	2.5
1	0	1202	A	2.5
10	D	61	PHE	2.5
22	P	116	SER	2.5
13	G	26	MET	2.5
1	0	1162	G	2.5
1	0	1951	G	2.5

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Mol	Chain	Res	Type	RSRZ
23	Q	95	GLU	2.5
26	T	115	GLU	2.5
15	I	106	GLN	2.5
20	N	148	ALA	2.5
30	X	83	ALA	2.5
27	U	47	ARG	2.5
20	N	41	LYS	2.5
26	T	40	VAL	2.5
20	N	159	TYR	2.5
18	L	130	ARG	2.5
1	0	130	C	2.5
1	0	969	G	2.5
1	0	1190	G	2.5
1	0	2768	A	2.5
10	D	135	VAL	2.4
10	D	138	GLY	2.4
3	2	42	TRP	2.4
9	C	133	ARG	2.4
18	L	60	GLU	2.4
1	0	2769	C	2.4
20	N	158	LEU	2.4
1	0	497	A	2.4
1	0	1178	G	2.4
11	E	11	VAL	2.4
12	F	119	ARG	2.4
12	F	90	GLU	2.4
3	2	36	ASN	2.4
1	0	2508	C	2.4
25	S	12	GLU	2.4
1	0	970	U	2.4
15	I	82	THR	2.4
28	V	46	ILE	2.4
14	H	35	LYS	2.4
17	K	119	GLN	2.4
1	0	2136	G	2.4
10	D	95	THR	2.4
10	D	155	HIS	2.4
15	I	95	LEU	2.4
18	L	110	GLY	2.3
7	A	34	ASP	2.3
1	0	1559	A	2.3
10	D	96	SER	2.3

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Mol	Chain	Res	Type	RSRZ
19	M	194	GLY	2.3
12	F	100	ASP	2.3
20	N	166	ALA	2.3
14	H	68	SER	2.3
18	L	105	TYR	2.3
25	S	81	ILE	2.3
10	D	72	LYS	2.3
1	0	1279	U	2.3
28	V	42	ASN	2.3
14	H	172	GLU	2.3
18	L	101	ASP	2.3
7	A	31	LYS	2.3
10	D	24	HIS	2.3
32	Z	20	ARG	2.3
10	D	21	VAL	2.3
12	F	102	GLY	2.3
18	L	59	GLU	2.3
8	B	56	ASP	2.3
3	2	43	ARG	2.3
8	B	29	TRP	2.3
10	D	58	VAL	2.3
7	A	236	GLY	2.3
10	D	134	LEU	2.2
4	3	83	TRP	2.2
10	D	153	THR	2.2
7	A	85	SER	2.2
7	A	33	GLU	2.2
28	V	47	LYS	2.2
14	H	40	GLN	2.2
15	I	103	ILE	2.2
28	V	6	GLN	2.2
3	2	31	ARG	2.2
14	H	114	ASP	2.2
18	L	104	ASP	2.2
7	A	35	GLY	2.2
1	0	716	G	2.2
1	0	1947	G	2.2
8	B	108	GLU	2.2
26	T	119	ALA	2.2
31	Y	235	GLU	2.2
20	N	146	HIS	2.2
15	I	110	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
7	A	32	VAL	2.2
10	D	25	MET	2.2
10	D	48	MET	2.2
32	Z	58	SER	2.2
10	D	40	ILE	2.2
1	0	1130	U	2.2
1	0	2004	U	2.2
32	Z	21	VAL	2.2
1	0	1182	C	2.2
20	N	163	PHE	2.2
10	D	88	LEU	2.2
7	A	86	ALA	2.2
1	0	1164	U	2.1
30	X	65	ASN	2.1
