



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:03 PM UTC

PDB ID : 2OTJ / pdb_00002otj
Title : 13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
Resolution : 2.90 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:

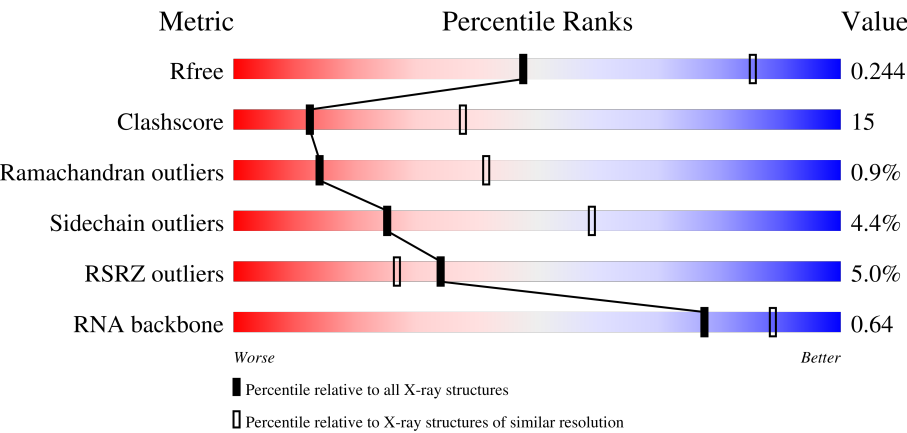
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.90 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.



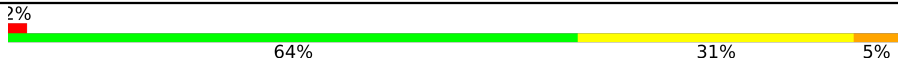
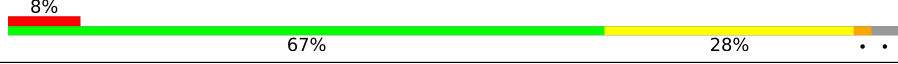
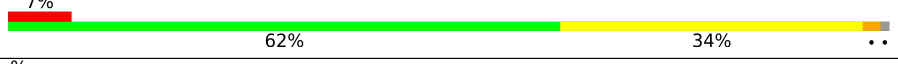
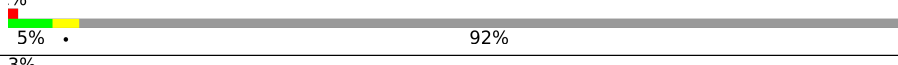
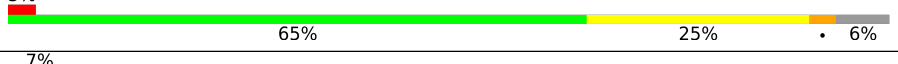
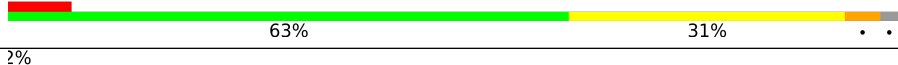
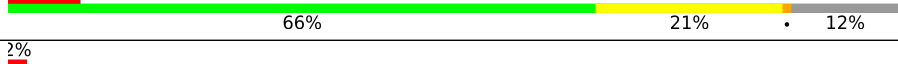
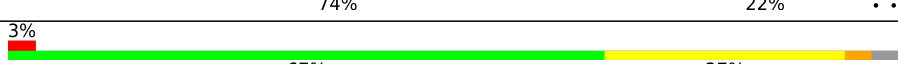
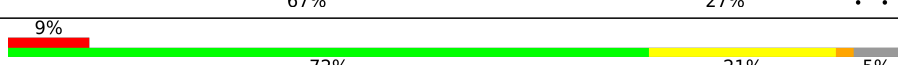
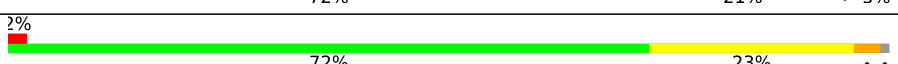
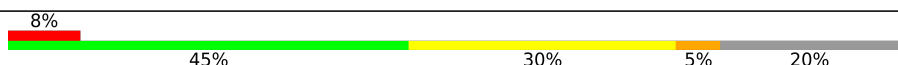
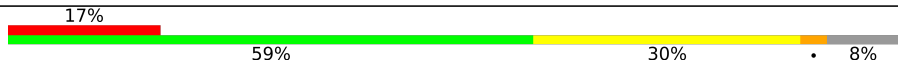
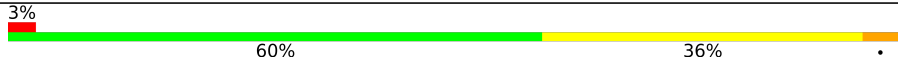
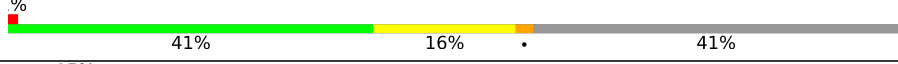
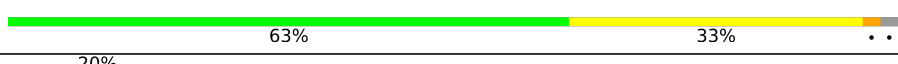
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	0	2922	2% 49%39%6%6%
2	9	122	2% 38%48%12%
3	A	240	5% 63%31%5%
4	B	338	7% 58%37%5%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	161	

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
32	13T	0	9000	-	-	X	-
33	MG	0	8024	-	-	-	X
35	NA	0	8542	-	-	X	-
35	NA	H	8522	-	-	-	X
36	CL	J	8801	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	-	insertion	UNP P60617
H	166	SER	-	insertion	UNP P60617
H	167	PRO	-	insertion	UNP P60617
H	168	ALA	-	insertion	UNP P60617
H	169	GLY	-	insertion	UNP P60617
H	170	ASN	-	insertion	UNP P60617
H	171	ALA	-	insertion	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	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 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	-	insertion	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	insertion	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

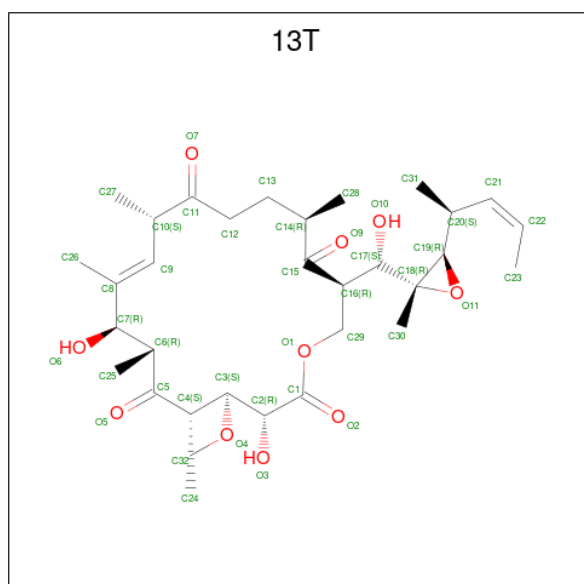
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is 13-DEOXYTEDANOLIDE (CCD ID: 13T) (formula: C₃₂H₅₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	0	1	Total	C	O	0	0
			42	32	10		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
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		
33	3	2	Total	Mg	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	74	Total	Na	0	0
			74	74		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	2	Total 2	Cl 2	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

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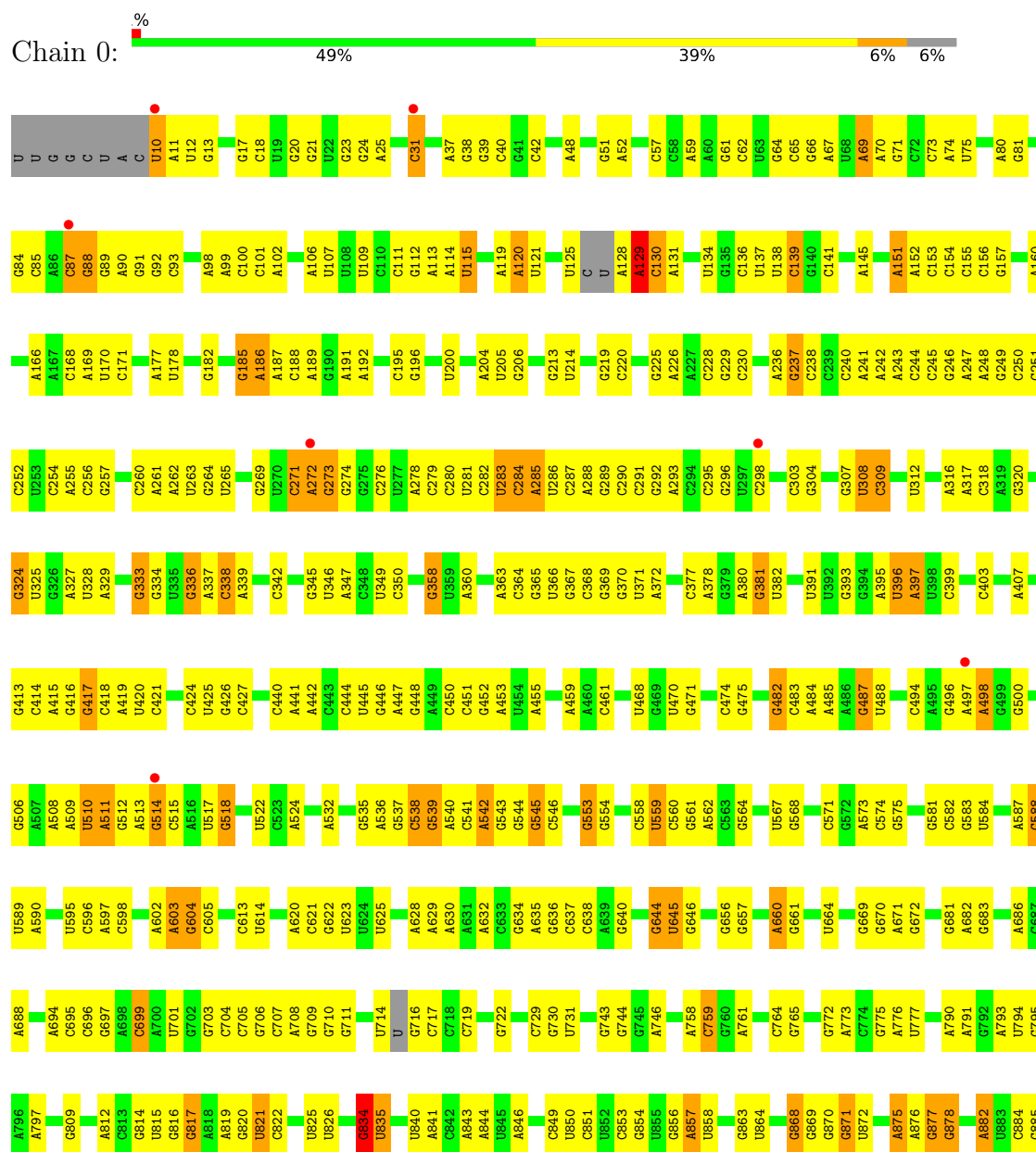
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	56	Total 56	O 56	0	0
38	Q	51	Total 51	O 51	0	0
38	R	80	Total 80	O 80	0	0
38	S	36	Total 36	O 36	0	0
38	T	33	Total 33	O 33	0	0
38	U	26	Total 26	O 26	0	0
38	V	11	Total 11	O 11	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	31	Total 31	O 31	0	0
38	1	56	Total 56	O 56	0	0
38	2	45	Total 45	O 45	0	0
38	3	66	Total 66	O 66	0	0
38	I	8	Total 8	O 8	0	0

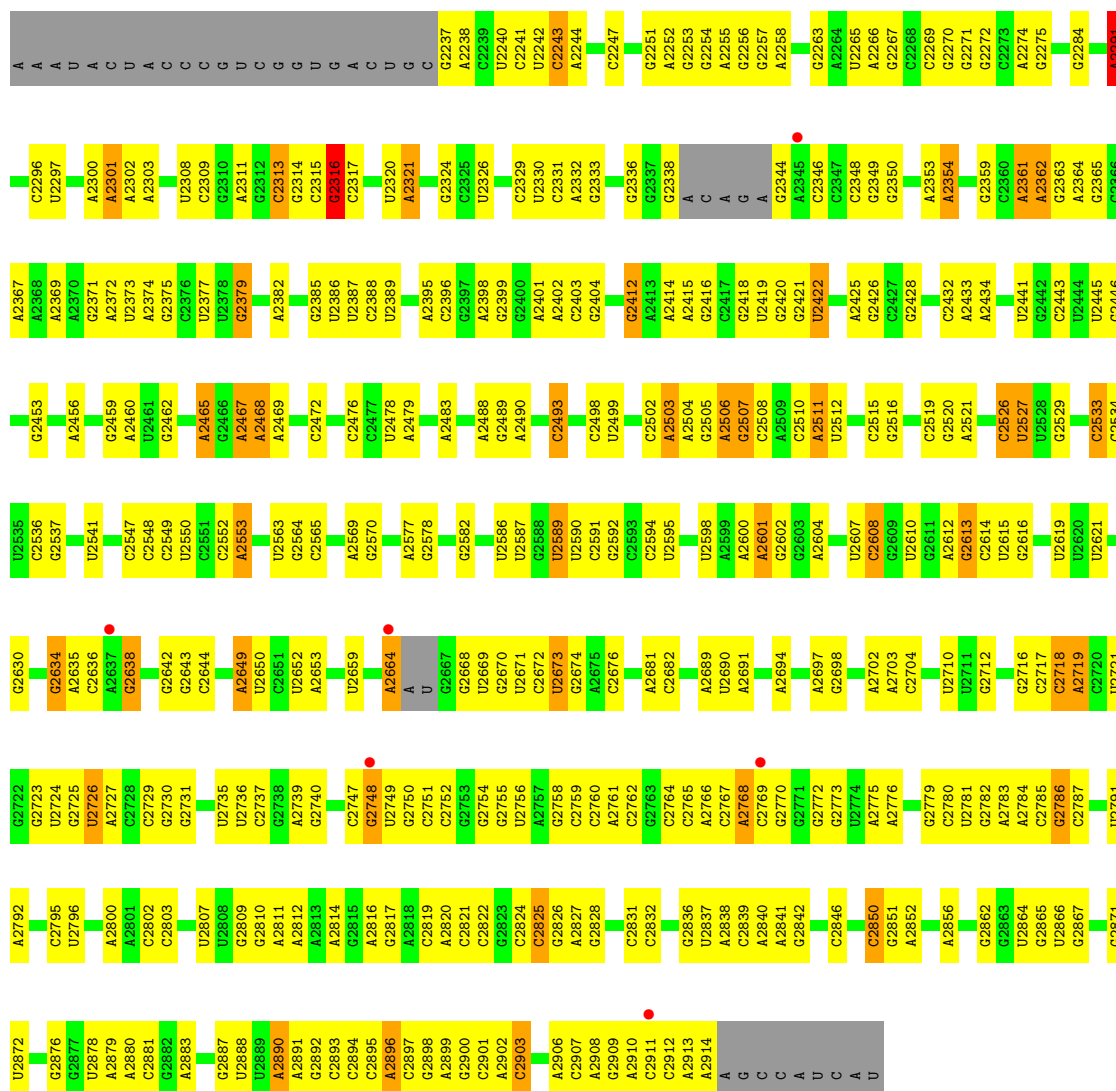
3 Residue-property plots

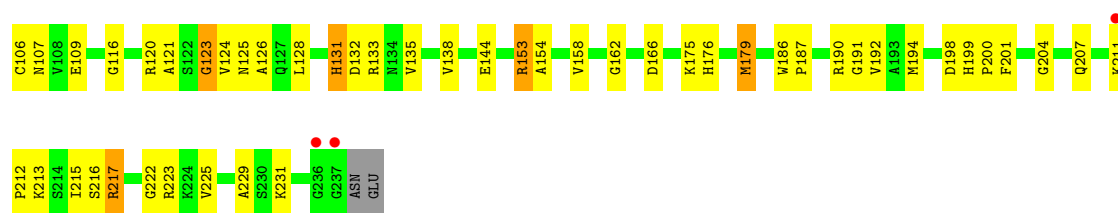
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

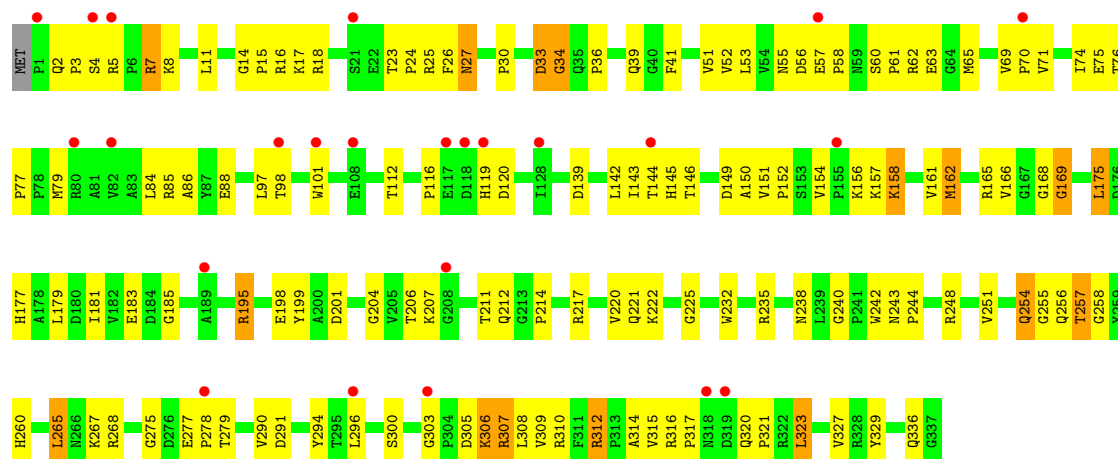


WORLDWIDE
PDB
PROTEIN DATA BANK

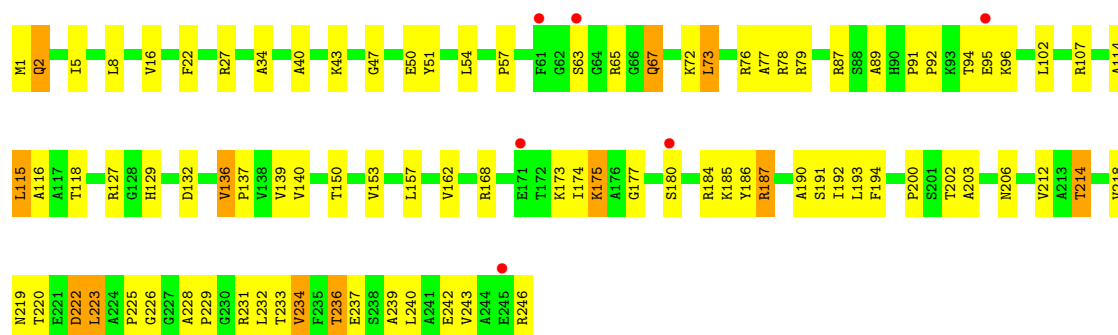




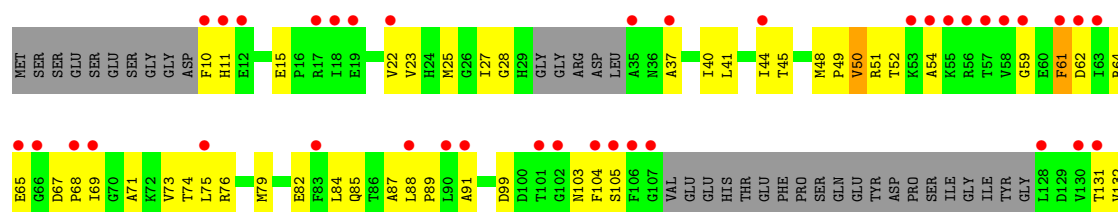
• Molecule 4: 50S ribosomal protein L3P

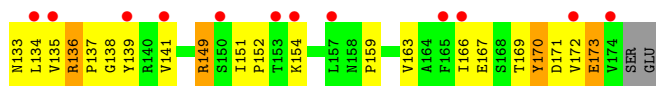


• Molecule 5: 50S ribosomal protein L4P

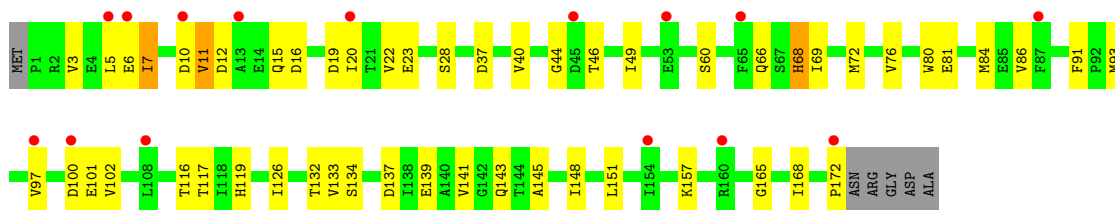


• Molecule 6: 50S ribosomal protein L5P

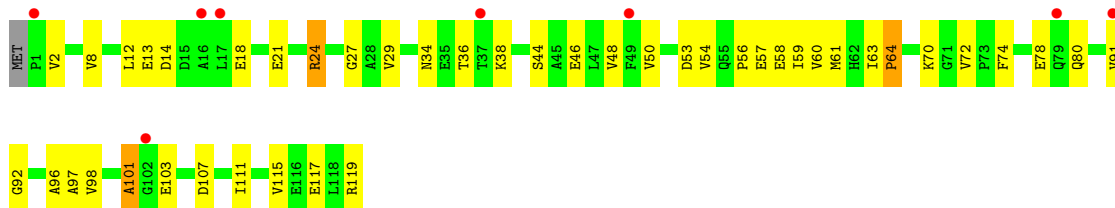




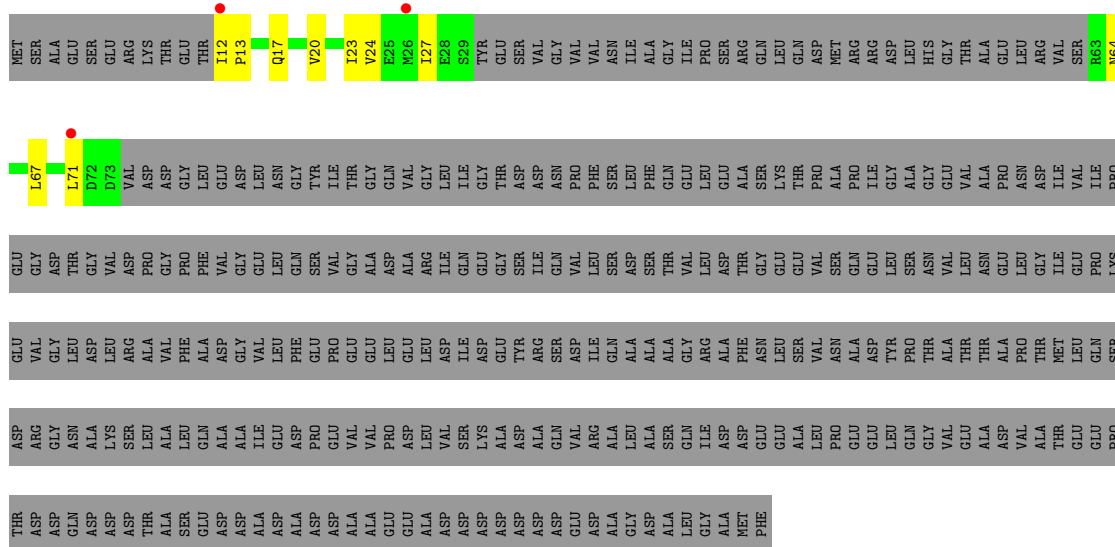
• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7Ae

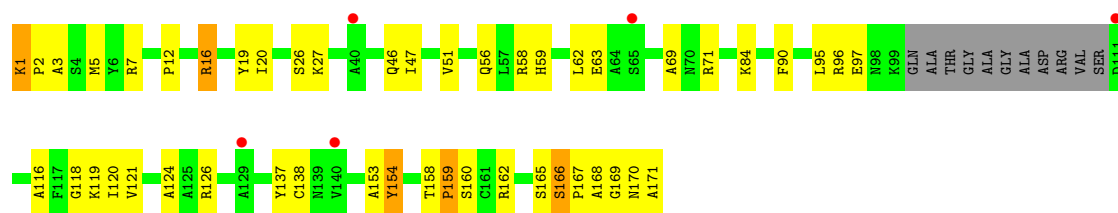


• Molecule 9: 50S ribosomal protein L10E

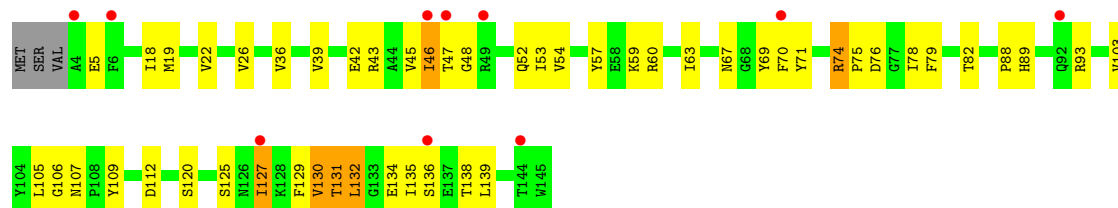


• Molecule 10: 50S ribosomal protein L10e

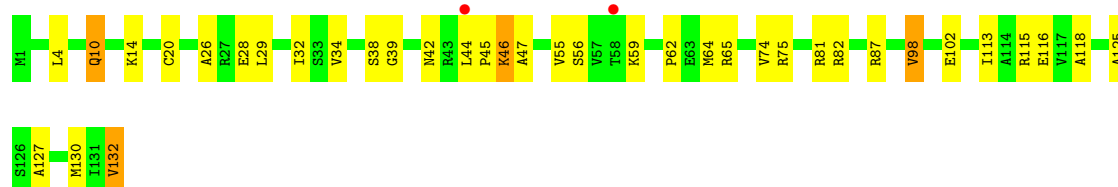
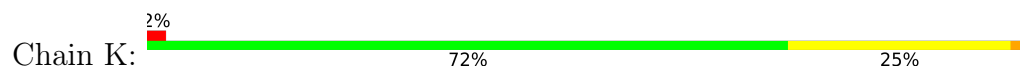