32	Z	26	VAL	2.1
26	T	117	ASP	2.1
1	0	285	A	2.1
1	0	288	A	2.1
1	0	2338	G	2.1
3	2	47	THR	2.1
15	I	70	THR	2.1
13	G	29	SER	2.1
1	0	1185	U	2.1
10	D	159	PRO	2.1
14	H	13	ASP	2.1
18	L	36	ASP	2.1
1	0	128	A	2.1
6	9	51	A	2.1
18	L	100	ALA	2.1
30	X	61	ARG	2.1
1	0	2507	G	2.1
15	I	72	GLU	2.1
30	X	80	GLU	2.1
13	G	64	ASN	2.1
15	I	123	VAL	2.1
19	M	80	GLY	2.1
4	3	41	GLU	2.1
16	J	5	GLU	2.1
1	0	272	A	2.1
1	0	1189	A	2.1
10	D	47	GLN	2.1
18	L	55	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
14	H	39	LYS	2.1
24	R	150	PRO	2.1
15	I	118	ASN	2.1
20	N	182	GLY	2.1
11	E	100	ASP	2.1
14	H	38	ARG	2.1
10	D	60	GLU	2.1
14	H	149	VAL	2.0
18	L	73	VAL	2.0
28	V	13	PRO	2.0
6	9	122	C	2.0
21	O	47	ARG	2.0
1	0	1205	U	2.0
1	0	2419	U	2.0
8	B	98	THR	2.0
27	U	52	THR	2.0
22	P	117	SER	2.0
18	L	145	LEU	2.0
32	Z	25	ARG	2.0
1	0	287	C	2.0
20	N	167	ASP	2.0
1	0	2256	G	2.0
10	D	22	VAL	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($\text{\AA}^2$)	Q<0.9
5	MHW	8	1	9/10	0.92	0.12	37,40,43,44	0
5	DBB	8	3	6/7	0.93	0.11	36,40,40,41	0
5	MEA	8	5	12/13	0.94	0.12	39,40,43,43	0
5	MHV	8	6	9/10	0.95	0.10	42,43,45,48	0
1	1MA	0	628	23/24	0.97	0.07	26,28,29,30	0
1	OMU	0	2587	21/22	0.97	0.07	31,34,37,40	0
1	UR3	0	2619	21/22	0.97	0.07	26,32,37,38	0
1	PSU	0	2621	20/21	0.97	0.06	25,29,33,34	0
5	004	8	7	10/11	0.97	0.10	41,45,48,49	0
1	OMG	0	2588	24/25	0.98	0.06	28,30,34,36	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
33	MG	0	8058	1/1	0.24	0.34	39,39,39,39	0
35	NA	0	8583	1/1	0.24	0.27	56,56,56,56	0
33	MG	0	8092	1/1	0.35	0.39	66,66,66,66	0
33	MG	B	8055	1/1	0.37	0.25	38,38,38,38	0
33	MG	0	8115	1/1	0.40	0.23	49,49,49,49	0
35	NA	0	8529	1/1	0.42	0.27	66,66,66,66	0
33	MG	0	8089	1/1	0.42	0.42	77,77,77,77	0
33	MG	0	8096	1/1	0.43	0.20	46,46,46,46	0
35	NA	0	8565	1/1	0.47	0.28	53,53,53,53	0
33	MG	0	8062	1/1	0.49	0.41	61,61,61,61	0
33	MG	0	8084	1/1	0.49	0.39	43,43,43,43	0
35	NA	0	8523	1/1	0.52	0.24	35,35,35,35	0