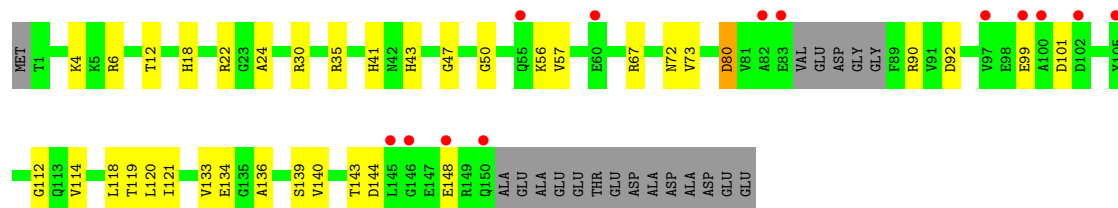
• Molecule 11: 50S ribosomal protein L13P



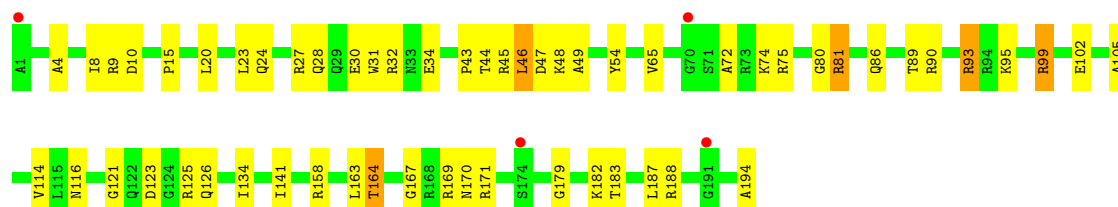
• Molecule 12: 50S ribosomal protein L14P



• Molecule 13: 50S ribosomal protein L15P

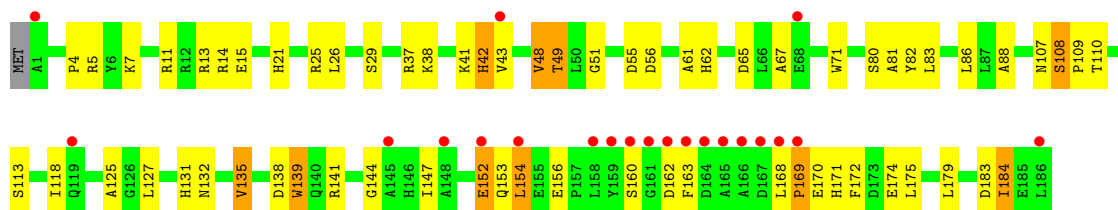


• Molecule 14: 50S ribosomal protein L15e



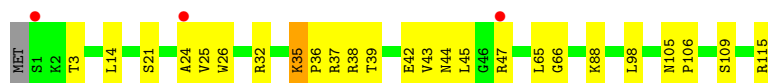
- Molecule 15: 50S ribosomal protein L18P

Chain N: 



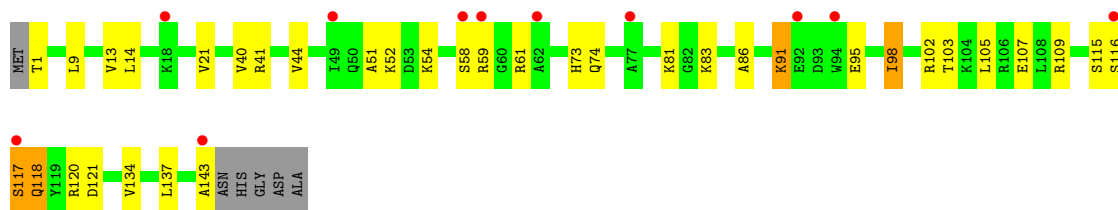
- Molecule 16: 50S ribosomal protein L18e

Chain O: 



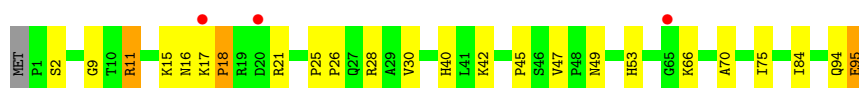
- Molecule 17: 50S ribosomal protein L19e

Chain P: 



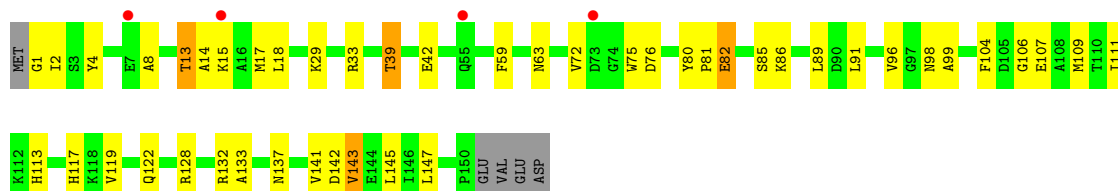
- Molecule 18: 50S ribosomal protein L21e

Chain Q: 

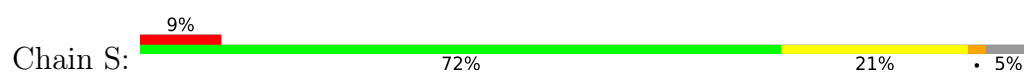


- Molecule 19: 50S ribosomal protein L22P

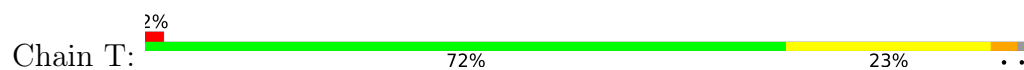
Chain R: 



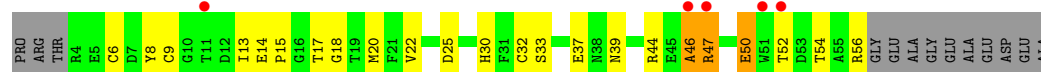
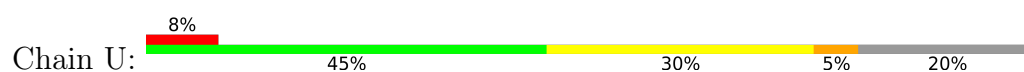
- Molecule 20: 50S ribosomal protein L23P



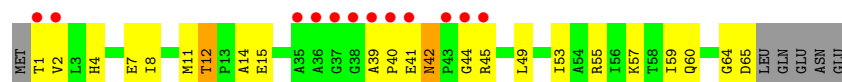
- Molecule 21: 50S ribosomal protein L24P



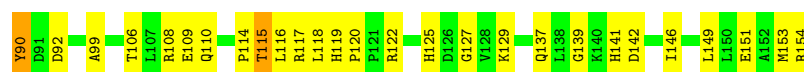
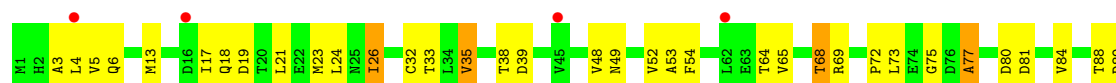
- Molecule 22: 50S ribosomal protein L24e



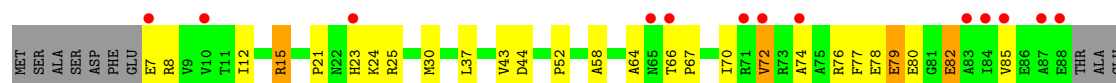
- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P

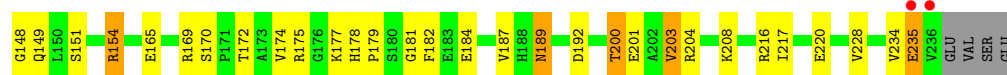


- Molecule 25: 50S ribosomal protein L31e

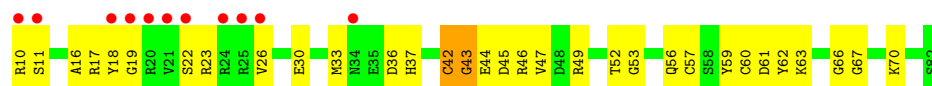


- Molecule 26: 50S ribosomal protein L32e





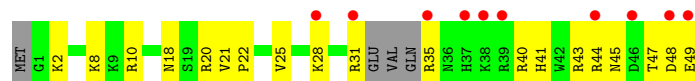
Chain Z: 15% 56% 41%



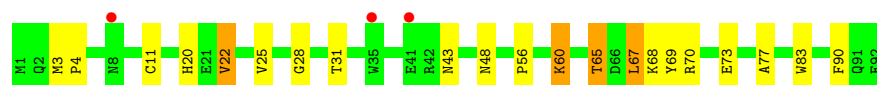
Chain 1: 63% 33% •



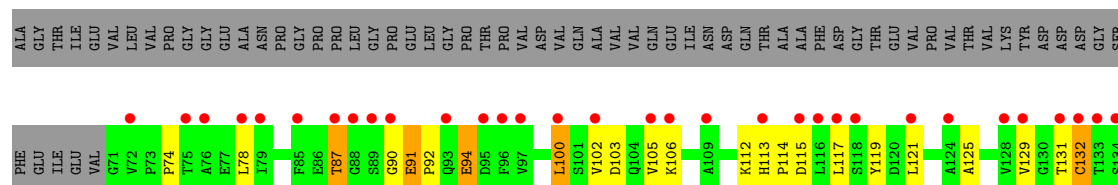
Chain 2:



Chain 3: 3% 77% 18%



Chain I:



L135	GLN	V137	I138	I139	E140	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	GLU	ALA	GLN	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 49.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 93.3 (49.70-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.238 0.211 , 0.244	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.1	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	99043	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 13T, 1MA, PSU, OMG, MG, K, OMU, NA, CL, UR3, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.39	0/65959	0.61	18/102870 (0.0%)
2	9	0.38	0/2905	0.60	2/4528 (0.0%)
3	A	0.46	0/1786	1.02	9/2408 (0.4%)
4	B	0.44	0/2690	1.03	18/3652 (0.5%)
5	C	0.48	0/1884	1.01	6/2551 (0.2%)
6	D	0.41	0/1111	0.96	5/1498 (0.3%)
7	E	0.41	0/1382	0.88	4/1880 (0.2%)
8	F	0.44	0/901	0.93	2/1224 (0.2%)
9	G	0.38	0/241	0.84	0/324
10	H	0.43	0/1287	0.99	10/1725 (0.6%)
11	J	0.43	0/1136	0.98	5/1530 (0.3%)
12	K	0.43	0/1001	0.99	1/1347 (0.1%)
13	L	0.41	0/1130	0.98	4/1509 (0.3%)
14	M	0.45	0/1584	0.93	5/2119 (0.2%)
15	N	0.38	0/1474	1.10	15/1999 (0.8%)
16	O	0.44	0/874	0.92	3/1181 (0.3%)
17	P	0.41	0/1147	0.89	1/1528 (0.1%)
18	Q	0.45	0/749	1.01	4/1005 (0.4%)
19	R	0.46	0/1172	0.95	3/1578 (0.2%)
20	S	0.39	0/648	0.89	2/875 (0.2%)
21	T	0.40	0/958	1.01	7/1289 (0.5%)
22	U	0.41	0/417	0.89	2/562 (0.4%)
23	V	0.44	0/502	1.05	2/675 (0.3%)
24	W	0.49	0/1219	1.00	5/1655 (0.3%)
25	X	0.44	0/664	0.97	3/895 (0.3%)
26	Y	0.45	0/1146	0.96	1/1536 (0.1%)
27	Z	0.41	0/590	0.98	1/787 (0.1%)
28	1	0.46	0/438	0.93	3/578 (0.5%)
29	2	0.46	0/401	0.82	0/529
30	3	0.41	0/771	0.82	3/1024 (0.3%)
31	I	0.47	0/526	1.08	4/716 (0.6%)
All	All	0.40	0/98693	0.73	148/147577 (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	1	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.74	130.11	109.50
17	P	118	GLN	N-CA-C	-8.86	101.70	111.36
1	0	1563	G	C4'-C3'-O3'	8.66	122.39	109.40
18	Q	17	LYS	N-CA-C	-8.39	99.52	109.93
21	T	52	ARG	N-CA-C	8.37	124.31	113.18
24	W	75	GLY	N-CA-C	8.15	119.69	111.95
3	A	222	GLY	N-CA-C	-8.07	104.20	114.37
4	B	222	LYS	N-CA-C	-7.92	99.11	110.59
4	B	175	LEU	N-CA-C	-7.91	102.60	111.14
15	N	51	GLY	CA-C-N	7.88	127.79	119.05
15	N	51	GLY	C-N-CA	7.88	127.79	119.05
15	N	169	PRO	N-CA-C	-7.79	104.12	113.86
6	D	170	TYR	N-CA-C	7.78	122.34	111.92
4	B	323	LEU	N-CA-C	7.26	119.94	110.43
10	H	160	SER	N-CA-C	-7.25	100.76	110.55
26	Y	143	TRP	N-CA-C	7.21	120.19	109.59
19	R	141	VAL	N-CA-C	7.16	118.79	108.48
6	D	136	ARG	CA-C-N	7.12	128.75	119.84
6	D	136	ARG	C-N-CA	7.12	128.75	119.84
3	A	48	ASP	CA-C-N	6.99	126.69	119.56
3	A	48	ASP	C-N-CA	6.99	126.69	119.56
2	9	3039	U	N1-C1'-C2'	6.97	122.45	112.00
31	I	91	GLU	CA-C-N	6.91	126.90	119.78
31	I	91	GLU	C-N-CA	6.91	126.90	119.78
10	H	1	LYS	CA-C-N	6.87	126.79	119.85
10	H	1	LYS	C-N-CA	6.87	126.79	119.85
21	T	3	GLN	CA-C-N	6.83	127.10	119.32
21	T	3	GLN	C-N-CA	6.83	127.10	119.32
14	M	89	THR	N-CA-C	6.83	118.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	80	ASP	N-CA-C	6.80	120.09	110.23
25	X	77	PHE	N-CA-C	6.68	116.69	107.73
10	H	7	ARG	N-CA-C	6.67	118.55	111.28
1	0	1942	A	C5'-C4'-C3'	6.61	125.92	116.00
1	0	920	C	C2'-C3'-O3'	-6.60	103.81	113.70
31	I	132	CYS	N-CA-C	6.58	118.14	110.97
15	N	135	VAL	N-CA-C	-6.57	106.27	113.43
14	M	121	GLY	N-CA-C	6.56	120.10	111.70
1	0	2316	G	C5'-C4'-C3'	-6.39	105.61	115.20
18	Q	47	VAL	CA-C-N	6.38	125.61	118.97
18	Q	47	VAL	C-N-CA	6.38	125.61	118.97
4	B	265	LEU	N-CA-C	6.36	118.92	110.53
7	E	11	VAL	N-CA-C	6.35	118.54	108.89
15	N	163	PHE	N-CA-C	-6.34	95.66	107.71
4	B	151	VAL	CA-C-N	6.31	125.88	119.19
4	B	151	VAL	C-N-CA	6.31	125.88	119.19
30	3	60	LYS	N-CA-C	-6.30	101.04	110.24
21	T	89	ARG	CA-C-N	6.29	126.32	119.90
21	T	89	ARG	C-N-CA	6.29	126.32	119.90
24	W	35	VAL	N-CA-C	6.29	115.09	107.61
5	C	191	SER	N-CA-C	6.27	113.92	108.78
15	N	14	ARG	N-CA-C	-6.25	104.38	111.07
14	M	125	ARG	N-CA-C	6.23	120.77	112.30
5	C	177	GLY	N-CA-C	6.16	118.32	112.04
13	L	47	GLY	N-CA-C	6.12	118.26	112.08
1	0	1504	A	N9-C1'-C2'	6.11	121.17	112.00
5	C	219	ASN	N-CA-C	6.08	118.44	109.69
13	L	57	VAL	N-CA-C	-6.05	106.86	112.43
15	N	48	VAL	N-CA-C	6.04	117.00	108.36
3	A	213	LYS	N-CA-C	6.04	118.83	111.82
30	3	43	ASN	N-CA-C	6.04	120.48	113.18
5	C	89	ALA	N-CA-C	6.01	118.35	111.02
21	T	78	THR	N-CA-C	6.00	117.70	109.18
23	V	42	ASN	CA-C-N	5.99	127.33	119.84
23	V	42	ASN	C-N-CA	5.99	127.33	119.84
18	Q	49	ASN	N-CA-C	5.98	118.63	110.55
11	J	71	TYR	CA-C-N	5.89	125.83	119.76
11	J	71	TYR	C-N-CA	5.89	125.83	119.76
25	X	12	ILE	N-CA-C	5.89	113.71	107.76
16	O	66	GLY	N-CA-C	5.86	127.06	113.18
15	N	108	SER	CA-C-N	5.86	127.16	119.84
15	N	108	SER	C-N-CA	5.86	127.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	35	LYS	CA-C-N	5.85	125.86	119.89
16	O	35	LYS	C-N-CA	5.85	125.86	119.89
11	J	67	ASN	N-CA-C	-5.84	104.99	111.36
5	C	175	LYS	N-CA-C	5.83	117.82	110.24
3	A	166	ASP	N-CA-C	5.83	117.63	111.28
28	1	21	ARG	N-CA-C	5.81	118.74	111.24
15	N	162	ASP	N-CA-C	5.80	118.91	108.17
1	0	2291	A	N9-C1'-C2'	5.80	120.70	112.00
1	0	2291	A	C4'-C3'-O3'	-5.79	104.31	113.00
4	B	120	ASP	CA-C-N	5.77	125.44	119.56
4	B	120	ASP	C-N-CA	5.77	125.44	119.56
1	0	1819	G	C5'-C4'-C3'	5.76	124.64	116.00
24	W	118	LEU	N-CA-C	5.74	117.47	110.41
10	H	116	ALA	N-CA-C	5.73	120.11	113.18
6	D	15	GLU	CA-C-N	5.68	126.95	119.84
6	D	15	GLU	C-N-CA	5.68	126.95	119.84
20	S	27	ALA	N-CA-C	-5.66	98.53	108.20
1	0	1592	G	N9-C1'-C2'	5.65	120.47	112.00
3	A	133	ARG	N-CA-C	-5.63	106.45	113.38
1	0	2726	U	N1-C1'-C2'	5.62	120.44	112.00
14	M	74	LYS	N-CA-C	5.60	118.53	109.40
28	1	54	ALA	N-CA-C	5.58	118.08	111.33
1	0	2301	A	N9-C1'-C2'	5.57	120.36	112.00
28	1	43	ALA	N-CA-C	-5.55	105.31	111.36
15	N	42	HIS	N-CA-C	5.55	117.84	109.41
5	C	192	ILE	N-CA-C	5.52	116.71	109.21
4	B	161	VAL	N-CA-C	5.51	116.32	107.73
1	0	1559	A	C2'-C3'-O3'	5.49	121.94	113.70
8	F	8	VAL	CA-C-N	5.49	125.41	119.76
8	F	8	VAL	C-N-CA	5.49	125.41	119.76
7	E	7	ILE	N-CA-C	5.49	113.35	108.63
21	T	54	ASP	N-CA-C	-5.48	106.10	112.89
10	H	90	PHE	CA-C-N	5.47	126.68	119.84
10	H	90	PHE	C-N-CA	5.47	126.68	119.84
27	Z	18	TYR	N-CA-C	5.47	122.44	110.80
11	J	22	VAL	N-CA-C	-5.45	105.19	110.42
15	N	13	ARG	N-CA-C	-5.45	106.77	113.41
20	S	59	ASP	N-CA-C	-5.44	105.86	112.88
3	A	135	VAL	N-CA-C	5.41	116.46	108.45
15	N	153	GLN	N-CA-C	-5.41	104.01	111.81
14	M	8	ILE	N-CA-C	-5.41	105.45	110.53
15	N	168	LEU	N-CA-C	5.39	120.39	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	158	LYS	CA-C-N	5.38	125.32	119.78
4	B	158	LYS	C-N-CA	5.38	125.32	119.78
30	3	67	LEU	N-CA-C	5.36	118.32	109.85
24	W	68	THR	N-CA-C	5.36	118.03	111.82
1	0	834	G	C2'-C3'-O3'	-5.35	105.68	113.70
4	B	303	GLY	CA-C-N	5.31	126.59	120.85
4	B	303	GLY	C-N-CA	5.31	126.59	120.85
22	U	46	ALA	N-CA-C	5.31	117.75	111.33
22	U	50	GLU	N-CA-C	5.31	117.75	111.33
2	9	3065	A	N9-C1'-C2'	5.31	119.96	112.00
4	B	217	ARG	N-CA-C	5.29	117.13	111.36
31	I	94	GLU	N-CA-C	-5.28	107.39	113.88
3	A	198	ASP	N-CA-C	5.27	119.80	112.90
3	A	123	GLY	N-CA-C	5.24	122.34	115.47
24	W	115	THR	N-CA-C	5.24	117.44	108.90
12	K	46	LYS	N-CA-C	5.24	118.65	110.32
10	H	118	GLY	N-CA-C	5.24	119.24	112.54
19	R	122	GLN	N-CA-C	-5.23	99.99	108.41
11	J	112	ASP	N-CA-C	-5.19	101.24	109.96
4	B	143	ILE	N-CA-C	-5.19	102.04	108.89
15	N	131	HIS	N-CA-C	5.16	115.09	108.34
4	B	157	LYS	N-CA-C	-5.14	107.67	114.04
19	R	137	ASN	N-CA-C	5.11	118.03	110.46
7	E	157	LYS	N-CA-C	5.10	117.16	109.41
4	B	154	VAL	CA-C-N	5.10	124.71	119.05
4	B	154	VAL	C-N-CA	5.10	124.71	119.05
10	H	158	THR	N-CA-C	5.10	119.88	113.25
25	X	79	GLU	N-CA-C	5.09	118.75	112.54
1	0	1878	G	O4'-C1'-C2'	-5.09	102.51	107.60
1	0	2313	C	O4'-C4'-C3'	-5.07	98.93	104.00
13	L	12	THR	N-CA-C	5.07	119.33	113.20
7	E	119	HIS	N-CA-C	5.07	116.56	108.41
10	H	159	PRO	N-CA-C	5.04	118.63	111.13
1	0	206	G	C5'-C4'-C3'	-5.03	108.45	116.00
1	0	129	A	C2'-C3'-O3'	5.02	121.23	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1131	G	Sidechain
1	0	1309	U	Sidechain
1	0	131	A	Sidechain
1	0	1376	G	Sidechain
1	0	1445	G	Sidechain
1	0	1458	A	Sidechain
1	0	1635	U	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	1993	C	Sidechain
1	0	220	C	Sidechain
1	0	2308	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	2552	C	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	391	U	Sidechain
1	0	396	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
2	9	3039	U	Sidechain