33	MG	2	8076	1/1	0.54	0.25	57,57,57,57	0
35	NA	0	8580	1/1	0.54	0.19	49,49,49,49	0
33	MG	0	8068	1/1	0.54	0.57	77,77,77,77	0
35	NA	0	8581	1/1	0.55	0.34	89,89,89,89	0
33	MG	0	8014	1/1	0.55	0.17	22,22,22,22	0
33	MG	0	8013	1/1	0.57	0.24	32,32,32,32	0
33	MG	0	8009	1/1	0.57	0.25	28,28,28,28	0
33	MG	0	8018	1/1	0.58	0.29	43,43,43,43	0
33	MG	0	8075	1/1	0.58	0.31	51,51,51,51	0
33	MG	0	8031	1/1	0.58	0.20	27,27,27,27	0
33	MG	0	8088	1/1	0.58	0.11	21,21,21,21	0
33	MG	0	8072	1/1	0.59	0.52	63,63,63,63	0
35	NA	R	8537	1/1	0.59	0.21	44,44,44,44	0
33	MG	0	8012	1/1	0.60	0.34	36,36,36,36	0
33	MG	0	8040	1/1	0.60	0.33	56,56,56,56	0
35	NA	0	8511	1/1	0.61	0.23	48,48,48,48	0
33	MG	0	8091	1/1	0.62	0.35	55,55,55,55	0
33	MG	0	8044	1/1	0.62	0.17	43,43,43,43	0
33	MG	0	8063	1/1	0.62	0.47	62,62,62,62	0
33	MG	0	8097	1/1	0.62	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8066	1/1	0.62	0.22	62,62,62,62	0
33	MG	0	8110	1/1	0.63	0.23	52,52,52,52	0
33	MG	0	8023	1/1	0.63	0.30	41,41,41,41	0
33	MG	0	8102	1/1	0.63	0.26	80,80,80,80	0
33	MG	0	8105	1/1	0.63	0.17	50,50,50,50	0
33	MG	0	8054	1/1	0.64	0.30	32,32,32,32	0
35	NA	9	8551	1/1	0.65	0.29	49,49,49,49	0
35	NA	0	8513	1/1	0.65	0.31	56,56,56,56	0
33	MG	0	8043	1/1	0.66	0.19	45,45,45,45	0
33	MG	0	8001	1/1	0.66	0.20	33,33,33,33	0
33	MG	0	8071	1/1	0.66	0.59	68,68,68,68	0
33	MG	0	8100	1/1	0.66	0.52	63,63,63,63	0
33	MG	0	8049	1/1	0.67	0.41	73,73,73,73	0
35	NA	0	8518	1/1	0.67	0.15	30,30,30,30	0
33	MG	0	8039	1/1	0.67	0.26	42,42,42,42	0
33	MG	0	8019	1/1	0.67	0.27	27,27,27,27	0
33	MG	0	8111	1/1	0.67	0.25	42,42,42,42	0
33	MG	0	8113	1/1	0.68	0.15	52,52,52,52	0
33	MG	0	8032	1/1	0.68	0.19	26,26,26,26	0
33	MG	0	8107	1/1	0.68	0.30	49,49,49,49	0
33	MG	0	8047	1/1	0.68	0.40	70,70,70,70	0
33	MG	0	8079	1/1	0.68	0.28	36,36,36,36	0
33	MG	0	8022	1/1	0.69	0.32	59,59,59,59	0
35	NA	R	8585	1/1	0.69	0.45	82,82,82,82	0
33	MG	0	8004	1/1	0.70	0.30	39,39,39,39	0