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Mol	Chain	Res	Type	Group
2	9	3090	G	Sidechain
24	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1341	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	81	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	76	0
6	D	1094	0	1085	57	0
7	E	1357	0	1266	41	0
8	F	890	0	843	33	0
9	G	240	0	231	9	0
10	H	1266	0	1268	40	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	41	0
13	L	1118	0	1076	29	0
14	M	1560	0	1568	46	0
15	N	1445	0	1401	47	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	45	0
20	S	641	0	605	15	0
21	T	950	0	923	25	0
22	U	410	0	364	23	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	23	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	20	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	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	2	0	0	0	0
35	0	74	0	0	2	0
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	1	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	9	0	0	2	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	2	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	8	0
38	B	142	0	0	20	0
38	C	170	0	0	17	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2297) 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)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H5'	1:0:871:G:H8	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5''	1.37	1.07
1:0:1474:C:H6	1:0:1474:C:H5'	1.16	1.06
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.34	1.05
1:0:1242:A:H5'	11:J:82:THR:HG23	1.34	1.04
1:0:541:C:H2'	1:0:542:A:H5''	1.41	1.03
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.41	1.02
1:0:542:A:H5'	1:0:542:A:H8	1.25	1.01
1:0:1559:A:H1'	38:0:5876:HOH:O	1.59	1.01
1:0:2717:C:C2'	1:0:2718:C:H5''	1.91	1.01
1:0:381:G:H5''	38:0:4329:HOH:O	1.61	1.00
4:B:62:ARG:HA	4:B:65:MET:HE3	1.43	1.00
1:0:1474:C:H5'	1:0:1474:C:C6	1.99	0.98
1:0:1701:A:H4'	1:0:1702:U:H5''	1.44	0.98
1:0:1666:C:O2'	1:0:1667:A:H5''	1.64	0.98
1:0:1162:G:H1'	31:I:117:LEU:HD11	1.45	0.98
1:0:156:C:H5''	14:M:171:ARG:HD3	1.41	0.97
1:0:1118:A:H62	1:0:1244:U:H3	1.09	0.97
1:0:2717:C:H2'	1:0:2718:C:H5''	1.46	0.96
1:0:2460:A:H5'	32:0:9000:13T:C23	1.96	0.96
2:9:3092:G:H2'	2:9:3093:A:C8	2.01	0.96
2:9:3076:G:H3'	2:9:3077:A:H5''	1.43	0.95
5:C:236:THR:HG22	5:C:239:ALA:H	1.28	0.95
1:0:871:G:H8	1:0:871:G:C5'	1.80	0.95
10:H:166:SER:HB2	10:H:167:PRO:HD3	1.49	0.94
1:0:1205:U:H2'	1:0:1206:U:H5''	1.50	0.94
1:0:2460:A:H5'	32:0:9000:13T:H233	1.46	0.93
1:0:1667:A:H8	1:0:1667:A:H5'	1.34	0.93
29:2:41:HIS:H	29:2:45:ASN:HD22	1.16	0.93
26:Y:200:THR:HG22	26:Y:201:GLU:HG3	1.49	0.93
1:0:289:G:H22	1:0:363:A:H2	0.97	0.93
1:0:1172:G:H5''	38:0:7252:HOH:O	1.69	0.93
1:0:877:G:H5'	1:0:878:G:OP1	1.69	0.93
24:W:149:LEU:HG	24:W:153:MET:HE2	1.49	0.93
1:0:282:C:H1'	1:0:368:C:N4	1.84	0.93
1:0:545:G:H5'	1:0:545:G:H8	1.34	0.92
1:0:1372:A:H3'	38:0:7182:HOH:O	1.69	0.92
1:0:2710:U:H1'	38:0:7605:HOH:O	1.68	0.92
12:K:10:GLN:HE21	12:K:10:GLN:H	0.93	0.92
1:0:2506:A:HO2'	1:0:2507:G:H8	0.93	0.92
1:0:506:G:H22	1:0:509:A:C5'	1.82	0.91
1:0:1118:A:C8	1:0:1118:A:H3'	2.05	0.91
1:0:1118:A:H3'	1:0:1118:A:H8	1.33	0.91
1:0:2812:A:H2	1:0:2814:A:H62	1.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:C2'	1:0:542:A:H5''	1.99	0.91
1:0:870:G:H2'	1:0:871:G:H5''	1.50	0.90
1:0:1184:C:H1'	38:0:7452:HOH:O	1.70	0.90
1:0:1603:A:H5'	1:0:1605:G:O4'	1.72	0.90
1:0:93:C:H5''	23:V:1:THR:HB	1.51	0.90
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.54	0.89
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.53	0.89
24:W:5:VAL:HG11	24:W:153:MET:HE1	1.52	0.89
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.54	0.89
1:0:2529:G:H3'	38:0:7177:HOH:O	1.70	0.89
1:0:289:G:N2	1:0:363:A:H2	1.70	0.89
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.55	0.88
1:0:317:A:H4'	38:0:3775:HOH:O	1.73	0.88
17:P:115:SER:H	17:P:118:GLN:HE21	1.20	0.88
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.56	0.88
1:0:1209:C:H2'	1:0:1210:G:H8	1.39	0.87
1:0:2508:C:H2'	38:0:6748:HOH:O	1.72	0.87
1:0:1165:G:H4'	1:0:1174:A:O2'	1.74	0.87
1:0:506:G:H22	1:0:509:A:H5''	1.37	0.87
2:9:3049:G:H5''	38:N:8842:HOH:O	1.73	0.87
1:0:1641:A:H2'	1:0:1642:A:H5'	1.55	0.86
8:F:58:GLU:HA	8:F:61:MET:HE2	1.57	0.86
1:0:1116:U:H3	1:0:1246:A:H62	1.21	0.86
1:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.84
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.84
1:0:1701:A:H5'	38:0:6285:HOH:O	1.77	0.84
12:K:10:GLN:HE21	12:K:10:GLN:N	1.76	0.84
1:0:2769:C:C2'	1:0:2770:G:H5'	2.08	0.84
12:K:10:GLN:H	12:K:10:GLN:NE2	1.76	0.84
1:0:182:G:H5'	38:0:5159:HOH:O	1.78	0.83
1:0:2291:A:C8	1:0:2309:C:H5'	2.13	0.83
1:0:21:G:H5'	19:R:2:ILE:HA	1.61	0.83
1:0:272:A:H3'	38:0:7515:HOH:O	1.79	0.83
1:0:272:A:H5'	1:0:273:G:OP2	1.79	0.83
15:N:113:SER:HB2	38:N:8855:HOH:O	1.78	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.76	0.83
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.25	0.83
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.61	0.83
1:0:282:C:O2'	1:0:283:U:H5'	1.79	0.83
2:9:3056:A:C2'	2:9:3057:A:H5''	2.09	0.83
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.42	0.82
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.61	0.82
1:0:559:U:H6	1:0:559:U:H5'	1.44	0.82
1:0:69:A:H5'	1:0:69:A:C8	2.14	0.82
1:0:797:A:H4'	27:Z:10:ARG:N	1.94	0.82
24:W:88:THR:HB	38:W:6679:HOH:O	1.79	0.82
1:0:1183:C:H2'	38:0:6249:HOH:O	1.79	0.81
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.62	0.81
1:0:1187:U:HO2'	1:0:1189:A:H2	1.26	0.81
38:0:5223:HOH:O	12:K:39:GLY:HA2	1.81	0.81
4:B:221:GLN:HE22	12:K:42:ASN:HD22	1.23	0.81
1:0:236:A:H4'	1:0:237:G:H5'	1.63	0.81
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.62	0.81
1:0:2717:C:O2'	1:0:2718:C:H5''	1.80	0.81
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.62	0.80
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.29	0.80
1:0:515:C:H5''	38:0:5657:HOH:O	1.81	0.80
3:A:199:HIS:HD2	3:A:201:PHE:H	1.27	0.80
1:0:558:C:O2'	1:0:559:U:H5''	1.81	0.80
1:0:1160:G:H5'	1:0:1161:A:H5'	0.88	0.80
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.64	0.80
1:0:541:C:H2'	1:0:542:A:C5'	2.12	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.79
1:0:1835:U:H5	1:0:1840:A:N7	1.79	0.79
1:0:1206:U:H5'	1:0:1206:U:H6	1.47	0.79
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.63	0.79
1:0:292:G:H2'	1:0:358:G:N2	1.97	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.61	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.63	0.79
1:0:2716:G:H5''	4:B:206:THR:HG21	1.63	0.79
12:K:98:VAL:HG13	12:K:102:GLU:HA	1.64	0.79
1:0:1615:A:H5'	38:0:4195:HOH:O	1.83	0.79
1:0:2054:A:N3	19:R:128:ARG:NH2	2.30	0.79
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.18	0.79
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.79
1:0:1119:G:N2	1:0:1246:A:C2	2.51	0.79
1:0:1667:A:H5'	1:0:1667:A:C8	2.18	0.79
20:S:57:THR:HG22	20:S:59:ASP:H	1.48	0.79
27:Z:46:ARG:HD3	27:Z:59:TYR:HB2	1.64	0.79
1:0:1002:G:C2'	1:0:1003:U:H5''	2.13	0.78
1:0:1741:U:H5'	1:0:1742:A:OP1	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:13:MET:HE3	24:W:17:ILE:HG22	1.66	0.78
1:0:1441:G:H1'	38:0:7748:HOH:O	1.82	0.78
32:0:9000:13T:H262	32:0:9000:13T:H2	1.65	0.78
1:0:514:G:H4'	38:0:5657:HOH:O	1.83	0.78
1:0:1919:A:H4'	38:0:4858:HOH:O	1.83	0.78
1:0:1878:G:H1'	38:0:6128:HOH:O	1.83	0.78
1:0:1666:C:C2'	1:0:1667:A:H5''	2.14	0.78
1:0:2908:A:H2'	1:0:2909:G:O4'	1.83	0.78
1:0:681:G:N3	1:0:681:G:H5'	1.99	0.77
1:0:871:G:C8	1:0:871:G:C5'	2.59	0.77
1:0:1474:C:H6	1:0:1474:C:C5'	1.97	0.77
1:0:21:G:C5'	19:R:2:ILE:HA	2.13	0.77
1:0:130:C:H2'	38:0:3162:HOH:O	1.84	0.77
1:0:2426:G:H1'	38:0:6098:HOH:O	1.85	0.77
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.66	0.77
1:0:1679:C:H5'	38:0:9320:HOH:O	1.85	0.77
1:0:542:A:H5'	1:0:542:A:C8	2.15	0.77
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.66	0.77
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.50	0.77
5:C:127:ARG:NH2	5:C:225:PRO:HG2	2.00	0.77
32:0:9000:13T:H21	32:0:9000:13T:C30	2.14	0.76
1:0:1205:U:H2'	1:0:1206:U:C5'	2.15	0.76
32:0:9000:13T:H262	32:0:9000:13T:C2	2.14	0.76
1:0:2769:C:H2'	1:0:2770:G:H5'	1.68	0.76
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.66	0.76
6:D:154:LYS:H	6:D:154:LYS:HD2	1.50	0.76
1:0:12:U:H2'	1:0:13:G:H5'	1.67	0.76
1:0:1603:A:H5''	1:0:1605:G:H5'	1.67	0.75
1:0:1058:A:H2'	1:0:1060:C:H5''	1.67	0.75
1:0:1701:A:H4'	1:0:1702:U:C5'	2.15	0.75
1:0:2851:G:O2'	1:0:2852:A:H5'	1.87	0.75
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.66	0.75
1:0:2502:C:C2'	1:0:2503:A:H5'	2.16	0.74
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.68	0.74
1:0:558:C:C2'	1:0:559:U:H5''	2.17	0.74
1:0:2010:A:H2'	38:0:5968:HOH:O	1.86	0.74
1:0:2570:G:H5''	38:0:4917:HOH:O	1.86	0.74
1:0:2766:A:H5'	38:B:8824:HOH:O	1.87	0.74
1:0:1205:U:C2'	1:0:1206:U:H5''	2.18	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.31	0.74
1:0:2005:G:H3'	1:0:2005:G:OP2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2768:A:O2'	1:0:2769:C:H5'	1.86	0.74
1:0:396:U:H1'	38:0:7612:HOH:O	1.88	0.74
1:0:899:C:H5'	38:0:3205:HOH:O	1.86	0.74
24:W:84:VAL:HG12	38:W:6679:HOH:O	1.88	0.74
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.68	0.74
1:0:949:U:H4'	18:Q:95:GLU:HA	1.68	0.74
1:0:69:A:H5'	1:0:69:A:H8	1.52	0.74
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.70	0.74
1:0:711:G:H1'	38:0:7092:HOH:O	1.87	0.73
1:0:797:A:C4'	27:Z:10:ARG:N	2.51	0.73
1:0:1926:G:H2'	1:0:1927:A:H8	1.53	0.73
1:0:2768:A:H2'	1:0:2769:C:O4'	1.87	0.73
2:9:3014:G:H5'	2:9:3014:G:H8	1.51	0.73
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.86	0.73
1:0:2578:G:H5'	1:0:2578:G:H8	1.53	0.73
1:0:961:A:H4'	38:0:6766:HOH:O	1.89	0.73
1:0:2468:A:H61	30:3:48:ASN:HD21	1.35	0.73
3:A:35:GLY:O	3:A:36:ASP:HB3	1.87	0.73
1:0:2748:G:H1'	38:0:7883:HOH:O	1.87	0.73
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.71	0.73
3:A:51:ARG:HB2	38:A:8897:HOH:O	1.89	0.73
11:J:127:ILE:HG22	36:J:8801:CL:CL	2.25	0.73
22:U:14:GLU:O	22:U:17:THR:HB	1.88	0.73
1:0:288:A:H61	1:0:364:C:H42	1.36	0.73
1:0:544:G:H2'	1:0:545:G:H5''	1.70	0.72
5:C:233:THR:HG22	5:C:234:VAL:H	1.54	0.72
1:0:545:G:H5'	1:0:545:G:C8	2.22	0.72
1:0:587:A:H5''	38:0:7279:HOH:O	1.89	0.72
1:0:2781:U:C2'	1:0:2782:G:H5'	2.19	0.72
1:0:1926:G:H2'	1:0:1927:A:C8	2.24	0.72
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.07	0.72
1:0:2781:U:H2'	1:0:2782:G:H5'	1.70	0.72
1:0:1634:G:H3'	38:0:3901:HOH:O	1.89	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.17	0.72
1:0:1080:C:H4'	1:0:1081:A:OP1	1.89	0.72
1:0:1350:U:H4'	38:0:5124:HOH:O	1.88	0.72
1:0:1593:C:H5'	17:P:116:SER:O	1.89	0.71
1:0:2505:G:O2'	1:0:2506:A:H5'	1.89	0.71
1:0:2507:G:H2'	1:0:2510:C:H42	1.55	0.71
1:0:2243:C:H5''	38:0:3753:HOH:O	1.88	0.71
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:3759:HOH:O	21:T:9:LYS:HD3	1.88	0.71
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.55	0.71
1:O:1189:A:H1'	1:O:1209:C:C1'	2.19	0.71
1:O:1189:A:H1'	1:O:1209:C:O4'	1.91	0.71
1:O:2420:G:O2'	1:O:2421:G:H5'	1.90	0.71
1:O:2827:A:H2'	1:O:2828:G:O4'	1.90	0.71
1:O:2862:G:H4'	4:B:336:GLN:O	1.91	0.71
1:O:2878:U:H2'	1:O:2879:A:O4'	1.90	0.71
16:O:32:ARG:HE	16:O:35:LYS:HD2	1.56	0.71
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.73	0.71
2:9:3039:U:H3'	2:9:3040:C:H5''	1.73	0.71
1:O:156:C:H5''	14:M:171:ARG:CD	2.19	0.71
1:O:308:U:H5'	1:O:309:C:OP1	1.90	0.71
1:O:271:C:H41	1:O:378:A:H2	1.36	0.70
1:O:2717:C:H2'	1:O:2718:C:C5'	2.21	0.70
5:C:236:THR:HG22	5:C:239:ALA:N	2.04	0.70
13:L:133:VAL:HA	38:L:8872:HOH:O	1.90	0.70
1:O:1342:C:C2'	1:O:1343:C:H5'	2.20	0.70
1:O:2364:A:H5''	18:Q:15:LYS:HD3	1.73	0.70
19:R:81:PRO:O	19:R:85:SER:HB2	1.91	0.70
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.72	0.70
1:O:214:U:H5'	38:O:6147:HOH:O	1.91	0.70
1:O:2526:C:O2'	1:O:2527:U:H5'	1.91	0.70
1:O:544:G:C2'	1:O:545:G:H5''	2.22	0.70
3:A:191:GLY:HA2	3:A:194:MET:CE	2.22	0.69
1:O:962:C:H1'	15:N:5:ARG:NH1	2.07	0.69
17:P:115:SER:H	17:P:118:GLN:NE2	1.90	0.69
1:O:2748:G:H2'	38:O:7526:HOH:O	1.91	0.69
17:P:143:ALA:HA	38:P:5521:HOH:O	1.93	0.69
24:W:72:PRO:HG2	24:W:77:ALA:HB3	1.74	0.69
1:O:338:C:H4'	5:C:174:ILE:CD1	2.21	0.69
1:O:2748:G:H5'	38:O:7526:HOH:O	1.92	0.69
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.74	0.69
1:O:960:G:H4'	38:O:7420:HOH:O	1.92	0.69
1:O:1299:G:O6	13:L:6:ARG:HD3	1.92	0.69
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.74	0.69
24:W:80:ASP:O	24:W:84:VAL:HG23	1.92	0.69
1:O:559:U:H5'	1:O:559:U:C6	2.27	0.69
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.73	0.69
6:D:103:ASN:ND2	6:D:134:LEU:H	1.90	0.69
1:O:2004:U:H4'	38:O:5313:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:88:THR:HG22	24:W:89:ASP:H	1.58	0.69
1:0:558:C:H2'	1:0:559:U:C5'	2.23	0.69
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.08	0.69
4:B:238:ASN:HD22	4:B:240:GLY:H	1.41	0.69
1:0:560:C:H42	1:0:597:A:H61	1.39	0.68
1:0:1189:A:H3'	38:0:7666:HOH:O	1.93	0.68
1:0:1242:A:H5'	11:J:82:THR:CG2	2.18	0.68
1:0:657:G:OP1	5:C:27:ARG:NH2	2.26	0.68
32:0:9000:13T:H21	32:0:9000:13T:H301	1.74	0.68
1:0:821:U:H2'	1:0:822:C:H6	1.57	0.68
1:0:1641:A:C2'	1:0:1642:A:H5'	2.23	0.68
36:0:8813:CL:CL	38:0:4691:HOH:O	2.48	0.68
2:9:3054:A:O2'	2:9:3055:U:H5'	1.94	0.68
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.94	0.68
10:H:166:SER:HB2	10:H:167:PRO:CD	2.21	0.68
1:0:1183:C:H42	1:0:1184:C:H41	1.42	0.68
1:0:2635:A:O2'	1:0:2636:C:H5'	1.94	0.68
3:A:199:HIS:CD2	3:A:201:PHE:H	2.10	0.68
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.75	0.68
1:0:1244:U:OP1	11:J:18:ILE:HD13	1.93	0.68
1:0:2459:G:H2'	32:0:9000:13T:C23	2.24	0.68
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.22	0.68
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.76	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.93	0.68
1:0:2812:A:C2	1:0:2814:A:N6	2.55	0.68
24:W:125:HIS:HD2	24:W:127:GLY:H	1.40	0.68
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.68
14:M:134:ILE:HG23	14:M:141:ILE:HD13	1.76	0.68
1:0:138:U:H5''	1:0:139:C:OP2	1.95	0.67
1:0:500:G:H21	19:R:98:ASN:HD21	1.41	0.67
1:0:2374:A:H2'	1:0:2375:G:C8	2.29	0.67
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.67
29:2:35:ARG:HB2	38:2:2691:HOH:O	1.95	0.67
1:0:1189:A:O2'	1:0:1208:C:H2'	1.95	0.67
1:0:1213:C:O2'	1:0:1214:G:H5'	1.94	0.67
1:0:506:G:H22	1:0:509:A:H5'	1.57	0.67
1:0:1118:A:N6	1:0:1244:U:H3	1.87	0.67
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.29	0.67
23:V:57:LYS:HA	23:V:60:GLN:HE21	1.60	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.28	0.67
11:J:107:ASN:HD22	11:J:109:TYR:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:OP1	4:B:207:LYS:HG3	1.95	0.67
11:J:76:ASP:HA	38:J:8868:HOH:O	1.94	0.67
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.77	0.67
1:0:1973:A:H5'	1:0:1973:A:H8	1.59	0.67
1:0:280:C:H2'	1:0:281:U:O4'	1.95	0.66
1:0:2563:U:H2'	1:0:2565:C:O5'	1.96	0.66
4:B:267:LYS:HD3	38:B:8824:HOH:O	1.95	0.66
1:0:2100:A:H5'	38:C:8662:HOH:O	1.93	0.66
1:0:2256:G:H2'	1:0:2257:G:C5'	2.25	0.66
1:0:485:A:N3	1:0:487:G:H5''	2.10	0.66
11:J:74:ARG:HB3	11:J:74:ARG:HH11	1.61	0.66
27:Z:10:ARG:HA	38:Z:8715:HOH:O	1.96	0.66
1:0:284:C:H4'	1:0:285:A:O5'	1.96	0.66
1:0:2256:G:H2'	1:0:2257:G:H5'	1.78	0.66
1:0:2489:G:H1'	38:0:7268:HOH:O	1.95	0.66
5:C:1:MET:HG2	5:C:2:GLN:H	1.61	0.66
30:3:73:GLU:HB3	38:3:8854:HOH:O	1.94	0.66
1:0:1162:G:H1'	31:I:117:LEU:CD1	2.24	0.66
1:0:1209:C:H2'	1:0:1210:G:C8	2.26	0.66
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.96	0.66
1:0:1524:U:OP1	1:0:1524:U:H4'	1.94	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.72	0.66
1:0:2521:A:OP2	10:H:3:ALA:HB3	1.96	0.66
1:0:694:A:H2'	1:0:695:C:H5'	1.77	0.66
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.78	0.66
19:R:99:ALA:HB1	19:R:109:MET:CE	2.26	0.66
1:0:21:G:H5''	19:R:1:GLY:O	1.97	0.65
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.61	0.65
1:0:2638:G:H1'	38:0:7742:HOH:O	1.96	0.65
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.25	0.65
2:9:3029:C:C2'	2:9:3030:C:H5'	2.26	0.65
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.31	0.65
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.79	0.65
1:0:2460:A:C5'	32:0:9000:13T:H233	2.23	0.65
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.26	0.65
1:0:136:C:H2'	1:0:137:U:O4'	1.97	0.65
1:0:2890:A:H1'	22:U:56:ARG:NH2	2.11	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.95	0.65
5:C:140:VAL:HB	38:C:8651:HOH:O	1.94	0.65
1:0:1666:C:H2'	1:0:1667:A:C5'	2.26	0.65
1:0:447:A:O2'	1:0:448:G:H5'	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.65
1:0:2414:A:H2'	1:0:2415:A:C8	2.31	0.65
1:0:407:A:H8	38:0:4466:HOH:O	1.79	0.65
1:0:584:U:H3'	38:0:6101:HOH:O	1.96	0.65
1:0:1187:U:O2'	1:0:1189:A:H2	1.78	0.65
1:0:2795:C:O2'	1:0:2796:U:H5'	1.96	0.65
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.79	0.65
2:9:3003:A:N6	2:9:3022:G:H1'	2.12	0.65
1:0:1701:A:H5''	1:0:1702:U:H3'	1.77	0.65
1:0:2320:U:H4'	1:0:2321:A:O4'	1.97	0.64
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.62	0.64
10:H:169:GLY:HA3	38:H:8591:HOH:O	1.95	0.64
1:0:403:C:H3'	38:0:6307:HOH:O	1.97	0.64
1:0:1342:C:H2'	1:0:1343:C:H5'	1.79	0.64
1:0:2241:C:O2'	1:0:2242:U:H5'	1.96	0.64
1:0:2787:C:H5	38:0:4641:HOH:O	1.80	0.64
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.28	0.64
24:W:88:THR:HG23	24:W:110:GLN:HE21	1.62	0.64
1:0:281:U:O2'	1:0:282:C:H5'	1.96	0.64
1:0:441:A:H1'	1:0:442:A:N7	2.13	0.64
1:0:2896:A:H5''	38:0:6105:HOH:O	1.97	0.64
6:D:99:ASP:HB3	6:D:103:ASN:H	1.62	0.64
1:0:958:G:H2'	1:0:959:C:C6	2.32	0.64
38:0:4678:HOH:O	4:B:300:SER:HB3	1.97	0.64
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.79	0.64
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.32	0.64
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.79	0.64
2:9:3091:C:H2'	2:9:3092:G:O4'	1.97	0.64
3:A:121:ALA:O	3:A:124:VAL:HG22	1.97	0.64
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.27	0.64
1:0:1185:U:H2'	1:0:1186:C:C6	2.33	0.64
1:0:2459:G:H2'	32:0:9000:13T:H233	1.80	0.64
1:0:2769:C:O2'	1:0:2770:G:H5'	1.96	0.64
1:0:1044:C:H5	38:0:6599:HOH:O	1.81	0.64
2:9:3048:C:H4'	15:N:141:ARG:HH21	1.63	0.64
2:9:3039:U:H1'	2:9:3044:A:H61	1.63	0.64
11:J:19:MET:HE2	11:J:79:PHE:HA	1.80	0.64
23:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.64
14:M:23:LEU:HD13	14:M:27:ARG:NH2	2.12	0.63
1:0:1200:A:H3'	38:0:5765:HOH:O	1.98	0.63
1:0:1790:C:H2'	1:0:1791:U:H6	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:H2'	1:0:2770:G:C5'	2.27	0.63
2:9:3007:G:H5'	38:9:5071:HOH:O	1.98	0.63
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.45	0.63
5:C:236:THR:HG21	38:C:8571:HOH:O	1.98	0.63
13:L:114:VAL:HG11	38:L:8872:HOH:O	1.99	0.63
1:0:157:G:H4'	14:M:95:LYS:HE2	1.79	0.63
1:0:1165:G:H1'	1:0:1174:A:H1'	1.79	0.63
1:0:1189:A:H1'	1:0:1209:C:H1'	1.79	0.63
4:B:36:PRO:HG3	4:B:169:GLY:H	1.62	0.63
10:H:166:SER:CB	10:H:167:PRO:HD3	2.27	0.63
16:O:47:ARG:HH11	16:O:47:ARG:HG3	1.63	0.63
18:Q:26:PRO:O	18:Q:30:VAL:HG23	1.98	0.63
1:0:1185:U:H5'	38:0:7452:HOH:O	1.98	0.63
1:0:1211:G:H2'	1:0:1212:C:H6	1.63	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.99	0.63
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.81	0.63
1:0:447:A:P	21:T:1:SER:HB2	2.39	0.63
13:L:148:GLU:HB2	38:L:8889:HOH:O	1.99	0.63
27:Z:57:CYS:SG	27:Z:59:TYR:HB3	2.38	0.63
1:0:20:G:H21	19:R:117:HIS:HD2	1.47	0.63
4:B:71:VAL:HG21	4:B:296:LEU:HB3	1.81	0.63
24:W:13:MET:HE2	24:W:18:GLN:HA	1.81	0.63
1:0:289:G:O2'	1:0:290:C:H5'	1.99	0.63
1:0:567:U:H5''	38:0:6400:HOH:O	1.98	0.62
1:0:1164:U:H3	1:0:1192:A:H2	1.46	0.62
1:0:1666:C:C2'	1:0:1667:A:C5'	2.77	0.62
1:0:1878:G:O2'	1:0:1879:U:C6	2.49	0.62
1:0:1313:A:H5'	26:Y:208:LYS:O	1.99	0.62
2:9:3092:G:H2'	2:9:3093:A:H8	1.58	0.62
1:0:951:A:C2'	1:0:952:G:H5'	2.29	0.62
1:0:1307:A:H2'	1:0:1308:A:C8	2.34	0.62
1:0:1666:C:H2'	1:0:1667:A:H5'	1.81	0.62
5:C:67:GLN:HG2	38:C:8624:HOH:O	2.00	0.62
18:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
1:0:396:U:O2'	1:0:418:C:H4'	1.99	0.62
1:0:1537:C:H1'	38:0:6583:HOH:O	1.98	0.62
2:9:3036:C:C5	2:9:3037:C:C5	2.88	0.62
1:0:292:G:H2'	1:0:358:G:H22	1.65	0.62
1:0:1377:C:H5'	1:0:1377:C:H6	1.64	0.62
1:0:1667:A:H2'	1:0:1668:U:C6	2.34	0.62
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:80:SER:HB2	38:N:8832:HOH:O	1.99	0.62
1:0:960:G:N3	1:0:960:G:H2'	2.13	0.62
1:0:1625:U:H4'	38:0:4674:HOH:O	2.00	0.62
25:X:43:VAL:HG12	25:X:44:ASP:N	2.15	0.62
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.62
1:0:1636:G:O2'	1:0:1637:A:H5'	1.99	0.62
1:0:2256:G:C2'	1:0:2257:G:H5'	2.29	0.62
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.81	0.62
14:M:99:ARG:HH21	14:M:170:ASN:HD22	1.48	0.62
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.82	0.62
1:0:558:C:C2'	1:0:559:U:C5'	2.78	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.82	0.61
23:V:39:ALA:N	23:V:40:PRO:HD2	2.14	0.61
1:0:656:G:H5'	16:O:3:THR:HB	1.80	0.61
35:L:8580:NA:NA	38:L:8826:HOH:O	1.71	0.61
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.82	0.61
1:0:597:A:H2'	1:0:598:C:H6	1.65	0.61
35:0:8542:NA:NA	38:0:5663:HOH:O	1.71	0.61
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.80	0.61
23:V:55:ARG:O	23:V:59:ILE:HG12	1.99	0.61
1:0:308:U:C4	1:0:342:C:H1'	2.35	0.61
1:0:470:U:O2'	28:1:16:HIS:HD2	1.82	0.61
1:0:1406:A:H4'	1:0:1407:A:H5''	1.81	0.61
1:0:1528:A:H2'	1:0:1529:G:O4'	2.00	0.61
1:0:1603:A:C5'	1:0:1605:G:H5'	2.30	0.61
1:0:2445:U:H2'	1:0:2446:G:C8	2.36	0.61
1:0:2511:A:H2'	1:0:2512:U:O4'	2.00	0.61
23:V:1:THR:HG23	23:V:2:VAL:H	1.65	0.61
1:0:538:C:OP2	26:Y:134:HIS:HE1	1.84	0.61
1:0:1234:U:N3	4:B:244:PRO:HB3	2.15	0.61
1:0:2338:G:H1'	6:D:105:SER:OG	1.99	0.61
38:0:7359:HOH:O	12:K:45:PRO:HB2	2.01	0.61
12:K:81:ARG:HD3	12:K:87:ARG:NH2	2.15	0.61
18:Q:21:ARG:HA	38:Q:6597:HOH:O	2.00	0.61
1:0:128:A:O2'	1:0:129:A:H5'	2.01	0.61
2:9:3041:C:O4'	6:D:50:VAL:HG22	2.00	0.61
1:0:1477:C:H5'	1:0:1868:G:C5'	2.30	0.61
2:9:3064:C:H2'	2:9:3065:A:H5'	1.83	0.61
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.82	0.61
1:0:281:U:H2'	1:0:282:C:O4'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2507:G:H2'	1:0:2510:C:N4	2.16	0.61
2:9:3064:C:C2'	2:9:3065:A:H5'	2.31	0.61
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.82	0.61
24:W:137:GLN:NE2	24:W:141:HIS:HE1	1.98	0.61
1:0:1762:C:H2'	1:0:1763:C:H6	1.65	0.61
1:0:2433:A:H2'	1:0:2434:A:C8	2.36	0.61
10:H:27:LYS:H	10:H:59:HIS:CD2	2.19	0.61
1:0:656:G:OP2	16:O:37:ARG:HD2	2.00	0.60
1:0:2134:G:N2	1:0:2242:U:C2	2.69	0.60
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.81	0.60
1:0:517:U:H1'	38:0:7561:HOH:O	2.00	0.60
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.60
2:9:3006:C:H5''	15:N:37:ARG:HH12	1.62	0.60
1:0:338:C:H4'	5:C:174:ILE:HD11	1.83	0.60
20:S:11:THR:H	20:S:14:ALA:HB3	1.65	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.01	0.60
1:0:669:G:O2'	1:0:670:G:H5'	2.01	0.60
1:0:2659:U:H5''	38:0:4135:HOH:O	2.00	0.60
32:0:9000:13T:H262	32:0:9000:13T:O3	2.01	0.60
29:2:20:ARG:HG2	29:2:21:VAL:H	1.66	0.60
30:3:65:THR:HG23	30:3:67:LEU:HG	1.84	0.60
1:0:255:A:H2'	1:0:256:C:C6	2.36	0.60
1:0:1118:A:C8	1:0:1118:A:C3'	2.70	0.60
27:Z:11:SER:HB3	27:Z:23:ARG:HB2	1.83	0.60
1:0:510:U:H6	38:0:7427:HOH:O	1.85	0.60
1:0:602:A:O2'	1:0:605:C:H4'	2.01	0.60
1:0:1819:G:H2'	1:0:1820:G:H4'	1.83	0.60
1:0:512:G:O3'	1:0:513:A:H8	1.85	0.60
1:0:2359:G:H3'	38:0:5701:HOH:O	2.01	0.60
14:M:187:LEU:CD2	14:M:194:ALA:HB3	2.32	0.60
3:A:48:ASP:HB3	38:A:8897:HOH:O	2.02	0.60
1:0:255:A:H2'	1:0:256:C:H6	1.66	0.59
1:0:2301:A:H5''	1:0:2302:A:H5'	1.84	0.59
4:B:214:PRO:HD2	38:B:8820:HOH:O	2.02	0.59
6:D:65:GLU:HA	38:D:4069:HOH:O	2.02	0.59
6:D:103:ASN:ND2	6:D:133:ASN:HA	2.17	0.59
27:Z:22:SER:O	27:Z:26:VAL:HG23	2.01	0.59
1:0:450:C:OP1	5:C:184:ARG:NH2	2.34	0.59
1:0:1202:A:H2'	1:0:1203:G:H5'	1.85	0.59
1:0:1266:U:H4'	26:Y:115:ARG:HH21	1.66	0.59
1:0:1525:G:H5'	1:0:1526:A:OP2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:50:VAL:O	6:D:71:ALA:HA	2.02	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.02	0.59
32:0:9000:13T:H3	30:3:56:PRO:HB2	1.83	0.59
2:9:3039:U:H3'	2:9:3040:C:C5'	2.32	0.59
4:B:86:ALA:HA	38:B:8876:HOH:O	2.01	0.59
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.83	0.59
14:M:114:VAL:HG23	36:M:8818:CL:CL	2.39	0.59
19:R:111:ILE:HG23	19:R:145:LEU:HD11	1.83	0.59
27:Z:42:CYS:SG	27:Z:43:GLY:N	2.75	0.59
1:0:1504:A:H5'	38:0:4423:HOH:O	2.02	0.59
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.33	0.59
1:0:966:U:H5'	38:0:3861:HOH:O	2.01	0.59
1:0:1060:C:H6	1:0:1060:C:H5'	1.65	0.59
1:0:2807:U:P	4:B:27:ASN:HD21	2.24	0.59
8:F:58:GLU:CD	14:M:27:ARG:HH22	2.10	0.59
11:J:45:VAL:HG21	11:J:129:PHE:CD1	2.38	0.59
1:0:249:G:O2'	1:0:250:C:H5'	2.03	0.59
1:0:1163:G:H2'	1:0:1164:U:C5	2.37	0.59
23:V:12:THR:HG23	23:V:14:ALA:H	1.68	0.59
1:0:1167:G:O2'	1:0:1168:C:H5'	2.02	0.59
1:0:1183:C:N3	1:0:1184:C:C5	2.71	0.59
1:0:1736:A:H1'	38:0:7569:HOH:O	2.03	0.59
7:E:100:ASP:HB2	38:E:2789:HOH:O	2.02	0.59
23:V:49:LEU:O	23:V:53:ILE:HG13	2.01	0.59
1:0:39:G:N2	1:0:444:C:C2	2.71	0.59
1:0:84:G:O2'	1:0:85:C:H5'	2.02	0.59
1:0:2781:U:H2'	1:0:2782:G:C5'	2.31	0.59
38:0:9354:HOH:O	28:1:1:THR:HA	2.03	0.59
10:H:3:ALA:HA	10:H:58:ARG:HH12	1.67	0.59
14:M:30:GLU:O	14:M:34:GLU:HG3	2.02	0.59
19:R:104:PHE:HB3	19:R:109:MET:HE2	1.83	0.59
1:0:121:U:OP2	29:2:10:ARG:NH2	2.35	0.59
1:0:947:U:H2'	1:0:948:G:C8	2.38	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
27:Z:44:GLU:HG2	27:Z:46:ARG:HD2	1.85	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.34	0.59
35:0:8542:NA:NA	38:0:3317:HOH:O	1.75	0.59
1:0:364:C:H2'	1:0:365:G:O4'	2.03	0.58
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.84	0.58
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.85	0.58
1:0:1014:A:H2'	1:0:1015:C:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1015:C:H2'	1:0:1016:U:H6	1.67	0.58
1:0:2676:C:H4'	11:J:70:PHE:HE1	1.66	0.58
11:J:107:ASN:ND2	11:J:109:TYR:H	2.01	0.58
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.85	0.58
31:I:132:CYS:HB3	31:I:137:VAL:HB	1.83	0.58
1:0:1202:A:C2'	1:0:1203:G:H5'	2.33	0.58
1:0:2252:A:C5	1:0:2253:G:H1'	2.36	0.58
5:C:139:VAL:HG13	38:C:8648:HOH:O	2.02	0.58
8:F:117:GLU:C	8:F:119:ARG:H	2.10	0.58
25:X:43:VAL:HG12	25:X:44:ASP:H	1.69	0.58
19:R:14:ALA:HB3	19:R:147:LEU:HB2	1.86	0.58
1:0:1377:C:H5'	1:0:1377:C:C6	2.38	0.58
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.84	0.58
5:C:180:SER:HB2	38:C:8645:HOH:O	2.02	0.58
2:9:3035:C:H5''	38:9:4078:HOH:O	2.03	0.58
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.85	0.58
16:O:42:GLU:HB2	38:O:2176:HOH:O	2.04	0.58
24:W:21:LEU:HD21	24:W:48:VAL:CG1	2.32	0.58
1:0:42:C:H3'	38:0:4179:HOH:O	2.03	0.58
1:0:87:C:H2'	29:2:28:LYS:O	2.04	0.58
1:0:1168:C:H4'	38:I:5128:HOH:O	2.04	0.58
1:0:2816:A:H5''	1:0:2817:G:H5'	1.86	0.58
13:L:136:ALA:HB3	38:L:8872:HOH:O	2.03	0.58
4:B:25:ARG:HA	4:B:310:ARG:HH21	1.68	0.58
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.31	0.58
13:L:143:THR:HG22	13:L:144:ASP:N	2.18	0.58
1:0:282:C:H1'	1:0:368:C:H42	1.69	0.58
1:0:661:G:C5	1:0:686:A:C2	2.92	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.58
1:0:2703:A:H2'	1:0:2704:C:H6	1.67	0.58
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.85	0.58
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.86	0.58
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.84	0.58
11:J:103:VAL:HG12	38:J:8868:HOH:O	2.03	0.58
15:N:144:GLY:O	15:N:147:ILE:HG22	2.02	0.58
1:0:875:A:C2	3:A:194:MET:SD	2.97	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
2:9:3057:A:H8	6:D:141:VAL:HG21	1.69	0.57
8:F:53:ASP:OD1	8:F:80:GLN:HB2	2.05	0.57
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.44	0.57
1:0:1183:C:H2'	1:0:1183:C:O2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:68:HIS:O	7:E:72:MET:HG3	2.04	0.57
10:H:63:GLU:HA	38:H:8582:HOH:O	2.03	0.57
1:0:2498:C:O2'	1:0:2499:U:H5'	2.04	0.57
38:0:7344:HOH:O	26:Y:149:GLN:HG3	2.02	0.57
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.70	0.57
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.68	0.57
11:J:131:THR:HB	11:J:134:GLU:HG3	1.85	0.57
1:0:877:G:C5'	1:0:878:G:OP1	2.49	0.57
1:0:2478:U:O2'	1:0:2479:A:H5'	2.04	0.57
4:B:258:GLY:H	4:B:260:HIS:CE1	2.21	0.57
1:0:1202:A:H2'	1:0:1203:G:C5'	2.34	0.57
1:0:1226:G:H5'	38:0:4537:HOH:O	2.05	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.57
1:0:1972:U:H2'	1:0:1973:A:C5'	2.35	0.57
1:0:2256:G:O2'	1:0:2257:G:H5'	2.04	0.57
2:9:3072:C:O2'	2:9:3073:G:H5'	2.05	0.57
14:M:24:GLN:NE2	14:M:27:ARG:HH11	2.02	0.57
1:0:31:C:H2'	38:0:7673:HOH:O	2.03	0.57
1:0:92:G:H4'	23:V:44:GLY:HA3	1.87	0.57
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.05	0.57
24:W:13:MET:HE2	24:W:18:GLN:CA	2.35	0.57
30:3:70:ARG:HG2	30:3:77:ALA:HB2	1.85	0.57
1:0:671:A:O2'	1:0:672:G:H2'	2.05	0.57
23:V:64:GLY:O	23:V:65:ASP:HB2	2.03	0.57
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.85	0.57
1:0:1028:U:H1'	38:0:3649:HOH:O	2.04	0.57
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.70	0.57
2:9:3095:C:O2'	2:9:3096:C:H5'	2.05	0.57
4:B:254:GLN:HG2	4:B:255:GLY:N	2.19	0.57
1:0:88:G:H8	1:0:88:G:H5'	1.70	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.40	0.57
1:0:1118:A:H8	1:0:1119:G:H5''	1.69	0.57
1:0:1291:A:H2	38:0:5297:HOH:O	1.86	0.57
1:0:1393:A:H2'	1:0:1394:C:C6	2.40	0.57
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.39	0.57
2:9:3091:C:H1'	38:9:7454:HOH:O	2.04	0.57
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.03	0.57
30:3:11:CYS:HB2	30:3:20:HIS:CE1	2.40	0.57
1:0:2781:U:O2'	1:0:2782:G:H5'	2.05	0.57
4:B:152:PRO:HA	38:B:8866:HOH:O	2.04	0.57
10:H:138:CYS:HB2	38:H:8544:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
1:0:1193:A:C2	1:0:1194:A:N6	2.73	0.56
1:0:2291:A:N9	1:0:2309:C:H5'	2.20	0.56
2:9:3052:A:H2'	2:9:3053:G:O4'	2.05	0.56
1:0:564:G:H1'	38:0:6311:HOH:O	2.03	0.56
2:9:3057:A:C8	6:D:141:VAL:HG21	2.40	0.56
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.87	0.56
4:B:225:GLY:HA3	38:B:8863:HOH:O	2.05	0.56
10:H:26:SER:HA	10:H:59:HIS:HD2	1.70	0.56
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.56
1:0:2385:G:H2'	1:0:2386:U:C6	2.40	0.56
1:0:2445:U:H2'	1:0:2446:G:H8	1.69	0.56
1:0:2604:A:H5'	38:0:5801:HOH:O	2.05	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.56
2:9:3044:A:O4'	6:D:76:ARG:NE	2.38	0.56
3:A:99:ILE:O	3:A:131:HIS:HE1	1.87	0.56
21:T:64:ASN:HB3	21:T:73:HIS:HB2	1.88	0.56
24:W:139:GLY:O	24:W:141:HIS:HD2	1.89	0.56
26:Y:187:VAL:HG23	26:Y:192:ASP:HB3	1.86	0.56
26:Y:189:ASN:C	26:Y:189:ASN:HD22	2.14	0.56
1:0:941:G:O2'	1:0:942:U:H5'	2.04	0.56
15:N:147:ILE:HB	38:N:8842:HOH:O	2.04	0.56
1:0:1154:A:H2'	1:0:1155:G:C8	2.40	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.06	0.56
4:B:254:GLN:HG3	38:B:8828:HOH:O	2.06	0.56
8:F:91:VAL:HG12	8:F:92:GLY:N	2.20	0.56
20:S:43:GLU:HB3	38:S:8546:HOH:O	2.04	0.56
1:0:776:A:OP1	28:1:28:HIS:HE1	1.87	0.56
1:0:870:G:OP2	3:A:3:ARG:HD3	2.06	0.56
1:0:1717:A:H5''	17:P:54:LYS:HB2	1.88	0.56
38:0:5467:HOH:O	9:G:12:ILE:HA	2.05	0.56
1:0:111:C:O2'	28:1:20:ARG:HG2	2.06	0.56
1:0:380:A:OP2	14:M:9:ARG:HD2	2.06	0.56
1:0:821:U:H5''	38:0:3050:HOH:O	2.05	0.56
1:0:1181:A:C2	1:0:1192:A:C8	2.94	0.56
1:0:1329:A:H2	38:0:4691:HOH:O	1.89	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.06	0.56
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.88	0.56
12:K:29:LEU:HB3	12:K:55:VAL:CG1	2.31	0.56
16:O:32:ARG:O	16:O:32:ARG:HD3	2.05	0.56
24:W:88:THR:HG23	24:W:110:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:43:VAL:HG11	25:X:82:GLU:HA	1.86	0.56
1:0:573:A:O2'	1:0:574:C:H5'	2.06	0.56
1:0:1167:G:H4'	31:I:135:LEU:HD22	1.88	0.56
1:0:1527:A:H1'	1:0:1528:A:C8	2.41	0.56
1:0:2403:C:H2'	1:0:2404:G:O5'	2.06	0.56
19:R:119:VAL:HG21	19:R:142:ASP:CG	2.31	0.56
22:U:47:ARG:HG2	38:U:4381:HOH:O	2.05	0.56
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.71	0.56
1:0:1167:G:H2'	1:0:1168:C:O4'	2.06	0.56
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.38	0.56
1:0:2255:A:N1	1:0:2256:G:C4	2.74	0.56
5:C:114:ALA:HB1	5:C:223:LEU:HB3	1.88	0.56
21:T:71:VAL:HG11	21:T:90:PRO:CB	2.33	0.56
1:0:21:G:H4'	19:R:2:ILE:HG22	1.88	0.56
1:0:1172:G:H1'	38:0:4978:HOH:O	2.05	0.56
38:0:9539:HOH:O	17:P:81:LYS:HG2	2.05	0.56
2:9:3006:C:C5'	15:N:37:ARG:NH1	2.58	0.56
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.87	0.56
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.88	0.56
1:0:1168:C:H5''	31:I:87:THR:HG22	1.88	0.55
1:0:1377:C:H2'	1:0:1723:G:O6	2.06	0.55
2:9:3106:C:O2'	2:9:3107:C:H5'	2.07	0.55
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.36	0.55
5:C:65:ARG:HG3	5:C:67:GLN:HB2	1.88	0.55
11:J:107:ASN:HD22	11:J:107:ASN:C	2.14	0.55
1:0:333:G:O2'	1:0:334:G:H5'	2.06	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.89	0.55
6:D:159:PRO:O	6:D:163:VAL:HG23	2.06	0.55
1:0:1309:U:O2'	1:0:1310:U:H5'	2.06	0.55
38:0:6860:HOH:O	3:A:211:LYS:HD3	2.07	0.55
6:D:149:ARG:HH12	15:N:15:GLU:HA	1.72	0.55
20:S:57:THR:HG22	20:S:59:ASP:N	2.18	0.55
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.05	0.55
25:X:74:ALA:HB2	25:X:85:VAL:HG13	1.88	0.55
1:0:2839:C:H2'	1:0:2840:A:H5''	1.88	0.55
2:9:3001:U:H5''	2:9:3003:A:OP1	2.07	0.55
24:W:6:GLN:HB2	24:W:26:ILE:CD1	2.36	0.55
1:0:1873:G:H3'	38:0:5213:HOH:O	2.06	0.55
24:W:88:THR:HG22	24:W:89:ASP:N	2.20	0.55
26:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:O2'	13:L:41:HIS:CD2	2.60	0.55
1:0:1169:U:H2'	1:0:1170:U:O4'	2.07	0.55
1:0:1180:U:H2'	1:0:1181:A:O4'	2.07	0.55
5:C:246:ARG:NE	38:C:8623:HOH:O	2.38	0.55
7:E:137:ASP:O	7:E:141:VAL:HG23	2.06	0.55
8:F:27:GLY:HA3	8:F:101:ALA:O	2.07	0.55
19:R:99:ALA:HB1	19:R:109:MET:HE1	1.88	0.55
22:U:52:THR:CG2	22:U:54:THR:HB	2.37	0.55
1:0:553:G:P	26:Y:204:ARG:HH22	2.30	0.55
1:0:960:G:N3	1:0:960:G:C2'	2.69	0.55
1:0:1687:C:O2	28:1:9:GLY:HA2	2.06	0.55
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.88	0.55
1:0:88:G:H2'	1:0:89:G:C8	2.41	0.55
1:0:559:U:H6	1:0:559:U:C5'	2.18	0.55
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.07	0.55
1:0:958:G:H2'	1:0:959:C:H6	1.72	0.55