33	MG	0	8006	1/1	0.70	0.14	32,32,32,32	0
33	MG	0	8029	1/1	0.70	0.25	37,37,37,37	0
33	MG	0	8045	1/1	0.70	0.29	54,54,54,54	0
35	NA	A	8545	1/1	0.70	0.30	49,49,49,49	0
33	MG	0	8061	1/1	0.70	0.20	31,31,31,31	0
33	MG	B	8056	1/1	0.70	0.28	50,50,50,50	0
33	MG	0	8048	1/1	0.71	0.26	49,49,49,49	0
33	MG	0	8106	1/1	0.71	0.23	38,38,38,38	0
33	MG	0	8036	1/1	0.71	0.28	36,36,36,36	0
35	NA	0	8534	1/1	0.71	0.18	40,40,40,40	0
35	NA	0	8535	1/1	0.71	0.25	44,44,44,44	0
35	NA	0	8555	1/1	0.71	0.30	72,72,72,72	0
35	NA	0	8559	1/1	0.71	0.35	52,52,52,52	0
35	NA	0	8560	1/1	0.71	0.22	56,56,56,56	0
33	MG	0	8093	1/1	0.72	0.28	49,49,49,49	0
33	MG	0	8027	1/1	0.72	0.29	44,44,44,44	0
33	MG	0	8052	1/1	0.72	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	3	8078	1/1	0.72	0.12	45,45,45,45	0
33	MG	0	8083	1/1	0.72	0.22	39,39,39,39	0
33	MG	0	8053	1/1	0.72	0.18	40,40,40,40	0
33	MG	0	8003	1/1	0.73	0.17	31,31,31,31	0
33	MG	0	8114	1/1	0.74	0.28	47,47,47,47	0
35	NA	9	8582	1/1	0.74	0.27	78,78,78,78	0
35	NA	0	8525	1/1	0.74	0.28	51,51,51,51	0
33	MG	0	8008	1/1	0.74	0.21	35,35,35,35	0
33	MG	0	8011	1/1	0.74	0.33	11,11,11,11	0
35	NA	0	8568	1/1	0.75	0.22	58,58,58,58	0
35	NA	0	8571	1/1	0.75	0.34	62,62,62,62	0
35	NA	0	8502	1/1	0.75	0.16	44,44,44,44	0
35	NA	0	8517	1/1	0.75	0.13	46,46,46,46	0
33	MG	0	8041	1/1	0.75	0.12	42,42,42,42	0
33	MG	0	8080	1/1	0.76	0.18	36,36,36,36	0
33	MG	0	8090	1/1	0.76	0.26	53,53,53,53	0
35	NA	0	8508	1/1	0.76	0.20	56,56,56,56	0
33	MG	0	8050	1/1	0.76	0.20	77,77,77,77	0
33	MG	A	8065	1/1	0.76	0.27	43,43,43,43	0
33	MG	0	8109	1/1	0.76	0.12	20,20,20,20	0
35	NA	0	8576	1/1	0.76	0.37	69,69,69,69	0
35	NA	0	8578	1/1	0.76	0.39	58,58,58,58	0
33	MG	0	8021	1/1	0.77	0.32	36,36,36,36	0
33	MG	0	8117	1/1	0.77	0.41	47,47,47,47	0
33	MG	0	8060	1/1	0.77	0.41	51,51,51,51	0
35	NA	0	8569	1/1	0.77	0.68	73,73,73,73	0
33	MG	0	8087	1/1	0.77	0.23	51,51,51,51	0
33	MG	0	8016	1/1	0.78	0.16	32,32,32,32	0