1:0:1132:A:N6	1:0:1229:C:H2'	2.22	0.55
5:C:77:ALA:O	5:C:78:ARG:HD2	2.06	0.55
29:2:20:ARG:HG2	29:2:21:VAL:N	2.22	0.55
1:0:941:G:C5	1:0:942:U:C4	2.95	0.55
1:0:947:U:H2'	1:0:948:G:H8	1.70	0.55
1:0:1118:A:C8	1:0:1119:G:H5''	2.41	0.55
1:0:856:G:C8	38:0:5435:HOH:O	2.54	0.55
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.55
1:0:1741:U:HO2'	1:0:2723:G:H4'	1.71	0.55
3:A:97:ALA:HA	3:A:131:HIS:HE2	1.71	0.55
5:C:236:THR:H	5:C:239:ALA:HB3	1.72	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.54
1:0:1790:C:H2'	1:0:1791:U:C6	2.40	0.54
1:0:2456:A:H5'	38:0:5705:HOH:O	2.06	0.54
38:0:4844:HOH:O	11:J:47:THR:HB	2.07	0.54
5:C:129:HIS:HE1	5:C:231:ARG:HA	1.69	0.54
1:0:120:A:H2'	1:0:120:A:N3	2.22	0.54
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.54
24:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.54
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.87	0.54
1:0:255:A:C5	1:0:256:C:C4	2.96	0.54
1:0:468:U:H3'	38:0:7553:HOH:O	2.07	0.54
1:0:1137:G:H1'	38:0:3885:HOH:O	2.07	0.54
1:0:1588:G:C6	1:0:1589:G:N1	2.75	0.54
3:A:33:GLU:O	3:A:34:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:24:GLN:HE22	14:M:27:ARG:HH11	1.55	0.54
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.88	0.54
31:I:113:HIS:N	31:I:114:PRO:HD2	2.22	0.54
1:O:2266:A:OP2	14:M:90:ARG:NH2	2.41	0.54
1:O:2425:A:H2'	38:O:9228:HOH:O	2.06	0.54
1:O:2780:C:H1'	7:E:143:GLN:NE2	2.22	0.54
1:O:2826:G:C6	1:O:2913:A:N6	2.75	0.54
2:9:3076:G:C3'	2:9:3077:A:H5''	2.30	0.54
38:9:3472:HOH:O	15:N:41:LYS:HD3	2.08	0.54
19:R:39:THR:HB	19:R:42:GLU:HG3	1.90	0.54
19:R:111:ILE:HG23	19:R:145:LEU:CD1	2.37	0.54
1:O:226:A:H1'	1:O:393:G:C5	2.43	0.54
1:O:705:C:O2	1:O:705:C:H2'	2.08	0.54
1:O:2718:C:H6	1:O:2718:C:H5'	1.73	0.54
5:C:22:PHE:HA	5:C:116:ALA:HA	1.88	0.54
5:C:233:THR:HG22	5:C:234:VAL:N	2.21	0.54
8:F:29:VAL:HG12	8:F:98:VAL:HA	1.90	0.54
21:T:53:GLY:HA3	38:T:6384:HOH:O	2.08	0.54
1:O:506:G:N2	1:O:509:A:H5''	2.16	0.54
1:O:1171:A:H2'	1:O:1172:G:H5'	1.90	0.54
1:O:1595:G:O2'	1:O:1596:U:H5'	2.08	0.54
1:O:1603:A:H5'	1:O:1605:G:C4'	2.38	0.54
1:O:1783:A:O2'	1:O:1784:U:H5'	2.08	0.54
1:O:2001:G:O2'	1:O:2002:C:H5'	2.07	0.54
1:O:2346:C:H6	1:O:2346:C:O5'	1.90	0.54
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.88	0.54
2:9:3003:A:OP2	2:9:3025:G:N2	2.40	0.54
5:C:236:THR:CG2	5:C:239:ALA:H	2.11	0.54
8:F:21:GLU:O	8:F:24:ARG:HG2	2.07	0.54
1:O:1667:A:H2'	1:O:1668:U:H6	1.72	0.54
38:O:4623:HOH:O	16:O:39:THR:HB	2.07	0.54
2:9:3076:G:H3'	2:9:3077:A:C5'	2.28	0.54
5:C:1:MET:HG2	5:C:2:GLN:N	2.21	0.54
7:E:93:MET:HE1	7:E:165:GLY:N	2.22	0.54
10:H:46:GLN:HG3	10:H:137:TYR:CE2	2.43	0.54
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.90	0.54
1:O:1421:C:H2'	1:O:1422:U:H6	1.73	0.54
1:O:1446:U:H2'	20:S:55:GLN:NE2	2.23	0.54
1:O:1568:G:O2'	1:O:1569:U:H5'	2.07	0.54
38:O:4376:HOH:O	3:A:212:PRO:HB2	2.08	0.54
2:9:3055:U:H4'	2:9:3056:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:58:GLU:HG3	8:F:61:MET:HE2	1.89	0.54
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.38	0.54
1:0:1319:G:H1'	38:0:4701:HOH:O	2.07	0.54
1:0:1450:C:C4'	1:0:1451:C:OP2	2.53	0.54
1:0:1931:A:H2'	1:0:1932:G:H5'	1.90	0.54
1:0:328:U:O4'	5:C:202:THR:HG22	2.07	0.54
1:0:645:U:OP2	13:L:4:LYS:HE2	2.08	0.54
1:0:794:U:H3	1:0:819:A:H61	1.54	0.54
1:0:1173:A:H2	38:0:6282:HOH:O	1.91	0.54
1:0:1762:C:H2'	1:0:1763:C:C6	2.43	0.54
1:0:2064:U:H4'	1:0:2653:A:OP1	2.08	0.54
3:A:51:ARG:NH1	3:A:120:ARG:O	2.41	0.54
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.54
5:C:236:THR:HA	38:C:8651:HOH:O	2.08	0.54
17:P:91:LYS:O	17:P:95:GLU:HG3	2.08	0.54
1:0:125:U:H2'	38:0:3769:HOH:O	2.07	0.53
1:0:349:U:O2'	1:0:350:C:H5'	2.09	0.53
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.53
1:0:820:G:H5'	1:0:821:U:H5'	1.90	0.53
1:0:841:A:H5''	38:0:6906:HOH:O	2.08	0.53
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.08	0.53
1:0:1396:C:H1'	17:P:1:THR:O	2.08	0.53
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.43	0.53
4:B:279:THR:OG1	4:B:290:VAL:HB	2.08	0.53
1:0:2361:A:H5'	1:0:2361:A:H8	1.73	0.53
1:0:2488:A:H61	1:0:2534:C:H42	1.54	0.53
4:B:74:ILE:HG22	4:B:76:THR:HG23	1.91	0.53
1:0:1444:G:O2'	1:0:1445:G:H5'	2.08	0.53
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.36	0.53
23:V:4:HIS:O	23:V:8:ILE:HG13	2.08	0.53
1:0:40:C:H4'	38:0:6998:HOH:O	2.08	0.53
1:0:399:C:H5'	14:M:179:GLY:O	2.09	0.53
1:0:660:A:H4'	1:0:661:G:O5'	2.08	0.53
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.53
1:0:2784:A:H1'	7:E:60:SER:OG	2.08	0.53
8:F:56:PRO:HG2	14:M:43:PRO:O	2.08	0.53
20:S:57:THR:HG22	20:S:59:ASP:HB2	1.90	0.53
22:U:9:CYS:HA	22:U:52:THR:HG23	1.90	0.53
1:0:2064:U:H5'	1:0:2652:U:H4'	1.91	0.53
1:0:2526:C:C6	1:0:2526:C:H5'	2.43	0.53
4:B:162:MET:CE	4:B:308:LEU:HD21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:64:THR:O	24:W:68:THR:HG22	2.08	0.53
1:0:271:C:H4'	1:0:272:A:OP1	2.08	0.53
1:0:622:G:O2'	1:0:623:U:H5'	2.08	0.53
1:0:2382:A:H5'	38:3:8831:HOH:O	2.09	0.53
1:0:2735:U:H2'	1:0:2736:U:C6	2.44	0.53
4:B:23:THR:HG23	4:B:308:LEU:HD23	1.91	0.53
5:C:40:ALA:O	5:C:43:LYS:HB2	2.08	0.53
8:F:96:ALA:HA	38:F:3111:HOH:O	2.09	0.53
11:J:46:ILE:HA	38:J:8828:HOH:O	2.09	0.53
14:M:49:ALA:C	14:M:54:TYR:HB3	2.34	0.53
18:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.90	0.53
24:W:68:THR:HG23	24:W:69:ARG:HG2	1.91	0.53
1:0:420:U:H2'	1:0:421:C:C6	2.44	0.53
1:0:821:U:H2'	1:0:822:C:C6	2.41	0.53
1:0:1314:U:H2'	38:0:5885:HOH:O	2.09	0.53
1:0:2071:C:H5'	38:0:9529:HOH:O	2.09	0.53
7:E:69:ILE:HA	7:E:72:MET:HE3	1.91	0.53
17:P:14:LEU:HD13	17:P:51:ALA:HB2	1.91	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.90	0.53
20:S:52:VAL:HG22	20:S:66:VAL:HG22	1.90	0.53
24:W:129:LYS:HG2	38:W:1990:HOH:O	2.07	0.53
31:I:103:ASP:HA	31:I:106:LYS:HD2	1.91	0.53
1:0:12:U:C2'	1:0:13:G:H5'	2.38	0.53
1:0:282:C:O2'	1:0:283:U:C5'	2.53	0.53
1:0:1342:C:O2'	1:0:1343:C:H5'	2.09	0.53
1:0:1456:C:H2'	1:0:1457:U:C6	2.44	0.53
1:0:1855:G:H4'	1:0:1856:C:O5'	2.09	0.53
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.44	0.53
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.09	0.53
6:D:163:VAL:HA	38:D:6326:HOH:O	2.07	0.53
6:D:166:ILE:HB	38:D:6326:HOH:O	2.09	0.53
1:0:1181:A:N1	1:0:1192:A:O2'	2.38	0.53
1:0:1213:C:C2'	1:0:1214:G:H5'	2.39	0.53
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.42	0.53
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.43	0.53
9:G:64:ASN:HD22	9:G:64:ASN:N	2.06	0.53
21:T:32:ARG:NH1	21:T:38:ARG:HH12	2.07	0.53
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.89	0.53
1:0:1159:G:H21	1:0:1189:A:H8	1.55	0.53
1:0:1236:A:H2'	1:0:1237:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1309:U:C2'	1:0:1310:U:H5'	2.40	0.53
1:0:2269:C:C2'	1:0:2270:G:H5'	2.39	0.53
6:D:135:VAL:HG22	6:D:136:ARG:H	1.74	0.53
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.89	0.53
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.06	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.38	0.52
1:0:625:U:H5''	1:0:1044:C:N4	2.24	0.52
1:0:1733:A:H4'	4:B:212:GLN:HA	1.90	0.52
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.52
1:0:2837:U:H2'	38:0:6833:HOH:O	2.08	0.52
2:9:3031:C:H2'	2:9:3032:G:O4'	2.10	0.52
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.91	0.52
10:H:56:GLN:HE21	10:H:126:ARG:NE	2.00	0.52
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.39	0.52
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.90	0.52
23:V:39:ALA:C	23:V:41:GLU:H	2.16	0.52
1:0:371:U:H2'	1:0:372:A:H8	1.75	0.52
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.38	0.52
2:9:3060:C:O2'	2:9:3061:C:H5'	2.09	0.52
4:B:16:ARG:NH1	38:B:8913:HOH:O	2.42	0.52
14:M:169:ARG:HD2	38:M:8886:HOH:O	2.09	0.52
1:0:603:A:H4'	1:0:604:G:O5'	2.09	0.52
1:0:1588:G:C6	1:0:1589:G:C6	2.98	0.52
10:H:69:ALA:HB2	10:H:153:ALA:HB2	1.90	0.52
15:N:38:LYS:HE2	15:N:107:ASN:ND2	2.24	0.52
20:S:76:GLU:HB3	38:S:8547:HOH:O	2.09	0.52
1:0:544:G:H2'	1:0:545:G:C5'	2.40	0.52
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.91	0.52
1:0:2601:A:N1	12:K:38:SER:HB2	2.25	0.52
1:0:2894:C:O2'	1:0:2895:C:H5'	2.09	0.52
1:0:304:G:H1'	1:0:347:A:N6	2.24	0.52
1:0:1384:C:H5'	25:X:30:MET:HG2	1.92	0.52
1:0:1755:A:H2'	1:0:1756:G:O4'	2.09	0.52
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.52
1:0:1972:U:C2'	1:0:1973:A:H5''	2.39	0.52
1:0:2237:G:H1'	38:0:4862:HOH:O	2.10	0.52
19:R:33:ARG:NH1	38:R:8838:HOH:O	2.41	0.52
30:3:3:MET:O	30:3:90:PHE:HA	2.10	0.52
1:0:289:G:N2	1:0:363:A:C2	2.57	0.52
1:0:1421:C:H2'	1:0:1422:U:C6	2.45	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3029:C:H2'	2:9:3030:C:C5'	2.36	0.52
6:D:82:GLU:HA	6:D:85:GLN:HE21	1.74	0.52
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.57	0.52
21:T:26:THR:HA	21:T:39:ASN:HB3	1.91	0.52
1:0:204:A:H2'	1:0:205:U:H5'	1.91	0.52
1:0:346:U:H4'	38:0:6837:HOH:O	2.08	0.52
1:0:707:C:C2	1:0:708:A:C8	2.97	0.52
1:0:1169:U:C5	1:0:1170:U:C4	2.97	0.52
1:0:1641:A:H2'	1:0:1642:A:C5'	2.33	0.52
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.90	0.52
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.91	0.52
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.25	0.52
13:L:148:GLU:HA	38:L:8871:HOH:O	2.10	0.52
22:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.52
24:W:88:THR:HG22	24:W:90:TYR:HD1	1.74	0.52
1:0:567:U:C5'	38:0:6400:HOH:O	2.57	0.52
1:0:951:A:O2'	1:0:952:G:H5'	2.10	0.52
9:G:23:ILE:O	9:G:27:ILE:HG13	2.10	0.52
24:W:21:LEU:HD22	24:W:26:ILE:CD1	2.40	0.52
1:0:59:A:H5'	38:0:4342:HOH:O	2.09	0.52
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.52
1:0:1661:A:C8	38:0:5210:HOH:O	2.55	0.52
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.52
1:0:2460:A:H5'	32:0:9000:13T:H231	1.90	0.52
1:0:2766:A:O2'	1:0:2767:C:H5'	2.10	0.52
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.16	0.52
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.52
5:C:95:GLU:HG3	38:C:8673:HOH:O	2.09	0.52
1:0:475:G:OP1	5:C:73:LEU:HD22	2.09	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.48	0.51
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.32	0.51
38:0:7541:HOH:O	30:3:60:LYS:HG3	2.10	0.51
2:9:3020:G:O2'	2:9:3021:G:H5'	2.10	0.51
14:M:164:THR:HG22	14:M:167:GLY:H	1.74	0.51
24:W:6:GLN:HB2	24:W:26:ILE:HD12	1.92	0.51
1:0:291:C:H2'	1:0:292:G:O4'	2.10	0.51
1:0:2010:A:C2'	38:0:5968:HOH:O	2.50	0.51
1:0:2361:A:H5''	38:0:9001:HOH:O	2.08	0.51
1:0:2388:C:O2'	1:0:2389:U:H5'	2.10	0.51
1:0:2467:A:O2'	1:0:2468:A:H2'	2.10	0.51
38:0:4733:HOH:O	19:R:29:LYS:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:242:GLU:HB2	38:C:8579:HOH:O	2.09	0.51
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.91	0.51
1:0:64:G:H2'	1:0:65:C:O4'	2.10	0.51
1:0:119:A:H2'	1:0:120:A:H5''	1.93	0.51
1:0:254:C:O2	1:0:254:C:H2'	2.09	0.51
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.51
1:0:1500:U:P	17:P:41:ARG:HH22	2.33	0.51
1:0:1545:C:H2'	1:0:1546:G:O4'	2.10	0.51
1:0:2266:A:H2'	1:0:2267:G:C8	2.45	0.51
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.74	0.51
8:F:91:VAL:HG12	8:F:92:GLY:H	1.76	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.93	0.51
1:0:1398:G:O2'	1:0:1399:A:H5'	2.11	0.51
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.11	0.51
1:0:2036:C:O4'	12:K:44:LEU:HG	2.10	0.51
2:9:3034:A:H2'	2:9:3035:C:O4'	2.11	0.51
2:9:3092:G:C6	2:9:3093:A:C6	2.98	0.51
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.09	0.51
18:Q:75:ILE:HD13	18:Q:84:ILE:HD11	1.93	0.51
27:Z:37:HIS:HB2	27:Z:47:VAL:HB	1.93	0.51
1:0:714:U:H3'	38:0:6939:HOH:O	2.09	0.51
1:0:894:A:C2	5:C:87:ARG:NH2	2.78	0.51
1:0:1249:U:H2'	1:0:1250:C:C6	2.46	0.51
1:0:2887:G:H2'	1:0:2888:U:C6	2.45	0.51
4:B:85:ARG:NH1	38:B:8930:HOH:O	2.42	0.51
13:L:72:ASN:HB2	38:L:8881:HOH:O	2.09	0.51
15:N:132:ASN:O	15:N:135:VAL:HG12	2.09	0.51
1:0:2379:G:N3	1:0:2418:G:H2'	2.25	0.51
1:0:2871:G:H2'	1:0:2872:U:C6	2.46	0.51
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.10	0.51
11:J:54:VAL:HG11	11:J:138:THR:HG21	1.93	0.51
17:P:115:SER:N	17:P:118:GLN:HE21	2.00	0.51
17:P:134:VAL:O	17:P:137:LEU:HB3	2.11	0.51
1:0:558:C:H2'	1:0:559:U:H5''	1.88	0.51
1:0:1314:U:H5''	1:0:1316:G:O4'	2.11	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.92	0.51
1:0:1819:G:H5'	38:0:4720:HOH:O	2.09	0.51
1:0:2578:G:H5'	1:0:2578:G:C8	2.41	0.51
2:9:3013:A:O2'	2:9:3014:G:H5''	2.11	0.51
2:9:3039:U:H1'	2:9:3044:A:N6	2.26	0.51
6:D:62:ASP:HA	38:D:4233:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:69:ILE:HA	7:E:72:MET:CE	2.40	0.51
15:N:169:PRO:O	15:N:172:PHE:HB3	2.11	0.51
1:0:324:G:C6	1:0:325:U:C5	2.99	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:589:U:H2'	1:0:590:A:H8	1.74	0.51
1:0:1163:G:H5'	31:I:115:ASP:O	2.10	0.51
1:0:1543:G:N1	1:0:1641:A:OP2	2.38	0.51
1:0:1787:C:H4'	1:0:2883:A:O4'	2.11	0.51
1:0:1856:C:H5'	1:0:1858:A:O4'	2.10	0.51
4:B:145:HIS:HD2	4:B:146:THR:O	1.94	0.51
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.92	0.51
1:0:228:C:H2'	1:0:229:G:H5'	1.92	0.51
1:0:1116:U:O2'	1:0:1118:A:C2	2.50	0.51
1:0:1878:G:C1'	38:0:6128:HOH:O	2.49	0.51
1:0:2893:C:O2'	1:0:2894:C:H5'	2.11	0.51
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.93	0.51
7:E:101:GLU:HB3	7:E:117:THR:HA	1.92	0.51
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.93	0.51
1:0:168:C:O5'	1:0:168:C:H6	1.93	0.51
1:0:329:A:OP2	5:C:206:ASN:HB2	2.11	0.51
1:0:1119:G:H8	11:J:52:GLN:HE22	1.59	0.51
1:0:1600:G:OP2	1:0:1600:G:H8	1.94	0.51
1:0:2765:C:H2'	1:0:2766:A:H8	1.76	0.51
5:C:132:ASP:HB3	38:C:8560:HOH:O	2.10	0.51
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.08	0.51
1:0:1119:G:H8	11:J:52:GLN:NE2	2.08	0.50
1:0:1586:G:O2'	1:0:1587:U:H5'	2.11	0.50
1:0:2106:C:H5'	1:0:2284:G:H21	1.77	0.50
1:0:2135:A:O2'	1:0:2136:G:H5'	2.10	0.50
1:0:2269:C:O2'	1:0:2270:G:H5'	2.11	0.50
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.93	0.50
1:0:17:G:H2'	1:0:18:C:C6	2.47	0.50
1:0:588:G:O6	24:W:154:ARG:NH1	2.43	0.50
1:0:710:G:C2'	1:0:711:G:H5'	2.41	0.50
1:0:1556:G:O2'	1:0:1557:G:H5'	2.11	0.50
1:0:1862:C:H1'	38:0:7211:HOH:O	2.10	0.50
1:0:2515:C:H2'	1:0:2516:G:O4'	2.11	0.50
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.93	0.50
6:D:103:ASN:HD22	6:D:134:LEU:H	1.57	0.50
24:W:4:LEU:HB2	24:W:33:THR:HG22	1.92	0.50
26:Y:117:LEU:HD12	26:Y:174:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:28:HIS:CE1	28:1:31:LYS:HE2	2.46	0.50
1:0:814:G:H4'	38:0:3133:HOH:O	2.12	0.50
1:0:1287:A:O4'	24:W:117:ARG:HD3	2.12	0.50
1:0:1413:A:H2'	1:0:1414:A:O4'	2.11	0.50
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.27	0.50
1:0:1188:A:H5'	38:0:7415:HOH:O	2.11	0.50
1:0:1406:A:H4'	1:0:1407:A:C5'	2.42	0.50
32:0:9000:13T:C23	32:0:9000:13T:C31	2.90	0.50
2:9:3023:U:O2'	2:9:3024:U:H4'	2.11	0.50
11:J:19:MET:HE1	11:J:78:ILE:HG22	1.92	0.50
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.26	0.50
31:I:78:LEU:HD12	31:I:112:LYS:NZ	2.26	0.50
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.44	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:1985:U:C2	1:0:1996:U:O4'	2.64	0.50
1:0:2717:C:C2'	1:0:2718:C:C5'	2.78	0.50
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.45	0.50
2:9:3104:A:O2'	2:9:3105:A:H5'	2.12	0.50
5:C:102:LEU:HD12	38:C:8515:HOH:O	2.11	0.50
19:R:119:VAL:HG12	19:R:119:VAL:O	2.10	0.50
1:0:84:G:C2'	1:0:85:C:H5'	2.42	0.50
1:0:240:C:O2	1:0:240:C:H2'	2.12	0.50
1:0:793:A:H5''	17:P:83:LYS:HG2	1.94	0.50
1:0:2664:A:H8	1:0:2664:A:OP1	1.95	0.50
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.94	0.50
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.46	0.50
6:D:172:VAL:HG12	6:D:173:GLU:N	2.27	0.50
12:K:74:VAL:HG13	12:K:113:ILE:HG12	1.92	0.50
13:L:24:ALA:HB2	13:L:30:ARG:HD2	1.93	0.50
26:Y:189:ASN:HA	26:Y:217:ILE:HD11	1.93	0.50
28:1:10:LYS:HG3	38:1:8731:HOH:O	2.11	0.50
1:0:370:G:O2'	1:0:371:U:H5'	2.12	0.50
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.76	0.50
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.94	0.50
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.93	0.50
19:R:59:PHE:O	19:R:63:ASN:HB3	2.12	0.50
21:T:41:ARG:NH1	21:T:42:VAL:O	2.45	0.50
21:T:69:LYS:O	21:T:71:VAL:HG23	2.12	0.50
24:W:125:HIS:CD2	24:W:127:GLY:H	2.25	0.50
26:Y:203:VAL:HG12	26:Y:228:VAL:HG22	1.94	0.50
1:0:363:A:O2'	1:0:364:C:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1130:U:H5'	38:0:7657:HOH:O	2.11	0.50
1:0:1207:A:C8	1:0:1208:C:C5	3.00	0.50
1:0:1878:G:O2'	1:0:1879:U:H6	1.93	0.50
1:0:2253:G:C2	1:0:2254:G:C8	3.00	0.50
1:0:2336:G:H1'	38:0:6297:HOH:O	2.12	0.50
1:0:2506:A:N6	1:0:2511:A:O2'	2.44	0.50
1:0:2668:G:H2'	1:0:2669:U:C6	2.46	0.50
1:0:2779:G:H21	7:E:143:GLN:NE2	2.10	0.50
3:A:89:ALA:HB3	38:A:8913:HOH:O	2.11	0.50
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.93	0.50
5:C:214:THR:HG23	38:C:8636:HOH:O	2.10	0.50
9:G:12:ILE:N	9:G:13:PRO:HD3	2.27	0.50
22:U:20:MET:HE2	22:U:30:HIS:NE2	2.27	0.50
1:0:424:C:H2'	1:0:425:U:H6	1.77	0.50
1:0:1154:A:H2'	1:0:1155:G:H8	1.75	0.50
1:0:1163:G:N2	38:0:6056:HOH:O	2.45	0.50
10:H:47:ILE:HG12	10:H:165:SER:HA	1.93	0.50
25:X:25:ARG:HD3	25:X:64:ALA:O	2.12	0.50
27:Z:19:GLY:O	27:Z:23:ARG:HG2	2.11	0.50
1:0:93:C:H5''	23:V:1:THR:CB	2.33	0.49
1:0:635:A:H2'	1:0:636:G:H5''	1.92	0.49
1:0:2296:C:H2'	1:0:2297:U:C6	2.47	0.49
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.49
1:0:2831:C:H2'	1:0:2832:C:H5'	1.93	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
13:L:80:ASP:HB2	13:L:90:ARG:O	2.12	0.49
15:N:43:VAL:HG11	15:N:81:ALA:HA	1.94	0.49
21:T:71:VAL:HG12	21:T:72:ILE:N	2.27	0.49
1:0:710:G:O2'	1:0:711:G:H5'	2.12	0.49
1:0:1423:C:O2'	1:0:1424:A:H5'	2.12	0.49
1:0:2896:A:N3	1:0:2896:A:H2'	2.28	0.49
2:9:3055:U:H4'	2:9:3056:A:H8	1.77	0.49
4:B:26:PHE:HE1	4:B:310:ARG:HB3	1.77	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.49
10:H:162:ARG:HD3	38:H:8585:HOH:O	2.12	0.49
1:0:415:A:O2'	1:0:416:G:H5'	2.13	0.49
1:0:775:G:OP1	28:1:16:HIS:HE1	1.95	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.12	0.49
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.49
3:A:179:MET:HG2	3:A:186:TRP:CG	2.46	0.49
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:12:ILE:HG22	9:G:17:GLN:HE21	1.76	0.49
13:L:134:GLU:HG3	38:L:8855:HOH:O	2.12	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.12	0.49
1:0:1008:C:H5''	10:H:16:ARG:HH12	1.76	0.49
1:0:1642:A:C8	1:0:1643:C:C5	3.00	0.49
1:0:2363:G:O2'	18:Q:11:ARG:HG3	2.13	0.49
1:0:2493:C:O2	1:0:2493:C:H2'	2.11	0.49
1:0:2866:U:C5	22:U:50:GLU:HB2	2.47	0.49
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.77	0.49
26:Y:235:GLU:CD	26:Y:235:GLU:H	2.21	0.49
1:0:494:C:H2'	1:0:496:G:OP2	2.13	0.49
1:0:946:C:H2'	1:0:947:U:C6	2.47	0.49
1:0:1972:U:H2'	1:0:1973:A:H5''	1.93	0.49
1:0:2004:U:O2	1:0:2004:U:H2'	2.11	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.49
10:H:27:LYS:H	10:H:59:HIS:HD2	1.59	0.49
26:Y:107:PRO:HD3	26:Y:182:PHE:CE1	2.47	0.49
27:Z:53:GLY:HA2	27:Z:67:GLY:O	2.12	0.49
1:0:251:C:O2'	1:0:252:C:H5'	2.12	0.49
1:0:318:C:H5'	1:0:339:A:C2	2.48	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.78	0.49
1:0:1474:C:C6	1:0:1474:C:C5'	2.81	0.49
1:0:2122:C:H3'	38:0:5295:HOH:O	2.13	0.49
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.38	0.49
4:B:267:LYS:HA	38:B:8824:HOH:O	2.11	0.49
11:J:75:PRO:HD3	11:J:136:SER:OG	2.13	0.49
1:0:710:G:OP1	16:O:24:ALA:HB3	2.13	0.49
1:0:1278:A:H4'	1:0:1279:U:C4	2.48	0.49
1:0:1488:U:H4'	1:0:1489:G:OP1	2.12	0.49
1:0:1681:G:H5''	1:0:1682:A:H5'	1.94	0.49
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.27	0.49
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.43	0.49
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.11	0.49
1:0:645:U:O2	1:0:761:A:H2	1.96	0.49
1:0:1331:A:OP2	26:Y:142:SER:OG	2.27	0.49
1:0:2694:A:C6	1:0:2702:A:C8	3.01	0.49
38:0:5640:HOH:O	17:P:58:SER:HB3	2.11	0.49
10:H:51:VAL:HG13	10:H:159:PRO:HG3	1.95	0.49
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.49
1:0:514:G:OP1	1:0:514:G:H2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:558:C:H5'	38:0:5262:HOH:O	2.13	0.49
1:0:1422:U:H2'	1:0:1423:C:C6	2.48	0.49
1:0:1484:G:H2'	38:0:9098:HOH:O	2.13	0.49
1:0:2102:G:C2	1:0:2104:C:C4	3.01	0.49
1:0:2316:G:H4'	38:0:6098:HOH:O	2.12	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.49
4:B:36:PRO:HA	4:B:168:GLY:CA	2.39	0.49
4:B:294:TYR:HE2	38:B:8945:HOH:O	1.95	0.49
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.28	0.49
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.48	0.49
28:1:25:LYS:O	28:1:25:LYS:HG2	2.13	0.49
1:0:23:G:C6	1:0:24:G:N1	2.81	0.49
1:0:949:U:O2'	18:Q:40:HIS:HE1	1.96	0.49
1:0:1098:A:H2'	1:0:1099:G:O4'	2.12	0.49
1:0:1311:G:C2	1:0:1312:G:C8	3.01	0.49
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.49
1:0:1421:C:O2'	1:0:1422:U:H5'	2.13	0.49
1:0:1834:C:H2'	1:0:1840:A:N6	2.27	0.49
1:0:2300:A:H4'	1:0:2301:A:O5'	2.13	0.49
1:0:2387:U:H2'	1:0:2388:C:C6	2.48	0.49
1:0:2453:G:H3'	38:0:5931:HOH:O	2.13	0.49
38:0:6679:HOH:O	21:T:38:ARG:NH1	2.45	0.49
38:0:6699:HOH:O	26:Y:165:GLU:HB3	2.13	0.49
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.43	0.49
15:N:154:LEU:C	15:N:156:GLU:H	2.20	0.49
1:0:447:A:OP2	21:T:1:SER:HB2	2.12	0.48
1:0:522:U:O2'	1:0:1366:C:H5'	2.13	0.48
1:0:559:U:C6	1:0:559:U:C3'	2.96	0.48
1:0:1165:G:C4'	1:0:1174:A:O2'	2.55	0.48
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.39	0.48
17:P:115:SER:OG	17:P:118:GLN:HG3	2.12	0.48
24:W:13:MET:HE1	24:W:21:LEU:HD12	1.95	0.48
24:W:115:THR:HG23	38:W:5420:HOH:O	2.13	0.48
1:0:816:G:C6	1:0:817:G:N1	2.80	0.48
1:0:999:C:H2'	1:0:1000:C:O4'	2.14	0.48
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.48
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.95	0.48
13:L:67:ARG:HB2	13:L:112:GLY:HA3	1.94	0.48
30:3:65:THR:HB	30:3:83:TRP:H	1.78	0.48
1:0:292:G:H1'	1:0:360:A:N6	2.28	0.48
1:0:474:C:O2'	5:C:73:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H5'	1:0:1868:G:H5'	1.95	0.48
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.48
1:0:2349:G:O2'	1:0:2350:G:H5'	2.12	0.48
1:0:2703:A:H2'	1:0:2704:C:C6	2.48	0.48
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.28	0.48
5:C:107:ARG:NE	38:C:8657:HOH:O	2.35	0.48
10:H:170:ASN:HD22	10:H:170:ASN:N	2.10	0.48
12:K:130:MET:SD	22:U:25:ASP:O	2.71	0.48
14:M:99:ARG:CD	14:M:167:GLY:HA2	2.42	0.48
24:W:4:LEU:HD22	24:W:52:VAL:CG2	2.34	0.48
25:X:23:HIS:CD2	25:X:24:LYS:HG3	2.49	0.48
1:0:10:U:O4	1:0:532:A:OP2	2.32	0.48
1:0:154:C:H2'	1:0:155:C:H6	1.78	0.48
1:0:441:A:H8	1:0:441:A:O5'	1.96	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.48
1:0:1589:G:N2	1:0:1605:G:H1'	2.28	0.48
1:0:2374:A:H2'	1:0:2375:G:H8	1.78	0.48
38:0:9792:HOH:O	13:L:30:ARG:NH2	2.44	0.48
3:A:53:ALA:HB3	38:A:8897:HOH:O	2.12	0.48
14:M:164:THR:CG2	14:M:167:GLY:H	2.27	0.48
31:I:113:HIS:CE1	31:I:121:LEU:HD22	2.48	0.48
1:0:188:C:H5''	14:M:163:LEU:HD21	1.95	0.48
1:0:597:A:C4	1:0:598:C:C5	3.01	0.48
1:0:1193:A:H2	1:0:1194:A:N6	2.12	0.48
1:0:2055:A:H4'	19:R:132:ARG:NH2	2.28	0.48
2:9:3054:A:C2	2:9:3055:U:N3	2.81	0.48
4:B:17:LYS:O	4:B:260:HIS:HD2	1.95	0.48
10:H:97:GLU:HB3	10:H:121:VAL:HG11	1.96	0.48
16:O:47:ARG:HG3	16:O:47:ARG:NH1	2.29	0.48
19:R:39:THR:HB	19:R:42:GLU:CG	2.43	0.48
1:0:366:U:H2'	1:0:367:G:O4'	2.12	0.48
1:0:470:U:O2'	28:1:16:HIS:CD2	2.64	0.48
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.48
1:0:1081:A:C6	1:0:1082:A:N1	2.82	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.95	0.48
1:0:1942:A:O2'	1:0:1943:C:H5'	2.14	0.48
1:0:2403:C:H3'	38:0:5214:HOH:O	2.13	0.48
1:0:2616:G:H1'	38:0:9423:HOH:O	2.14	0.48
2:9:3058:G:C8	2:9:3059:C:C5	3.02	0.48
7:E:84:MET:HE1	7:E:148:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.44	0.48
1:0:613:C:H2'	1:0:614:U:H6	1.79	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:963:C:O2	1:0:1005:A:N1	2.46	0.48
1:0:1118:A:N6	1:0:1244:U:N3	2.57	0.48
1:0:1552:G:C6	1:0:1553:C:C4	3.01	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.48
1:0:2324:G:N2	1:0:2377:U:H1'	2.29	0.48
1:0:2553:A:H2'	1:0:2553:A:N3	2.28	0.48
4:B:221:GLN:HE22	12:K:42:ASN:ND2	2.03	0.48
11:J:42:GLU:O	11:J:131:THR:HG23	2.14	0.48
11:J:74:ARG:NH1	11:J:76:ASP:HB2	2.29	0.48
24:W:3:ALA:O	24:W:54:PHE:HA	2.14	0.48
27:Z:33:MET:SD	27:Z:49:ARG:HD2	2.53	0.48
29:2:41:HIS:HD2	29:2:44:ARG:H	1.62	0.48
1:0:886:A:OP2	1:0:2113:G:H5'	2.14	0.48
1:0:1217:G:C2	1:0:1218:U:C2	3.02	0.48
1:0:1842:A:C4	1:0:1979:G:C6	3.01	0.48
1:0:1921:A:O2'	1:0:1922:A:H5'	2.14	0.48
1:0:1942:A:H3'	38:0:7336:HOH:O	2.12	0.48
1:0:2032:U:H2'	1:0:2033:G:C5'	2.44	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.96	0.48
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.95	0.48
3:A:200:PRO:HD3	38:A:8819:HOH:O	2.14	0.48
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.42	0.48
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.14	0.48
11:J:45:VAL:HG23	11:J:130:VAL:O	2.14	0.48
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.93	0.48
1:0:1044:C:H5''	38:0:9021:HOH:O	2.12	0.48
1:0:1573:A:N7	1:0:1574:C:C2	2.82	0.48
1:0:1669:A:H2'	1:0:1670:G:C8	2.49	0.48
1:0:1747:A:C8	12:K:44:LEU:HD13	2.49	0.48
1:0:1789:G:O6	17:P:73:HIS:HE1	1.97	0.48
1:0:2070:G:H5''	38:0:3786:HOH:O	2.14	0.48
1:0:2488:A:H2	38:0:7268:HOH:O	1.96	0.48
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.95	0.48
5:C:51:TYR:HA	5:C:54:LEU:HD12	1.96	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.43	0.48
1:0:629:A:H2'	1:0:630:A:O4'	2.14	0.48
1:0:1587:U:H2'	1:0:1588:G:O4'	2.13	0.48
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3051:A:H5'	15:N:160:SER:HB3	1.96	0.48
6:D:51:ARG:HH11	6:D:68:PRO:HB3	1.79	0.48
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.96	0.48
15:N:67:ALA:HA	15:N:71:TRP:CB	2.42	0.48
16:O:39:THR:O	16:O:115:ARG:NH2	2.47	0.48
1:0:57:C:H5''	38:0:6753:HOH:O	2.14	0.47
1:0:324:G:O2'	1:0:325:U:H5'	2.14	0.47
1:0:397:A:O2'	1:0:417:G:N3	2.40	0.47
1:0:664:U:O4	1:0:681:G:H5''	2.14	0.47
1:0:2044:G:OP1	25:X:23:HIS:HE1	1.97	0.47
1:0:2114:C:OP1	3:A:1:GLY:HA2	2.13	0.47
1:0:2689:A:H2'	1:0:2690:U:H5'	1.96	0.47
1:0:2831:C:C2'	1:0:2832:C:H5'	2.44	0.47
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.95	0.47
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.44	0.47
25:X:66:THR:HG23	25:X:67:PRO:HD2	1.96	0.47
1:0:709:G:O2'	16:O:25:VAL:HG12	2.14	0.47
1:0:941:G:C6	1:0:942:U:C4	3.02	0.47
1:0:1188:A:C6	1:0:1189:A:C6	3.02	0.47
1:0:1477:C:C5'	1:0:1868:G:H5''	2.43	0.47
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.47
1:0:2765:C:H2'	1:0:2766:A:C8	2.49	0.47
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.79	0.47
7:E:10:ASP:HA	38:E:6017:HOH:O	2.14	0.47
12:K:125:ALA:C	12:K:127:ALA:H	2.22	0.47
28:1:25:LYS:HD2	29:2:48:ASP:HA	1.96	0.47
1:0:255:A:C8	1:0:256:C:C5	3.02	0.47
1:0:264:G:H1'	1:0:265:U:H5	1.79	0.47
1:0:1339:G:C6	1:0:1340:G:N1	2.82	0.47
1:0:1398:G:H2'	1:0:1399:A:C8	2.49	0.47
1:0:2112:A:H2'	1:0:2113:G:C8	2.49	0.47
1:0:2297:U:H1'	38:0:5179:HOH:O	2.13	0.47
1:0:2330:U:H4'	1:0:2331:C:OP1	2.15	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.31	0.47
1:0:2802:C:H2'	1:0:2803:C:C6	2.50	0.47
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.27	0.47
4:B:150:ALA:O	4:B:152:PRO:HD3	2.14	0.47
1:0:106:A:O2'	1:0:107:U:H5'	2.14	0.47
1:0:155:C:OP2	14:M:188:ARG:HD3	2.13	0.47
1:0:271:C:C2	1:0:273:G:O4'	2.67	0.47
1:0:293:A:C4	1:0:360:A:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:9215:HOH:O	3:A:11:ARG:HD3	2.15	0.47
2:9:3002:U:OP2	2:9:3002:U:H4'	2.15	0.47
2:9:3049:G:H2'	2:9:3050:G:O4'	2.14	0.47
2:9:3114:G:O6	15:N:11:ARG:HD3	2.13	0.47
4:B:112:THR:OG1	4:B:158:LYS:HG3	2.14	0.47
11:J:135:ILE:O	11:J:139:LEU:HG	2.15	0.47
21:T:73:HIS:CD2	21:T:88:PRO:HG3	2.49	0.47
1:0:80:A:H3'	21:T:43:ASN:OD1	2.15	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1592:G:O2'	1:0:1593:C:O5'	2.33	0.47
7:E:11:VAL:HG12	7:E:12:ASP:N	2.29	0.47
13:L:143:THR:HG21	38:L:8836:HOH:O	2.14	0.47
30:3:3:MET:HG3	30:3:4:PRO:HD2	1.96	0.47
1:0:69:A:H8	1:0:69:A:C5'	2.25	0.47
1:0:247:A:H2'	38:0:3931:HOH:O	2.13	0.47
1:0:876:A:H2'	1:0:876:A:N3	2.29	0.47
1:0:1562:C:O2	1:0:1562:C:H2'	2.12	0.47
1:0:1574:C:H2'	1:0:1575:C:C6	2.50	0.47
1:0:2026:C:O2'	1:0:2027:U:H5'	2.15	0.47
1:0:2115:U:H2'	1:0:2116:U:C6	2.49	0.47
1:0:2403:C:C2'	1:0:2404:G:O5'	2.62	0.47
15:N:108:SER:HA	15:N:109:PRO:HD3	1.74	0.47
24:W:52:VAL:HG22	24:W:53:ALA:H	1.79	0.47
26:Y:189:ASN:HD22	26:Y:192:ASP:H	1.63	0.47
1:0:475:G:H5'	5:C:73:LEU:CD2	2.44	0.47
1:0:524:A:C5'	19:R:29:LYS:HE2	2.45	0.47
1:0:644:G:H5'	1:0:644:G:N3	2.30	0.47
1:0:729:C:C2	1:0:743:G:C2	3.03	0.47
1:0:758:A:H2'	1:0:759:C:O4'	2.15	0.47
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.50	0.47
1:0:1069:C:C2'	1:0:1070:A:H5'	2.44	0.47
1:0:1079:A:H4'	1:0:2078:U:H5'	1.97	0.47
1:0:1202:A:O2'	1:0:1203:G:H5'	2.14	0.47
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.47
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.47	0.47
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.15	0.47
1:0:2274:A:O2'	1:0:2275:G:H5'	2.14	0.47
1:0:2371:G:H5'	38:0:5013:HOH:O	2.14	0.47
1:0:2419:U:H5''	1:0:2420:G:H5'	1.97	0.47
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.47
1:0:2421:G:H3'	1:0:2422:U:H5''	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2615:U:C5	1:0:2616:G:C6	3.03	0.47
1:0:2754:G:O2'	1:0:2755:G:H5'	2.15	0.47
2:9:3048:C:H4'	15:N:141:ARG:NH2	2.30	0.47
4:B:275:GLY:O	4:B:291:ASP:HA	2.15	0.47
10:H:2:PRO:HD2	10:H:5:MET:SD	2.55	0.47
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.97	0.47
14:M:65:VAL:HG21	14:M:105:ALA:HB2	1.97	0.47
16:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.47
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.45	0.47
24:W:21:LEU:HD22	24:W:26:ILE:HD11	1.97	0.47
24:W:90:TYR:CE2	24:W:99:ALA:HB2	2.50	0.47
27:Z:30:GLU:HA	27:Z:33:MET:HE2	1.97	0.47
31:I:102:VAL:HG12	31:I:106:LYS:HE3	1.96	0.47
1:0:920:C:H5'	1:0:921:G:C4	2.50	0.47
1:0:951:A:H2'	1:0:952:G:H5'	1.96	0.47
1:0:1731:C:H1'	38:0:6446:HOH:O	2.14	0.47
1:0:1746:A:O4'	1:0:1747:A:C2	2.67	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.47
1:0:2111:G:H1'	38:0:9044:HOH:O	2.14	0.47
3:A:17:ARG:HD2	38:A:8836:HOH:O	2.13	0.47
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.79	0.47
22:U:33:SER:O	22:U:37:GLU:HG3	2.14	0.47
26:Y:117:LEU:HD12	26:Y:174:VAL:HG11	1.97	0.47
28:1:28:HIS:HD2	28:1:30:LYS:H	1.61	0.47
1:0:329:A:C5	1:0:347:A:C2	3.03	0.47
1:0:524:A:H5'	19:R:29:LYS:HE2	1.97	0.47
1:0:905:C:H3'	38:0:5188:HOH:O	2.15	0.47
1:0:1013:A:H1'	38:0:9156:HOH:O	2.15	0.47
1:0:1114:A:O2'	1:0:1115:U:H5'	2.15	0.47
1:0:1268:C:O2'	1:0:1269:G:H5'	2.14	0.47
1:0:1593:C:OP1	17:P:117:SER:HB3	2.15	0.47
1:0:1921:A:C6	1:0:1922:A:C2	3.03	0.47
1:0:2244:A:H1'	38:M:8866:HOH:O	2.14	0.47
1:0:2274:A:H1'	14:M:86:GLN:NE2	2.30	0.47
1:0:2468:A:H4'	38:0:3550:HOH:O	2.14	0.47
1:0:2502:C:H2'	1:0:2503:A:C5'	2.43	0.47
1:0:2768:A:C2'	1:0:2769:C:O4'	2.61	0.47
38:0:6273:HOH:O	17:P:59:ARG:HD3	2.15	0.47
38:0:6996:HOH:O	18:Q:9:GLY:HA2	2.15	0.47
2:9:3047:A:C2	2:9:3048:C:C2	3.03	0.47
3:A:109:GLU:HG2	3:A:116:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:312:U:C2	1:0:320:G:N2	2.83	0.47
1:0:377:C:H5	38:0:3309:HOH:O	1.98	0.47
1:0:1015:C:O5'	1:0:1015:C:H6	1.98	0.47
1:0:1857:A:N6	1:0:2247:C:H1'	2.30	0.47
1:0:1878:G:H5'	38:0:4380:HOH:O	2.15	0.47
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
6:D:135:VAL:HG22	6:D:136:ARG:N	2.29	0.47
7:E:37:ASP:OD1	11:J:125:SER:HB3	2.15	0.47
8:F:34:ASN:HA	14:M:4:ALA:HB2	1.97	0.47
1:0:513:A:N3	38:0:3663:HOH:O	2.36	0.46
1:0:559:U:C6	1:0:559:U:H3'	2.51	0.46
1:0:812:A:H1'	38:0:3966:HOH:O	2.14	0.46
1:0:851:C:H5	38:0:6802:HOH:O	1.96	0.46
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.46
1:0:1773:G:N2	1:0:1774:G:C8	2.83	0.46
1:0:2047:C:H2'	1:0:2048:C:H6	1.80	0.46
1:0:2063:U:O4	1:0:2083:A:H2	1.98	0.46
1:0:2255:A:C6	1:0:2256:G:C5	3.03	0.46
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.46
2:9:3097:U:H2'	2:9:3098:C:H6	1.79	0.46
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.97	0.46
18:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.15	0.46
21:T:71:VAL:HG13	21:T:91:LEU:O	2.15	0.46
24:W:38:THR:HG22	24:W:39:ASP:N	2.30	0.46
26:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.48	0.46
1:0:31:C:H4'	38:0:7414:HOH:O	2.16	0.46
1:0:111:C:O2'	1:0:112:G:H5'	2.16	0.46
1:0:1183:C:C2	1:0:1184:C:C5	3.03	0.46
1:0:1447:U:H3'	1:0:1506:U:O2	2.15	0.46
1:0:1838:U:O2'	1:0:2644:C:H5'	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.16	0.46
1:0:2255:A:C2	1:0:2256:G:C4	3.03	0.46
1:0:2526:C:HO2'	1:0:2527:U:H5'	1.79	0.46
32:0:9000:13T:C23	32:0:9000:13T:H311	2.46	0.46
2:9:3028:U:H2'	2:9:3029:C:C6	2.50	0.46
1:0:694:A:C2'	1:0:695:C:H5'	2.43	0.46
1:0:1198:U:C6	1:0:1200:A:OP2	2.68	0.46
1:0:1207:A:N6	38:0:5644:HOH:O	2.48	0.46
1:0:1211:G:H2'	1:0:1212:C:C6	2.47	0.46
1:0:1523:G:C6	1:0:1524:U:O4	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.46
1:0:1878:G:O2'	1:0:1879:U:C5	2.65	0.46
1:0:1913:C:H2'	1:0:1914:C:H6	1.80	0.46
1:0:2269:C:H2'	1:0:2270:G:C5'	2.46	0.46
1:0:2764:C:H1'	38:0:7458:HOH:O	2.16	0.46
3:A:126:ALA:HB1	3:A:138:VAL:CG1	2.45	0.46
8:F:111:ILE:O	8:F:115:VAL:HG23	2.15	0.46
22:U:6:CYS:C	22:U:8:TYR:H	2.21	0.46
1:0:559:U:H2'	1:0:560:C:O4'	2.14	0.46
1:0:704:C:H2'	1:0:705:C:H6	1.81	0.46
1:0:843:A:C2	1:0:846:A:C8	3.04	0.46
1:0:1913:C:H2'	1:0:1914:C:C6	2.50	0.46
1:0:1931:A:C2'	1:0:1932:G:H5'	2.45	0.46
1:0:2459:G:C2'	32:0:9000:13T:C23	2.94	0.46
2:9:3006:C:OP1	15:N:37:ARG:NH1	2.48	0.46
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.31	0.46
16:O:105:ASN:HD21	16:O:109:SER:H	1.62	0.46
31:I:100:LEU:HD22	31:I:105:VAL:CG2	2.46	0.46
1:0:317:A:OP1	21:T:52:ARG:O	2.33	0.46
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.46
1:0:1204:C:H2'	1:0:1205:U:O4'	2.16	0.46
1:0:2459:G:H2'	32:0:9000:13T:H232	1.98	0.46
1:0:2821:C:H2'	1:0:2822:C:H6	1.80	0.46
15:N:65:ASP:HB3	38:N:8821:HOH:O	2.14	0.46
26:Y:112:GLU:CD	26:Y:115:ARG:NH1	2.74	0.46
1:0:39:G:C2	1:0:444:C:C2	3.04	0.46
1:0:1173:A:H3'	38:0:4360:HOH:O	2.16	0.46
1:0:1619:G:C5	1:0:1620:C:C4	3.03	0.46
1:0:2114:C:O2'	1:0:2115:U:H5'	2.16	0.46
1:0:2332:A:H3'	1:0:2333:G:H8	1.80	0.46
3:A:3:ARG:H	3:A:3:ARG:HG2	1.55	0.46
3:A:179:MET:HG2	3:A:186:TRP:CB	2.45	0.46