35	NA	0	8536	1/1	0.78	0.22	47,47,47,47	0
35	NA	0	8541	1/1	0.78	0.12	39,39,39,39	0
33	MG	0	8086	1/1	0.78	0.26	47,47,47,47	0
35	NA	0	8514	1/1	0.78	0.18	33,33,33,33	0
33	MG	0	8010	1/1	0.79	0.20	34,34,34,34	0
33	MG	K	8069	1/1	0.79	0.36	45,45,45,45	0
35	NA	0	8540	1/1	0.79	0.12	34,34,34,34	0
33	MG	0	8015	1/1	0.79	0.24	30,30,30,30	0
35	NA	0	8527	1/1	0.79	0.20	51,51,51,51	0
35	NA	0	8516	1/1	0.79	0.19	42,42,42,42	0
33	MG	0	8094	1/1	0.79	0.43	72,72,72,72	0
35	NA	0	8562	1/1	0.80	0.15	43,43,43,43	0
35	NA	0	8572	1/1	0.80	0.09	58,58,58,58	0
35	NA	0	8563	1/1	0.80	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8077	1/1	0.80	0.23	29,29,29,29	0
33	MG	0	8017	1/1	0.80	0.29	27,27,27,27	0
33	MG	0	8030	1/1	0.80	0.14	21,21,21,21	0
33	MG	0	8028	1/1	0.81	0.27	35,35,35,35	0
33	MG	0	8070	1/1	0.81	0.14	45,45,45,45	0
33	MG	0	8025	1/1	0.81	0.18	31,31,31,31	0
33	MG	0	8051	1/1	0.81	0.27	60,60,60,60	0
33	MG	0	8118	1/1	0.82	0.16	34,34,34,34	0
35	NA	0	8573	1/1	0.82	0.39	68,68,68,68	0
35	NA	0	8538	1/1	0.82	0.10	42,42,42,42	0
35	NA	0	8554	1/1	0.82	0.16	38,38,38,38	0
35	NA	0	8550	1/1	0.83	0.14	34,34,34,34	0
33	MG	0	8112	1/1	0.83	0.29	42,42,42,42	0
33	MG	0	8074	1/1	0.83	0.23	34,34,34,34	0
33	MG	0	8037	1/1	0.83	0.18	32,32,32,32	0
35	NA	0	8566	1/1	0.83	0.14	46,46,46,46	0
33	MG	0	8005	1/1	0.84	0.22	31,31,31,31	0
33	MG	0	8104	1/1	0.84	0.16	51,51,51,51	0
33	MG	0	8082	1/1	0.84	0.51	63,63,63,63	0
35	NA	0	8567	1/1	0.84	0.19	64,64,64,64	0
35	NA	0	8577	1/1	0.84	0.17	44,44,44,44	0
35	NA	0	8519	1/1	0.84	0.11	25,25,25,25	0
35	NA	0	8507	1/1	0.84	0.14	59,59,59,59	0
33	MG	0	8024	1/1	0.85	0.14	22,22,22,22	0
35	NA	0	8542	1/1	0.85	0.17	41,41,41,41	0
33	MG	0	8098	1/1	0.85	0.10	25,25,25,25	0
35	NA	0	8506	1/1	0.85	0.41	41,41,41,41	0
35	NA	0	8558	1/1	0.86	0.28	61,61,61,61	0
35	NA	0	8524	1/1	0.86	0.17	43,43,43,43	0
33	MG	0	8085	1/1	0.86	0.29	53,53,53,53	0