14:M:183:THR:HG22	14:M:194:ALA:HB1	1.96	0.46
22:U:13:ILE:HG12	22:U:32:CYS:HB3	1.97	0.46
1:0:281:U:C2'	1:0:282:C:H5'	2.46	0.46
1:0:857:A:H4'	3:A:176:HIS:CD2	2.51	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.98	0.46
1:0:1850:U:H2'	1:0:1851:G:C8	2.50	0.46
3:A:72:GLU:HG3	27:Z:66:GLY:HA2	1.98	0.46
6:D:10:PHE:CG	6:D:11:HIS:N	2.84	0.46
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:4:TYR:CE1	19:R:17:MET:HE2	2.51	0.46
19:R:39:THR:HG23	19:R:107:GLU:O	2.16	0.46
1:0:475:G:H5'	5:C:73:LEU:HD23	1.96	0.46
1:0:1684:A:O2'	1:0:1685:A:H5''	2.15	0.46
1:0:2121:G:O2'	1:0:2122:C:H5'	2.16	0.46
1:0:2729:C:O2'	1:0:2730:G:H5'	2.15	0.46
3:A:36:ASP:O	3:A:38:ILE:N	2.49	0.46
3:A:215:ILE:HG13	3:A:216:SER:N	2.30	0.46
13:L:56:LYS:NZ	38:L:8873:HOH:O	2.49	0.46
22:U:52:THR:HG22	22:U:54:THR:N	2.31	0.46
26:Y:216:ARG:HD2	38:Y:8868:HOH:O	2.14	0.46
1:0:1218:U:H2'	1:0:1219:U:C6	2.51	0.46
1:0:2263:G:H1'	38:0:6618:HOH:O	2.16	0.46
1:0:2329:C:O2'	1:0:2330:U:H5'	2.16	0.46
26:Y:184:GLU:OE2	26:Y:204:ARG:HD2	2.15	0.46
1:0:17:G:H2'	1:0:18:C:H6	1.81	0.46
1:0:101:C:H2'	1:0:102:A:C8	2.51	0.46
1:0:113:A:H2'	1:0:115:U:O4	2.16	0.46
1:0:1166:A:H1'	1:0:1192:A:C2	2.50	0.46
1:0:1182:C:O2'	1:0:1183:C:H5	1.99	0.46
1:0:2050:G:H5''	19:R:80:TYR:O	2.16	0.46
1:0:2549:C:H4'	38:0:7504:HOH:O	2.16	0.46
1:0:2672:C:H1'	38:B:8930:HOH:O	2.15	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
38:0:7403:HOH:O	31:I:90:GLY:HA2	2.16	0.46
6:D:51:ARG:NH1	6:D:68:PRO:HB3	2.31	0.46
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.98	0.46
8:F:107:ASP:O	8:F:111:ILE:HG13	2.15	0.46
10:H:170:ASN:N	10:H:170:ASN:ND2	2.64	0.46
11:J:26:VAL:HG13	11:J:36:VAL:HG11	1.98	0.46
14:M:134:ILE:CG2	14:M:141:ILE:HD13	2.43	0.46
20:S:57:THR:CG2	20:S:59:ASP:HB2	2.45	0.46
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.45	0.46
1:0:189:A:OP1	14:M:171:ARG:NH2	2.49	0.45
1:0:583:G:H2'	1:0:584:U:C6	2.51	0.45
1:0:1180:U:H4'	31:I:91:GLU:HG2	1.97	0.45
1:0:1583:U:H1'	38:0:9979:HOH:O	2.15	0.45
1:0:2000:G:O2'	1:0:2001:G:H5'	2.16	0.45
1:0:2253:G:O2'	1:0:2254:G:H5'	2.16	0.45
1:0:2730:G:O2'	1:0:2731:G:H5'	2.15	0.45
2:9:3107:C:H2'	2:9:3108:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.98	0.45
10:H:1:LYS:HA	10:H:2:PRO:HD3	1.73	0.45
11:J:45:VAL:HG22	11:J:46:ILE:N	2.30	0.45
20:S:77:VAL:O	20:S:80:ARG:HG2	2.17	0.45
1:0:706:G:O2'	1:0:707:C:H6	1.99	0.45
1:0:939:A:H5'	38:0:5419:HOH:O	2.16	0.45
1:0:1127:C:C5	1:0:1128:U:C4	3.04	0.45
1:0:1321:A:H2'	1:0:1322:G:C8	2.51	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.51	0.45
1:0:1741:U:C4	1:0:2033:G:C8	3.04	0.45
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.45
1:0:2092:G:H5''	1:0:2613:G:OP1	2.15	0.45
1:0:2570:G:H8	38:0:4917:HOH:O	2.00	0.45
1:0:2820:A:H2'	1:0:2821:C:O4'	2.17	0.45
10:H:95:LEU:HD11	10:H:124:ALA:HB2	1.99	0.45
16:O:32:ARG:HB2	38:O:4656:HOH:O	2.17	0.45
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.45
23:V:7:GLU:O	23:V:11:MET:HG3	2.15	0.45
26:Y:220:GLU:HG3	38:Y:8849:HOH:O	2.16	0.45
27:Z:56:GLN:HA	27:Z:62:TYR:O	2.16	0.45
1:0:365:G:C6	1:0:366:U:C4	3.04	0.45
1:0:419:A:H1'	1:0:1921:A:C2	2.51	0.45
1:0:512:G:O3'	1:0:513:A:C8	2.69	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.82	0.45
1:0:814:G:N2	1:0:815:U:H1'	2.31	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45
1:0:1855:G:H8	3:A:144:GLU:OE2	1.99	0.45
1:0:2314:G:C2'	1:0:2315:C:H5'	2.46	0.45
1:0:2582:G:H5''	4:B:3:PRO:HB3	1.98	0.45
1:0:2831:C:H2'	1:0:2832:C:C5'	2.46	0.45
2:9:3107:C:C5	38:9:3167:HOH:O	2.68	0.45
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.52	0.45
17:P:83:LYS:O	17:P:86:ALA:HB3	2.16	0.45
23:V:39:ALA:N	23:V:40:PRO:CD	2.80	0.45
23:V:45:ARG:HH11	23:V:45:ARG:HG3	1.82	0.45
27:Z:60:CYS:O	27:Z:61:ASP:HB2	2.16	0.45
29:2:20:ARG:HB3	38:2:5444:HOH:O	2.17	0.45
1:0:51:G:O2'	1:0:52:A:H5'	2.16	0.45
1:0:200:U:H2'	38:0:3446:HOH:O	2.15	0.45
1:0:229:G:O2'	1:0:230:C:H5'	2.16	0.45
1:0:1477:C:H5'	1:0:1868:G:H5''	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1588:G:C5	1:0:1589:G:C6	3.05	0.45
1:0:2105:C:H2'	1:0:2106:C:C6	2.52	0.45
1:0:2428:G:N7	30:3:60:LYS:NZ	2.61	0.45
1:0:2649:A:H5'	1:0:2649:A:C8	2.52	0.45
3:A:82:VAL:HG13	3:A:93:THR:HB	1.98	0.45
26:Y:130:ARG:HB2	26:Y:142:SER:O	2.16	0.45
1:0:407:A:H5'	38:0:6034:HOH:O	2.15	0.45
1:0:2016:U:H2'	1:0:2017:U:C6	2.51	0.45
1:0:2864:U:C5	1:0:2865:G:C6	3.04	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.81	0.45
38:0:9988:HOH:O	13:L:22:ARG:HG2	2.15	0.45
2:9:3008:G:O6	15:N:11:ARG:NH1	2.39	0.45
2:9:3026:C:O2'	2:9:3027:C:H5'	2.17	0.45
3:A:33:GLU:H	3:A:33:GLU:CD	2.24	0.45
3:A:109:GLU:HG2	3:A:116:GLY:N	2.31	0.45
4:B:162:MET:CE	4:B:310:ARG:HD3	2.47	0.45
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.45
1:0:453:A:H4'	1:0:455:A:N7	2.32	0.45
1:0:1730:G:H4'	1:0:1731:C:H6	1.82	0.45
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.51	0.45
25:X:76:ARG:HH11	25:X:76:ARG:CG	2.28	0.45
25:X:76:ARG:HG3	25:X:76:ARG:NH1	2.28	0.45
26:Y:117:LEU:HA	26:Y:174:VAL:HG11	1.98	0.45
1:0:111:C:C2'	1:0:112:G:H5'	2.47	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.16	0.45
1:0:560:C:H2'	1:0:561:G:H8	1.82	0.45
1:0:1164:U:OP1	31:I:74:PRO:HA	2.17	0.45
1:0:1544:U:O2'	1:0:1545:C:H5'	2.17	0.45
1:0:2110:G:C2	1:0:2478:U:C2	3.04	0.45
1:0:2326:U:H4'	1:0:2412:G:C4'	2.46	0.45
1:0:2772:G:O2'	1:0:2773:G:H5'	2.16	0.45
1:0:2891:A:C2	1:0:2892:G:C4	3.05	0.45
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.45
1:0:244:C:OP2	8:F:38:LYS:HE3	2.17	0.45
1:0:289:G:N1	1:0:363:A:C2	2.81	0.45
1:0:696:C:O2'	1:0:731:U:OP1	2.33	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.16	0.45
1:0:1029:U:O2'	1:0:1273:C:OP1	2.32	0.45
1:0:1123:A:N1	1:0:1238:C:H5'	2.32	0.45
1:0:1150:A:C2	9:G:20:VAL:HG21	2.52	0.45
1:0:1252:A:H2'	1:0:1253:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1682:A:O2'	1:0:1683:G:H5''	2.17	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45
1:0:1940:C:H4'	38:0:7336:HOH:O	2.17	0.45
1:0:1973:A:H5'	1:0:1973:A:C8	2.45	0.45
1:0:2073:G:OP2	1:0:2490:A:H5'	2.16	0.45
1:0:2453:G:H4'	13:L:50:GLY:C	2.42	0.45
7:E:15:GLN:HG2	7:E:19:ASP:O	2.17	0.45
13:L:143:THR:HG22	13:L:144:ASP:H	1.81	0.45
15:N:110:THR:HB	15:N:113:SER:OG	2.17	0.45
30:3:69:TYR:O	30:3:77:ALA:HA	2.16	0.45
31:I:78:LEU:HD12	31:I:112:LYS:HZ2	1.80	0.45
1:0:292:G:H1'	1:0:360:A:H61	1.81	0.45
1:0:542:A:C5'	1:0:542:A:C8	2.95	0.45
1:0:1076:G:C2	1:0:1084:C:C2	3.05	0.45
1:0:2075:G:C6	1:0:2076:U:C4	3.05	0.45
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.45
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.45
1:0:2906:A:H5'	1:0:2907:C:O4'	2.17	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
5:C:2:GLN:HB3	38:C:8582:HOH:O	2.15	0.45
8:F:70:LYS:C	8:F:72:VAL:H	2.25	0.45
1:0:488:U:O2'	21:T:82:THR:HG21	2.17	0.45
1:0:670:G:H2'	1:0:671:A:C8	2.52	0.45
1:0:926:A:O2'	13:L:41:HIS:HD2	2.00	0.45
1:0:1238:C:H5''	1:0:1239:G:OP2	2.17	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.98	0.45
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.98	0.45
5:C:236:THR:HG22	5:C:239:ALA:CB	2.47	0.45
17:P:9:LEU:O	17:P:13:VAL:HG23	2.17	0.45
19:R:75:TRP:CG	19:R:76:ASP:H	2.35	0.45
24:W:139:GLY:O	24:W:141:HIS:CD2	2.70	0.45
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.17	0.44
1:0:538:C:N4	1:0:2061:C:H1'	2.32	0.44
1:0:660:A:N6	1:0:746:A:O4'	2.50	0.44
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.44
1:0:1188:A:C5	1:0:1189:A:C2	3.05	0.44
1:0:1279:U:O2	1:0:1279:U:H2'	2.17	0.44
1:0:2346:C:O2'	6:D:52:THR:HG21	2.17	0.44
1:0:2354:A:C2	1:0:2367:A:C8	3.04	0.44
1:0:2594:C:O2'	1:0:2595:U:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:95:GLU:CD	5:C:95:GLU:H	2.25	0.44
6:D:40:ILE:HG23	38:D:5583:HOH:O	2.17	0.44
11:J:53:ILE:O	11:J:57:TYR:HD1	2.00	0.44
15:N:179:LEU:HD23	15:N:184:ILE:CD1	2.47	0.44
18:Q:75:ILE:CD1	18:Q:84:ILE:HD11	2.47	0.44
22:U:52:THR:HG22	22:U:54:THR:HB	1.98	0.44
25:X:78:GLU:HG2	25:X:79:GLU:H	1.82	0.44
1:O:256:C:H2'	1:O:257:G:O4'	2.18	0.44
1:O:536:A:H3'	38:O:5051:HOH:O	2.16	0.44
1:O:957:A:H8	1:O:957:A:O5'	2.00	0.44
1:O:1494:A:O2'	1:O:1505:U:O2	2.34	0.44
1:O:2719:A:C2	4:B:70:PRO:HG3	2.52	0.44
2:9:3058:G:H1'	38:9:3839:HOH:O	2.16	0.44
2:9:3097:U:H2'	2:9:3098:C:C6	2.51	0.44
3:A:107:ASN:OD1	3:A:116:GLY:HA3	2.17	0.44
4:B:60:SER:HA	4:B:61:PRO:HD3	1.85	0.44
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.52	0.44
11:J:45:VAL:CG2	11:J:129:PHE:HD1	2.30	0.44
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.98	0.44
26:Y:151:SER:HB3	26:Y:154:ARG:HB3	2.00	0.44
1:O:111:C:H2'	1:O:112:G:C5'	2.46	0.44
1:O:263:U:C2	8:F:59:ILE:CD1	3.01	0.44
1:O:697:G:H4'	1:O:730:G:O3'	2.17	0.44
1:O:834:G:H3'	1:O:835:U:H4'	1.99	0.44
1:O:1174:A:C5	1:O:1201:C:H4'	2.53	0.44
1:O:1244:U:H4'	1:O:1246:A:O4'	2.17	0.44
1:O:1269:G:H2'	1:O:1270:U:C6	2.53	0.44
1:O:1334:C:O2'	1:O:1335:C:H5'	2.18	0.44
1:O:1972:U:C2'	1:O:1973:A:C5'	2.96	0.44
1:O:2133:U:H4'	1:O:2134:G:C5'	2.47	0.44
1:O:2716:G:O2'	1:O:2717:C:H5'	2.18	0.44
1:O:2900:G:C2'	1:O:2901:C:H5'	2.47	0.44
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.44
14:M:15:PRO:HA	14:M:20:LEU:HD23	2.00	0.44
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.52	0.44
31:I:92:PRO:C	31:I:94:GLU:H	2.24	0.44
1:O:2256:G:H2'	1:O:2257:G:O5'	2.17	0.44
1:O:2610:U:H4'	38:O:9479:HOH:O	2.18	0.44
4:B:18:ARG:HE	4:B:256:GLN:NE2	2.15	0.44
4:B:307:ARG:HA	38:B:8850:HOH:O	2.17	0.44
5:C:34:ALA:HB3	5:C:220:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.85	0.44
1:0:710:G:N2	1:0:719:C:C2	2.86	0.44
1:0:1309:U:C4	1:0:1310:U:C5	3.06	0.44
1:0:1667:A:H8	1:0:1667:A:C5'	2.18	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.18	0.44
1:0:1748:U:C5	1:0:1749:U:C4	3.06	0.44
1:0:2846:C:H4'	4:B:156:LYS:HB3	1.98	0.44
4:B:144:THR:HB	38:B:8921:HOH:O	2.18	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.98	0.44
1:0:538:C:H5''	1:0:539:G:C8	2.53	0.44
1:0:816:G:H5'	1:0:1598:A:H4'	2.00	0.44
1:0:929:A:O5'	1:0:929:A:H8	2.01	0.44
1:0:1117:A:C2	1:0:1244:U:C2	3.06	0.44
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.51	0.44
1:0:1523:G:H2'	1:0:1524:U:C6	2.53	0.44
1:0:1602:C:OP2	27:Z:46:ARG:NH2	2.51	0.44
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.18	0.44
1:0:2504:A:H4'	10:H:71:ARG:HH11	1.83	0.44
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.44
32:0:9000:13T:O2	32:0:9000:13T:H323	2.18	0.44
4:B:199:TYR:CE2	4:B:268:ARG:HB2	2.53	0.44
7:E:132:THR:HB	38:E:2227:HOH:O	2.17	0.44
12:K:14:LYS:CB	12:K:45:PRO:HG2	2.46	0.44
23:V:45:ARG:HG3	23:V:45:ARG:NH1	2.32	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.53	0.44
1:0:1771:U:O2'	1:0:1773:G:N7	2.48	0.44
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.17	0.44
1:0:2432:C:H1'	32:0:9000:13T:O9	2.17	0.44
4:B:321:PRO:HA	38:B:8952:HOH:O	2.16	0.44
5:C:129:HIS:CE1	5:C:232:LEU:H	2.36	0.44
24:W:90:TYR:CD1	24:W:90:TYR:N	2.85	0.44
1:0:413:G:H2'	1:0:414:C:C6	2.52	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.44
1:0:500:G:H21	19:R:98:ASN:ND2	2.13	0.44
1:0:622:G:P	26:Y:148:GLY:HA3	2.58	0.44
1:0:637:C:H2'	1:0:638:C:C6	2.52	0.44
1:0:920:C:H4'	1:0:921:G:N2	2.32	0.44
1:0:1069:C:O2'	1:0:1070:A:H5'	2.18	0.44
1:0:1280:A:OP1	1:0:1280:A:H3'	2.18	0.44
1:0:1730:G:H4'	1:0:1731:C:C6	2.53	0.44
1:0:1773:G:C8	27:Z:16:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2361:A:H2'	1:0:2362:A:C8	2.52	0.44
1:0:2577:A:H5'	38:0:7734:HOH:O	2.17	0.44
1:0:2802:C:H2'	1:0:2803:C:H6	1.81	0.44
1:0:2899:A:O2'	1:0:2900:G:H5'	2.18	0.44
38:0:7396:HOH:O	21:T:2:LYS:HE2	2.17	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
15:N:171:HIS:CE1	38:N:8862:HOH:O	2.71	0.44
1:0:238:C:H4'	1:0:287:C:OP1	2.18	0.44
1:0:276:C:H6	1:0:276:C:O5'	2.01	0.44
1:0:303:C:O2'	1:0:304:G:H5'	2.18	0.44
1:0:307:G:C2	1:0:309:C:C4	3.05	0.44
1:0:821:U:H4'	27:Z:17:ARG:NH1	2.33	0.44
1:0:1236:A:C8	11:J:63:ILE:HD11	2.53	0.44
1:0:2385:G:H2'	1:0:2386:U:H6	1.79	0.44
1:0:2691:A:OP1	1:0:2691:A:H8	2.01	0.44
2:9:3039:U:H3	2:9:3042:C:H5''	1.83	0.44
4:B:185:GLY:HA2	38:B:8929:HOH:O	2.17	0.44
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
1:0:1159:G:H1	1:0:1208:C:H42	1.64	0.43
1:0:1191:A:H2'	1:0:1193:A:H5'	2.00	0.43
1:0:1205:U:C2'	1:0:1206:U:C5'	2.87	0.43
1:0:1761:U:H5'	17:P:81:LYS:O	2.18	0.43
4:B:75:GLU:C	4:B:77:PRO:HD3	2.43	0.43
27:Z:36:ASP:HB3	27:Z:45:ASP:HB3	1.99	0.43
1:0:37:A:H2'	1:0:38:G:C8	2.52	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.18	0.43
1:0:338:C:H4'	5:C:174:ILE:HD12	1.98	0.43
1:0:1183:C:H42	1:0:1184:C:N4	2.12	0.43
1:0:1215:A:O3'	1:0:1216:G:C4'	2.66	0.43
1:0:1829:A:H5''	38:0:3081:HOH:O	2.17	0.43
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.43
1:0:2101:A:H2'	5:C:63:SER:OG	2.18	0.43
1:0:2821:C:H4'	4:B:116:PRO:HG3	2.00	0.43
1:0:2850:C:H6	1:0:2850:C:H5'	1.83	0.43
5:C:51:TYR:CE2	28:1:53:LYS:HB3	2.53	0.43
12:K:87:ARG:NH1	38:K:4066:HOH:O	2.51	0.43
1:0:195:C:H2'	1:0:196:G:H5'	2.00	0.43
1:0:1377:C:H6	1:0:1377:C:C5'	2.28	0.43
1:0:1624:A:H5'	1:0:1626:A:O4'	2.17	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2089:A:O2'	1:0:2090:G:H5'	2.18	0.43
32:0:9000:13T:H2	32:0:9000:13T:C26	2.42	0.43
38:0:7442:HOH:O	4:B:211:THR:HG21	2.19	0.43
3:A:194:MET:HE3	3:A:199:HIS:CB	2.48	0.43
1:0:99:A:C8	1:0:100:C:C5	3.06	0.43
1:0:304:G:H1'	1:0:347:A:H61	1.83	0.43
1:0:634:G:O2'	1:0:1358:A:OP1	2.33	0.43
1:0:772:G:H2'	1:0:773:A:O4'	2.17	0.43
1:0:1118:A:N6	1:0:1244:U:C2	2.86	0.43
1:0:1343:C:H2'	1:0:1344:G:O5'	2.19	0.43
1:0:1409:G:C2	1:0:1410:G:C8	3.06	0.43
1:0:1903:U:O2'	1:0:1904:A:N7	2.49	0.43
1:0:2002:C:H2'	1:0:2003:U:H5'	2.00	0.43
1:0:2252:A:C6	1:0:2253:G:H1'	2.54	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.01	0.43
5:C:115:LEU:HD12	5:C:115:LEU:HA	1.87	0.43
6:D:170:TYR:O	6:D:171:ASP:HB3	2.18	0.43
7:E:22:VAL:O	7:E:76:VAL:HG11	2.18	0.43
8:F:101:ALA:HA	38:F:5413:HOH:O	2.18	0.43
12:K:34:VAL:HG21	12:K:46:LYS:O	2.19	0.43
12:K:132:VAL:HG21	22:U:22:VAL:HG11	2.00	0.43
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.34	0.43
19:R:39:THR:HB	19:R:42:GLU:CD	2.44	0.43
20:S:33:SER:O	20:S:37:VAL:HG23	2.18	0.43
1:0:137:U:H2'	1:0:139:C:C5	2.53	0.43
1:0:187:A:H3'	1:0:188:C:H6	1.83	0.43
1:0:242:A:N6	1:0:269:G:H1'	2.34	0.43
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.43
1:0:2786:G:H2'	38:0:7180:HOH:O	2.17	0.43
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.43
5:C:185:LYS:HD3	5:C:186:TYR:CE1	2.53	0.43
5:C:193:LEU:HD13	5:C:222:ASP:HB2	2.00	0.43
6:D:49:PRO:HA	6:D:73:VAL:HG22	2.01	0.43
7:E:80:TRP:O	7:E:134:SER:HA	2.17	0.43
15:N:7:LYS:HE3	18:Q:21:ARG:O	2.19	0.43
19:R:132:ARG:HG2	19:R:133:ALA:N	2.32	0.43
1:0:69:A:C8	1:0:69:A:C5'	2.95	0.43
1:0:645:U:H2'	1:0:646:G:C8	2.54	0.43
1:0:1130:U:H4'	38:0:6133:HOH:O	2.18	0.43
1:0:1183:C:O2	1:0:1183:C:C2'	2.67	0.43
1:0:1186:C:H5''	31:I:119:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1439:C:O5'	1:0:1439:C:H6	2.01	0.43
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.43
1:0:2779:G:N2	1:0:2796:U:C2	2.87	0.43
1:0:2812:A:H2	1:0:2814:A:N6	1.91	0.43
1:0:2840:A:OP1	4:B:211:THR:HG23	2.19	0.43
4:B:88:GLU:O	4:B:88:GLU:HG3	2.18	0.43
8:F:56:PRO:CG	14:M:44:THR:HA	2.48	0.43
9:G:20:VAL:O	9:G:24:VAL:HG23	2.19	0.43
24:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
1:0:365:G:C5	1:0:366:U:C5	3.07	0.43
1:0:947:U:O2'	1:0:948:G:H5'	2.18	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.43
1:0:1215:A:O3'	1:0:1216:G:H4'	2.19	0.43
1:0:1257:C:O2'	1:0:1258:G:H5'	2.18	0.43
1:0:1386:G:O2'	1:0:1387:G:H5'	2.19	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
1:0:1778:A:H2'	1:0:1779:A:H5'	2.00	0.43
1:0:1883:U:H5'	1:0:2012:U:OP2	2.19	0.43
1:0:1904:A:H2'	1:0:1905:U:O4'	2.19	0.43
1:0:2460:A:C4	32:0:9000:13T:H20	2.53	0.43
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.34	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
11:J:47:THR:HG22	11:J:48:GLY:N	2.34	0.43
14:M:46:LEU:HG	38:M:8913:HOH:O	2.18	0.43
24:W:13:MET:CE	24:W:18:GLN:HA	2.49	0.43
24:W:106:THR:OG1	24:W:109:GLU:HB2	2.19	0.43
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:445:U:O2'	1:0:446:G:H5'	2.18	0.43
1:0:1415:G:H5'	28:1:12:ASN:O	2.18	0.43
1:0:1434:A:H2'	1:0:1436:C:C5	2.53	0.43
1:0:1565:C:O2'	1:0:1566:C:H5'	2.19	0.43
1:0:1850:U:O4'	1:0:1941:A:C2	2.71	0.43
1:0:2036:C:C4'	12:K:44:LEU:HG	2.48	0.43
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
1:0:2856:A:OP1	25:X:15:ARG:NH2	2.51	0.43
38:0:6721:HOH:O	18:Q:2:SER:HA	2.19	0.43
38:0:9208:HOH:O	4:B:248:ARG:NH2	2.51	0.43
2:9:3069:U:OP1	15:N:4:PRO:HG3	2.18	0.43
4:B:33:ASP:HB3	4:B:34:GLY:H	1.60	0.43
11:J:127:ILE:CG2	36:J:8801:CL:CL	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.54	0.43
31:I:125:ALA:O	31:I:129:VAL:HG23	2.19	0.43
1:0:134:U:C2	1:0:145:A:C2	3.07	0.43
1:0:228:C:C2'	1:0:229:G:H5'	2.49	0.43
1:0:1191:A:H2	1:0:1206:U:H3	1.67	0.43
1:0:1825:U:O2'	1:0:1826:C:H5'	2.19	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.43
1:0:2254:G:C2	1:0:2255:A:C8	3.06	0.43
1:0:2372:A:H2'	1:0:2373:U:H6	1.82	0.43
32:0:9000:13T:H3	30:3:56:PRO:CB	2.48	0.43
6:D:138:GLY:N	38:D:7597:HOH:O	2.51	0.43
7:E:20:ILE:HD11	7:E:40:VAL:HG11	2.01	0.43