33	MG	0	8026	1/1	0.86	0.14	22,22,22,22	0
33	MG	0	8101	1/1	0.86	0.19	50,50,50,50	0
33	MG	0	8033	1/1	0.86	0.12	32,32,32,32	0
33	MG	0	8103	1/1	0.86	0.12	47,47,47,47	0
33	MG	0	8002	1/1	0.86	0.15	28,28,28,28	0
35	NA	0	8520	1/1	0.87	0.15	28,28,28,28	0
33	MG	T	8073	1/1	0.87	0.18	66,66,66,66	0
35	NA	0	8528	1/1	0.87	0.10	38,38,38,38	0
35	NA	0	8505	1/1	0.87	0.20	32,32,32,32	0
35	NA	Q	8548	1/1	0.87	0.07	32,32,32,32	0
35	NA	0	8532	1/1	0.87	0.09	42,42,42,42	0
35	NA	0	8556	1/1	0.87	0.21	40,40,40,40	0

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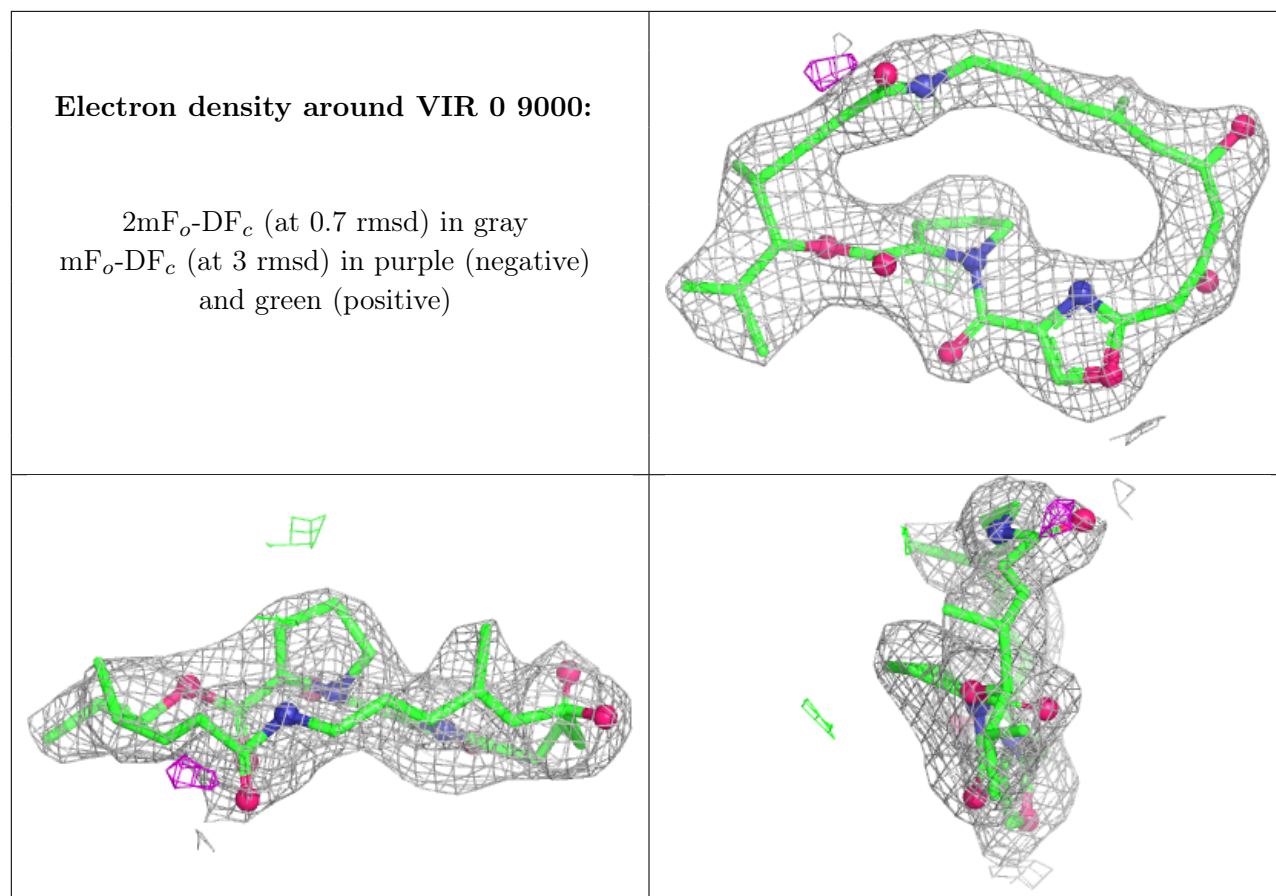
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	S	8512	1/1	0.87	0.08	35,35,35,35	0
36	CL	0	8822	1/1	0.87	0.21	81,81,81,81	0
33	MG	0	8057	1/1	0.88	0.07	38,38,38,38	0
35	NA	0	8557	1/1	0.88	0.22	50,50,50,50	0
33	MG	0	8020	1/1	0.88	0.21	20,20,20,20	0
35	NA	0	8515	1/1	0.88	0.19	47,47,47,47	0
35	NA	0	8552	1/1	0.88	0.23	59,59,59,59	0
35	NA	0	8510	1/1	0.88	0.12	40,40,40,40	0
33	MG	Y	8108	1/1	0.88	0.09	36,36,36,36	0
35	NA	0	8584	1/1	0.88	0.29	51,51,51,51	0
33	MG	0	8042	1/1	0.89	0.07	31,31,31,31	0
35	NA	0	8570	1/1	0.89	0.37	58,58,58,58	0
35	NA	0	8533	1/1	0.89	0.20	43,43,43,43	0
35	NA	0	8561	1/1	0.89	0.33	59,59,59,59	0
33	MG	0	8046	1/1	0.89	0.17	48,48,48,48	0
35	NA	C	8504	1/1	0.89	0.07	40,40,40,40	0
33	MG	0	8081	1/1	0.89	0.11	44,44,44,44	0
33	MG	0	8038	1/1	0.89	0.34	26,26,26,26	0
33	MG	0	8116	1/1	0.89	0.11	20,20,20,20	0
33	MG	0	8007	1/1	0.89	0.10	18,18,18,18	0
35	NA	0	8530	1/1	0.89	0.08	40,40,40,40	0
35	NA	0	8526	1/1	0.90	0.18	51,51,51,51	0
33	MG	0	8035	1/1	0.90	0.30	42,42,42,42	0
35	NA	0	8544	1/1	0.90	0.06	24,24,24,24	0
35	NA	0	8503	1/1	0.90	0.14	45,45,45,45	0
35	NA	0	8521	1/1	0.90	0.20	61,61,61,61	0
35	NA	0	8553	1/1	0.91	0.11	30,30,30,30	0
35	NA	0	8549	1/1	0.91	0.14	46,46,46,46	0
35	NA	H	8522	1/1	0.91	0.24	55,55,55,55	0
35	NA	0	8543	1/1	0.91	0.09	46,46,46,46	0
35	NA	0	8574	1/1	0.91	0.38	44,44,44,44	0
35	NA	0	8575	1/1	0.91	0.15	45,45,45,45	0
35	NA	0	8564	1/1	0.91	0.17	45,45,45,45	0
36	CL	0	8817	1/1	0.91	0.08	49,49,49,49	0
33	MG	0	8059	1/1	0.91	0.19	38,38,38,38	0
36	CL	J	8802	1/1	0.91	0.10	63,63,63,63	0
33	MG	9	8095	1/1	0.92	0.15	55,55,55,55	0
34	K	0	8402	1/1	0.92	0.15	66,66,66,66	0
33	MG	0	8034	1/1	0.92	0.17	24,24,24,24	0
35	NA	0	8531	1/1	0.92	0.14	46,46,46,46	0
33	MG	0	8099	1/1	0.92	0.14	49,49,49,49	0
36	CL	N	8807	1/1	0.92	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8501	1/1	0.93	0.16	23,23,23,23	0
33	MG	0	8064	1/1	0.93	0.07	30,30,30,30	0
36	CL	A	8809	1/1	0.93	0.14	68,68,68,68	0
35	NA	J	8546	1/1	0.93	0.07	48,48,48,48	0
35	NA	L	8579	1/1	0.93	0.21	67,67,67,67	0
38	CD	O	8705	1/1	0.93	0.06	88,88,88,88	0
35	NA	M	8547	1/1	0.94	0.11	31,31,31,31	0
36	CL	3	8804	1/1	0.94	0.11	68,68,68,68	0
35	NA	0	8539	1/1	0.94	0.12	35,35,35,35	0
36	CL	J	8801	1/1	0.94	0.10	63,63,63,63	0
36	CL	0	8805	1/1	0.94	0.08	58,58,58,58	0
36	CL	0	8815	1/1	0.94	0.14	84,84,84,84	0
36	CL	O	8808	1/1	0.94	0.18	84,84,84,84	0
36	CL	R	8806	1/1	0.94	0.10	41,41,41,41	0
35	NA	0	8509	1/1	0.94	0.06	38,38,38,38	0
36	CL	B	8819	1/1	0.95	0.15	46,46,46,46	0
36	CL	0	8813	1/1	0.95	0.10	50,50,50,50	0
33	MG	0	8067	1/1	0.95	0.08	44,44,44,44	0
37	VIR	0	9000	38/38	0.95	0.11	24,36,40,44	0
36	CL	J	8821	1/1	0.95	0.08	48,48,48,48	0
36	CL	0	8816	1/1	0.96	0.12	57,57,57,57	0
36	CL	0	8811	1/1	0.96	0.06	53,53,53,53	0
36	CL	Y	8820	1/1	0.97	0.07	43,43,43,43	0
36	CL	L	8810	1/1	0.97	0.08	53,53,53,53	0
36	CL	0	8803	1/1	0.97	0.07	54,54,54,54	0
36	CL	0	8812	1/1	0.98	0.09	43,43,43,43	0
38	CD	3	8704	1/1	0.98	0.03	69,69,69,69	0
36	CL	M	8818	1/1	0.98	0.09	40,40,40,40	0
36	CL	0	8814	1/1	0.99	0.04	49,49,49,49	0
38	CD	1	8702	1/1	0.99	0.05	58,58,58,58	0
38	CD	Z	8703	1/1	0.99	0.04	84,84,84,84	0
38	CD	U	8701	1/1	1.00	0.01	58,58,58,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.