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.49	0.43
20:S:57:THR:C	20:S:59:ASP:H	2.26	0.43
1:0:73:C:O2'	1:0:74:A:H5'	2.18	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.34	0.43
1:0:815:U:O2'	1:0:1598:A:H4'	2.18	0.43
1:0:1080:C:O5'	1:0:1080:C:H6	2.02	0.43
1:0:1114:A:H2'	1:0:1115:U:C6	2.54	0.43
1:0:1163:G:H1	1:0:1184:C:N4	2.17	0.43
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.52	0.43
1:0:1667:A:C2	1:0:1668:U:C2	3.07	0.43
1:0:1805:G:H2'	1:0:1806:G:H8	1.83	0.43
1:0:2255:A:H2'	1:0:2256:G:O4'	2.18	0.43
1:0:2255:A:O2'	1:0:2256:G:H5'	2.18	0.43
1:0:2348:C:H1'	6:D:131:THR:HG21	2.01	0.43
1:0:2598:U:O2	1:0:2600:A:H8	2.00	0.43
4:B:177:HIS:O	4:B:181:ILE:HG13	2.19	0.43
5:C:173:LYS:NZ	38:C:8612:HOH:O	2.44	0.43
6:D:167:GLU:C	6:D:169:THR:H	2.27	0.43
11:J:45:VAL:HG21	11:J:129:PHE:HD1	1.82	0.43
14:M:80:GLY:O	14:M:81:ARG:HD3	2.18	0.43
24:W:4:LEU:O	24:W:32:CYS:HA	2.18	0.43
26:Y:107:PRO:HD3	26:Y:182:PHE:CD1	2.54	0.43
29:2:40:ARG:HG3	29:2:45:ASN:CB	2.48	0.43
1:0:559:U:C5	1:0:560:C:C5	3.07	0.42
1:0:571:C:O5'	1:0:571:C:H6	2.01	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.42
1:0:1242:A:OP2	11:J:60:ARG:NH2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1930:A:H2'	1:0:1931:A:C8	2.54	0.42
1:0:2291:A:H8	38:0:6467:HOH:O	2.01	0.42
1:0:2504:A:H4'	10:H:71:ARG:NH1	2.34	0.42
1:0:2519:C:O2'	1:0:2520:G:H5'	2.19	0.42
1:0:2712:G:H5'	38:0:5223:HOH:O	2.18	0.42
32:0:9000:13T:H233	32:0:9000:13T:H311	2.01	0.42
38:0:6400:HOH:O	24:W:122:ARG:NH2	2.45	0.42
5:C:194:PHE:HA	5:C:234:VAL:HG13	2.01	0.42
6:D:103:ASN:HD22	6:D:133:ASN:HA	1.84	0.42
22:U:17:THR:HG22	22:U:18:GLY:N	2.34	0.42
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.34	0.42
28:1:53:LYS:HA	28:1:53:LYS:HD3	1.85	0.42
1:0:169:A:H1'	30:3:48:ASN:ND2	2.34	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.19	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
1:0:952:G:OP1	18:Q:42:LYS:HE2	2.20	0.42
1:0:1138:G:H4'	38:0:5719:HOH:O	2.19	0.42
1:0:1552:G:H2'	1:0:1553:C:C6	2.54	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
2:9:3041:C:C2	6:D:50:VAL:HG21	2.54	0.42
3:A:36:ASP:C	3:A:38:ILE:H	2.26	0.42
6:D:44:ILE:HG23	6:D:45:THR:HG23	2.00	0.42
10:H:47:ILE:HG21	38:H:8579:HOH:O	2.20	0.42
16:O:21:SER:OG	16:O:106:PRO:HB2	2.18	0.42
16:O:105:ASN:HD21	16:O:109:SER:N	2.18	0.42
19:R:4:TYR:CE1	19:R:15:LYS:HD3	2.53	0.42
21:T:28:SER:O	21:T:32:ARG:HG3	2.18	0.42
26:Y:178:HIS:CG	26:Y:179:PRO:HD2	2.54	0.42
1:0:151:A:H2'	1:0:152:A:O4'	2.18	0.42
1:0:284:C:C4'	1:0:285:A:O5'	2.64	0.42
1:0:644:G:O2'	36:0:8814:CL:CL	2.67	0.42
1:0:1544:U:H2'	1:0:1545:C:C6	2.54	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.35	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
1:0:2608:C:H3'	38:0:7790:HOH:O	2.18	0.42
1:0:2785:C:H4'	1:0:2786:G:OP2	2.19	0.42
38:0:4740:HOH:O	15:N:21:HIS:HD2	2.01	0.42
4:B:165:ARG:HG2	4:B:166:VAL:N	2.35	0.42
4:B:204:GLY:HA3	38:B:8948:HOH:O	2.18	0.42
6:D:91:ALA:HB1	38:D:5198:HOH:O	2.19	0.42
20:S:37:VAL:O	20:S:41:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1486:A:C5	29:2:2:LYS:HG3	2.55	0.42
1:0:2296:C:H2'	1:0:2297:U:H6	1.82	0.42
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.42
2:9:3001:U:H4'	2:9:3003:A:OP1	2.19	0.42
14:M:167:GLY:O	14:M:171:ARG:HG3	2.19	0.42
15:N:82:TYR:CD2	15:N:82:TYR:C	2.97	0.42
16:O:44:ASN:HA	16:O:65:LEU:O	2.19	0.42
22:U:6:CYS:HB2	22:U:32:CYS:HB3	2.00	0.42
1:0:263:U:C4	8:F:54:VAL:HG13	2.54	0.42
1:0:395:A:H4'	38:0:9964:HOH:O	2.20	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.19	0.42
1:0:958:G:O2'	1:0:959:C:H5'	2.19	0.42
1:0:2035:C:O5'	1:0:2035:C:H6	2.02	0.42
1:0:2395:A:C6	1:0:2396:C:C4	3.07	0.42
1:0:2502:C:O2'	1:0:2503:A:H5'	2.18	0.42
1:0:2909:G:O2'	1:0:2910:A:H5'	2.20	0.42
2:9:3031:C:H1'	38:9:1137:HOH:O	2.18	0.42
12:K:28:GLU:HB3	12:K:59:LYS:HB2	2.01	0.42
13:L:73:VAL:HG11	13:L:118:LEU:HD21	2.01	0.42
15:N:71:TRP:CE3	15:N:175:LEU:HD22	2.55	0.42
17:P:103:THR:O	17:P:107:GLU:HG3	2.20	0.42
28:1:26:SER:HB3	28:1:35:SER:OG	2.20	0.42
1:0:475:G:C5'	5:C:73:LEU:HD23	2.50	0.42
1:0:482:G:O4'	1:0:511:A:C2	2.72	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:1046:G:N3	1:0:1082:A:H2	2.17	0.42
1:0:1175:G:H1'	1:0:1193:A:H2'	2.01	0.42
1:0:2105:C:O2'	1:0:2284:G:N2	2.52	0.42
1:0:2265:U:H2'	1:0:2266:A:C8	2.55	0.42
1:0:2607:U:H4'	38:0:9438:HOH:O	2.18	0.42
2:9:3034:A:H8	2:9:3034:A:O5'	2.02	0.42
3:A:9:ARG:NH1	38:A:8822:HOH:O	2.53	0.42
11:J:39:VAL:HG13	11:J:106:GLY:O	2.20	0.42
14:M:28:GLN:O	14:M:32:ARG:HG3	2.18	0.42
15:N:170:GLU:O	15:N:174:GLU:HG3	2.20	0.42
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.42
25:X:80:GLU:HB3	38:X:5564:HOH:O	2.17	0.42
26:Y:151:SER:HB3	26:Y:154:ARG:CB	2.49	0.42
1:0:316:A:H5'	21:T:54:ASP:OD2	2.20	0.42
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.42
1:0:535:G:C6	1:0:2064:U:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:876:A:N3	1:0:876:A:C2'	2.83	0.42
1:0:1323:G:N2	1:0:1335:C:C2	2.88	0.42
32:0:9000:13T:H323	32:0:9000:13T:C1	2.49	0.42
38:0:3186:HOH:O	14:M:9:ARG:HG3	2.19	0.42
2:9:3059:C:H5'	38:9:5233:HOH:O	2.18	0.42
2:9:3110:G:C5	2:9:3111:U:C5	3.07	0.42
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.42
6:D:25:MET:HE1	6:D:37:ALA:O	2.19	0.42
8:F:117:GLU:C	8:F:119:ARG:N	2.76	0.42
11:J:59:LYS:O	11:J:63:ILE:HG13	2.19	0.42
14:M:47:ASP:CG	14:M:48:LYS:N	2.78	0.42
30:3:22:VAL:HG11	30:3:67:LEU:HD13	2.01	0.42
1:0:447:A:OP1	21:T:2:LYS:HG2	2.20	0.42
1:0:595:U:H2'	1:0:596:C:H6	1.85	0.42
1:0:1161:A:O5'	1:0:1161:A:H8	2.02	0.42
1:0:1579:C:H4'	1:0:1580:A:OP1	2.19	0.42
1:0:2078:U:O2'	1:0:2079:G:H5'	2.20	0.42
1:0:2256:G:C2'	1:0:2257:G:C5'	2.93	0.42
1:0:2836:G:O2'	1:0:2838:A:N7	2.52	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.42
38:0:3652:HOH:O	16:O:3:THR:HG21	2.19	0.42
38:0:4574:HOH:O	5:C:50:GLU:HG2	2.20	0.42
2:9:3013:A:H3'	2:9:3014:G:H5'	2.02	0.42
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.02	0.42
5:C:218:VAL:HG12	38:C:8623:HOH:O	2.19	0.42
12:K:4:LEU:HD23	12:K:4:LEU:HA	1.83	0.42
13:L:120:LEU:HD12	13:L:133:VAL:HG21	2.02	0.42
1:0:282:C:O2'	1:0:283:U:C4'	2.68	0.42
1:0:318:C:H5'	1:0:339:A:N3	2.35	0.42
1:0:589:U:H2'	1:0:590:A:C8	2.54	0.42
1:0:825:U:H5''	1:0:826:U:OP1	2.20	0.42
1:0:856:G:H2'	38:0:5435:HOH:O	2.18	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.20	0.42
1:0:1923:G:H2'	1:0:1924:A:H8	1.84	0.42
1:0:2758:G:H2'	1:0:2759:C:C6	2.55	0.42
2:9:3059:C:H2'	2:9:3060:C:C6	2.55	0.42
4:B:14:GLY:HA2	4:B:15:PRO:C	2.44	0.42
6:D:64:ARG:HD3	6:D:67:ASP:HB3	2.02	0.42
15:N:152:GLU:C	15:N:154:LEU:H	2.28	0.42
19:R:4:TYR:CZ	19:R:17:MET:HE2	2.54	0.42
26:Y:170:SER:OG	26:Y:175:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:561:G:C2	1:0:562:A:C5	3.08	0.42
1:0:1055:G:OP2	10:H:96:ARG:NH1	2.53	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.42
1:0:2240:U:O2'	1:0:2241:C:H5'	2.19	0.42
1:0:2521:A:P	10:H:3:ALA:HB3	2.60	0.42
1:0:2612:A:H4'	38:0:3685:HOH:O	2.19	0.42
1:0:2824:C:O3'	1:0:2825:C:H6	2.01	0.42
2:9:3114:G:H2'	2:9:3115:C:C6	2.55	0.42
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.01	0.42
4:B:305:ASP:O	4:B:306:LYS:CB	2.68	0.42
6:D:23:VAL:HG21	6:D:45:THR:HG21	2.02	0.42
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.50	0.42
19:R:132:ARG:NH2	38:R:8879:HOH:O	2.52	0.42
1:0:517:U:C2'	1:0:518:G:H5'	2.50	0.41
1:0:941:G:C2'	1:0:942:U:H5'	2.50	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
1:0:1019:C:O2	18:Q:94:GLN:NE2	2.53	0.41
1:0:1762:C:H4'	38:0:4662:HOH:O	2.19	0.41
1:0:2032:U:O2'	1:0:2033:G:H5'	2.20	0.41
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.55	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:2589:U:H2'	1:0:2590:U:C6	2.55	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
2:9:3059:C:H6	2:9:3059:C:O5'	2.03	0.41
2:9:3105:A:C2'	2:9:3106:C:H5'	2.49	0.41
3:A:65:ARG:C	3:A:66:ARG:HG3	2.44	0.41
3:A:76:VAL:HG23	27:Z:63:LYS:HB3	2.00	0.41
3:A:131:HIS:O	3:A:132:ASP:HB2	2.20	0.41
4:B:260:HIS:HE1	38:B:8883:HOH:O	2.03	0.41
6:D:25:MET:SD	6:D:40:ILE:HD11	2.60	0.41
6:D:48:MET:HA	6:D:49:PRO:HD3	1.87	0.41
12:K:26:ALA:HB2	12:K:64:MET:HE3	2.02	0.41
19:R:18:LEU:HD12	19:R:143:VAL:HG11	2.02	0.41
1:0:381:G:OP2	14:M:45:ARG:NH2	2.50	0.41
1:0:497:A:H2'	1:0:498:A:C5'	2.50	0.41
1:0:553:G:H2'	1:0:554:G:H5'	2.02	0.41
1:0:699:C:C6	1:0:744:G:C4	3.08	0.41
1:0:1904:A:C8	1:0:1905:U:C5	3.08	0.41
1:0:2112:A:H2'	1:0:2113:G:H8	1.85	0.41
1:0:2254:G:O2'	1:0:2255:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2402:A:H1'	38:0:3163:HOH:O	2.20	0.41
1:0:2689:A:C2'	1:0:2690:U:H5'	2.50	0.41
1:0:2754:G:C2'	1:0:2755:G:H5'	2.50	0.41
6:D:49:PRO:HG3	38:D:5828:HOH:O	2.21	0.41
8:F:14:ASP:O	8:F:18:GLU:HG3	2.20	0.41
8:F:48:VAL:HG23	8:F:74:PHE:HB3	2.01	0.41
14:M:164:THR:HG22	14:M:167:GLY:N	2.35	0.41
22:U:17:THR:CG2	22:U:18:GLY:N	2.83	0.41
28:1:25:LYS:HD2	29:2:49:GLU:H	1.84	0.41
31:I:100:LEU:HD22	31:I:105:VAL:HG23	2.02	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.41
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.41
1:0:459:A:H5''	38:0:9047:HOH:O	2.20	0.41
1:0:694:A:H4'	1:0:2441:U:OP1	2.21	0.41
1:0:902:G:N7	13:L:18:HIS:CD2	2.85	0.41
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
1:0:1225:C:H2'	1:0:1226:G:O4'	2.21	0.41
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.41
1:0:1576:G:H2'	1:0:1577:U:H6	1.85	0.41
1:0:2434:A:O3'	30:3:28:GLY:HA3	2.20	0.41
2:9:3033:U:H2'	38:9:3797:HOH:O	2.19	0.41
2:9:3042:C:O2	6:D:76:ARG:NH1	2.52	0.41
2:9:3105:A:H2'	2:9:3106:C:H5'	2.03	0.41
7:E:84:MET:HG2	7:E:168:ILE:HA	2.02	0.41
10:H:154:TYR:CD1	10:H:154:TYR:C	2.97	0.41
10:H:171:ALA:HA	38:H:8570:HOH:O	2.20	0.41
21:T:9:LYS:HE3	21:T:13:ARG:NH1	2.35	0.41
24:W:4:LEU:CD1	24:W:24:LEU:HD13	2.50	0.41
27:Z:30:GLU:HB2	38:Z:8715:HOH:O	2.20	0.41
28:1:25:LYS:HE2	38:2:7213:HOH:O	2.20	0.41
31:I:91:GLU:HA	31:I:92:PRO:HD2	1.84	0.41
1:0:81:G:N3	1:0:98:A:C2	2.89	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.54	0.41
1:0:1422:U:H4'	38:0:7732:HOH:O	2.19	0.41
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.41
1:0:1943:C:C4'	3:A:212:PRO:HA	2.50	0.41
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.86	0.41
1:0:2634:G:OP2	3:A:204:GLY:N	2.53	0.41
1:0:2825:C:H4'	1:0:2826:G:O5'	2.20	0.41
11:J:74:ARG:HH11	11:J:74:ARG:CB	2.30	0.41
15:N:42:HIS:CG	15:N:62:HIS:HE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:7:GLU:HA	25:X:74:ALA:O	2.20	0.41
1:0:61:G:C6	1:0:62:C:C4	3.09	0.41
1:0:308:U:C4	1:0:342:C:C1'	3.03	0.41
1:0:849:C:O2'	1:0:850:U:H5'	2.21	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.56	0.41
1:0:1024:G:C6	1:0:1025:C:C4	3.08	0.41
1:0:1052:G:N3	1:0:1052:G:H2'	2.35	0.41
1:0:1170:U:O2'	1:0:1172:G:N7	2.47	0.41
1:0:1400:C:O2'	1:0:1401:G:H5'	2.21	0.41
1:0:1923:G:H2'	1:0:1924:A:C8	2.56	0.41
2:9:3001:U:H5'	2:9:3121:C:O2	2.20	0.41
2:9:3001:U:O3'	2:9:3003:A:C5'	2.69	0.41
2:9:3092:G:C6	2:9:3093:A:N6	2.88	0.41
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.86	0.41
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.48	0.41
14:M:182:LYS:HB2	14:M:194:ALA:HB2	2.01	0.41
25:X:74:ALA:CB	25:X:85:VAL:HG22	2.51	0.41
27:Z:67:GLY:N	27:Z:70:LYS:O	2.54	0.41
1:0:255:A:C5	1:0:256:C:C5	3.09	0.41
1:0:863:G:C6	1:0:864:U:C4	3.08	0.41
1:0:1206:U:H6	1:0:1206:U:C5'	2.23	0.41
1:0:2775:A:C6	1:0:2776:A:C6	3.08	0.41
4:B:4:SER:O	4:B:5:ARG:HB2	2.19	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.51	0.41
18:Q:16:ASN:OD1	18:Q:45:PRO:HB2	2.20	0.41
24:W:19:ASP:O	24:W:23:MET:HG3	2.20	0.41
1:0:25:A:O2'	1:0:640:G:H5'	2.21	0.41
1:0:298:C:H6	1:0:298:C:O5'	2.04	0.41
1:0:1181:A:C2'	1:0:1182:C:H5'	2.51	0.41
1:0:1224:G:H2'	1:0:1225:C:C6	2.55	0.41
1:0:2549:C:O2'	1:0:2550:U:H5'	2.20	0.41
4:B:7:ARG:HH11	4:B:7:ARG:HG2	1.85	0.41
7:E:5:LEU:HD21	7:E:66:GLN:HG3	2.01	0.41
14:M:123:ASP:OD1	14:M:126:GLN:HG2	2.19	0.41
24:W:119:HIS:HD2	24:W:120:PRO:O	2.03	0.41
1:0:247:A:H1'	38:0:3892:HOH:O	2.21	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.20	0.41
1:0:539:G:H2'	1:0:540:A:C8	2.56	0.41
1:0:912:A:C4	1:0:1294:A:C2	3.09	0.41
1:0:1021:G:O2'	1:0:1022:A:H5'	2.19	0.41
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1622:G:H2'	1:0:1623:C:H5'	2.02	0.41
1:0:2036:C:C1'	12:K:44:LEU:HG	2.51	0.41
1:0:2303:A:H2	38:Q:5641:HOH:O	2.03	0.41
1:0:2365:G:H4'	18:Q:45:PRO:O	2.20	0.41
1:0:2716:G:H5''	4:B:206:THR:CG2	2.44	0.41
2:9:3003:A:H61	2:9:3022:G:H1'	1.83	0.41
12:K:132:VAL:HG21	22:U:22:VAL:CG1	2.50	0.41
13:L:92:ASP:HA	13:L:121:ILE:HB	2.02	0.41
14:M:158:ARG:HB2	14:M:163:LEU:HB2	2.03	0.41
19:R:72:VAL:CG1	19:R:75:TRP:HB3	2.50	0.41
20:S:45:TYR:O	20:S:80:ARG:NH2	2.53	0.41
26:Y:144:ARG:NH2	38:Y:8912:HOH:O	2.54	0.41
1:0:66:G:C2	1:0:109:U:C4	3.08	0.41
1:0:169:A:H4'	38:M:8837:HOH:O	2.20	0.41
1:0:287:C:H6	1:0:287:C:O5'	2.04	0.41
1:0:327:A:H4'	1:0:329:A:C8	2.55	0.41
1:0:368:C:H2'	1:0:369:G:H5'	2.02	0.41
1:0:483:C:C4	1:0:484:A:C6	3.09	0.41
1:0:567:U:O2'	1:0:568:G:H5'	2.20	0.41
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.41
1:0:911:G:H5'	1:0:932:U:OP1	2.21	0.41
1:0:1115:U:O2'	1:0:1116:U:H5'	2.20	0.41
1:0:1116:U:C2	1:0:1246:A:N6	2.89	0.41
1:0:1157:C:O2'	1:0:1158:G:H5'	2.20	0.41
1:0:1166:A:P	1:0:1174:A:H4'	2.61	0.41
1:0:1619:G:C6	1:0:1620:C:N3	2.89	0.41
1:0:1630:A:O2'	1:0:1631:A:H5'	2.21	0.41
1:0:1666:C:H2'	1:0:1667:A:H8	1.86	0.41
1:0:1786:C:OP1	17:P:74:GLN:HG2	2.21	0.41
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.21	0.41
1:0:2415:A:O2'	15:N:29:SER:HB3	2.21	0.41
1:0:2569:A:H2'	1:0:2570:G:O5'	2.20	0.41
1:0:2607:U:C4	4:B:242:TRP:CZ2	3.08	0.41
1:0:2727:A:N1	1:0:2756:U:C2	2.89	0.41
1:0:2768:A:H5''	38:0:4432:HOH:O	2.21	0.41
2:9:3001:U:C4'	2:9:3003:A:OP1	2.69	0.41
2:9:3040:C:OP1	2:9:3041:C:H5	2.04	0.41
2:9:3065:A:O2'	2:9:3066:G:P	2.79	0.41
2:9:3104:A:C2'	2:9:3105:A:H5'	2.50	0.41
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:186:TRP:CG	3:A:187:PRO:HA	2.56	0.41
4:B:23:THR:HG23	4:B:308:LEU:CD2	2.51	0.41
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.56	0.41
4:B:52:VAL:O	4:B:53:LEU:HD12	2.21	0.41
4:B:265:LEU:HD21	4:B:316:ARG:HD3	2.01	0.41
4:B:329:TYR:CE2	22:U:15:PRO:HG2	2.56	0.41
5:C:228:ALA:HA	5:C:229:PRO:HD3	1.90	0.41
6:D:59:GLY:C	6:D:61:PHE:H	2.29	0.41
6:D:151:ILE:HA	6:D:152:PRO:HD3	1.92	0.41
11:J:42:GLU:HG2	11:J:43:ARG:HG3	2.03	0.41
19:R:113:HIS:O	19:R:145:LEU:HD12	2.20	0.41
21:T:3:GLN:HA	21:T:4:PRO:HD3	1.76	0.41
21:T:32:ARG:NH1	21:T:38:ARG:NH1	2.69	0.41
22:U:6:CYS:C	22:U:8:TYR:N	2.79	0.41
24:W:81:ASP:OD1	24:W:92:ASP:HB2	2.20	0.41
31:I:131:THR:O	31:I:135:LEU:HG	2.21	0.41
1:0:380:A:O4'	1:0:382:U:H1'	2.21	0.41
1:0:397:A:H1'	1:0:417:G:H1'	2.02	0.41
1:0:716:G:C6	1:0:717:C:N4	2.89	0.41
1:0:1182:C:O5'	1:0:1182:C:H6	2.02	0.41
1:0:1299:G:N2	38:0:4691:HOH:O	2.53	0.41
1:0:1594:C:OP1	17:P:109:ARG:NH1	2.54	0.41
1:0:1662:C:H2'	1:0:1663:G:O4'	2.21	0.41
1:0:2004:U:H5''	1:0:2005:G:C8	2.56	0.41
1:0:2363:G:H2'	1:0:2364:A:O4'	2.21	0.41
1:0:2791:U:H4'	1:0:2792:A:OP1	2.21	0.41
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.41
1:0:2897:C:O2'	1:0:2898:G:H5'	2.21	0.41
32:0:9000:13T:H261	32:0:9000:13T:H10	1.80	0.41
3:A:68:ILE:HD11	38:A:8863:HOH:O	2.20	0.41
13:L:119:THR:HA	13:L:139:SER:O	2.21	0.41
17:P:115:SER:O	17:P:117:SER:N	2.46	0.41
26:Y:144:ARG:NE	38:Y:8912:HOH:O	2.54	0.41
1:0:228:C:H2'	1:0:229:G:C5'	2.51	0.40
1:0:445:U:C1'	38:0:7326:HOH:O	2.68	0.40
1:0:545:G:H2'	1:0:546:C:O4'	2.21	0.40
1:0:1449:G:N3	1:0:1449:G:H2'	2.36	0.40
1:0:1745:G:H5'	38:0:4341:HOH:O	2.20	0.40
1:0:1925:G:O2'	1:0:1926:G:H5'	2.21	0.40
1:0:2072:G:H3'	1:0:2073:G:C5'	2.52	0.40
1:0:2549:C:H2'	1:0:2550:U:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.40
1:0:2887:G:H2'	1:0:2888:U:O4'	2.21	0.40
4:B:198:GLU:HA	38:B:8952:HOH:O	2.20	0.40
4:B:305:ASP:O	4:B:306:LYS:HB2	2.21	0.40
4:B:336:GLN:NE2	38:B:8822:HOH:O	2.53	0.40
7:E:22:VAL:O	7:E:28:SER:HA	2.22	0.40
7:E:172:PRO:HB3	38:E:6931:HOH:O	2.21	0.40
9:G:67:LEU:O	9:G:71:LEU:HG	2.21	0.40
19:R:89:LEU:HD23	19:R:89:LEU:HA	1.84	0.40
26:Y:189:ASN:ND2	26:Y:192:ASP:N	2.69	0.40
1:0:535:G:O6	1:0:2064:U:C6	2.75	0.40
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.40
1:0:567:U:O5'	1:0:567:U:H6	2.04	0.40
1:0:699:C:H6	1:0:744:G:O4'	2.03	0.40
1:0:1310:U:P	5:C:168:ARG:HH11	2.44	0.40
1:0:1457:U:H5	38:0:7859:HOH:O	2.04	0.40
1:0:1494:A:H1'	1:0:1495:C:C6	2.56	0.40
1:0:1574:C:O5'	1:0:1574:C:H6	2.04	0.40
1:0:1642:A:N7	1:0:1643:C:C4	2.89	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2064:U:H2'	1:0:2065:C:H6	1.86	0.40
1:0:2344:G:H2'	1:0:2344:G:N3	2.36	0.40
1:0:2361:A:H2'	1:0:2362:A:O4'	2.21	0.40
1:0:2453:G:O3'	13:L:50:GLY:HA2	2.21	0.40
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.54	0.40
26:Y:134:HIS:H	26:Y:134:HIS:CD2	2.38	0.40
1:0:74:A:H2'	1:0:75:U:C6	2.55	0.40
1:0:574:C:H2'	1:0:575:G:O4'	2.21	0.40
1:0:844:A:C6	1:0:882:A:C6	3.09	0.40
1:0:1268:C:O2'	26:Y:169:ARG:HB2	2.21	0.40
1:0:1902:G:H2'	1:0:1903:U:O4'	2.21	0.40
1:0:2642:G:H2'	1:0:2643:G:O4'	2.22	0.40
1:0:2902:A:H4'	1:0:2903:C:OP1	2.21	0.40
3:A:105:VAL:HG12	3:A:106:CYS:N	2.36	0.40
14:M:72:ALA:HB2	14:M:93:ARG:HG2	2.03	0.40
17:P:121:ASP:HB2	38:P:5891:HOH:O	2.21	0.40
24:W:65:VAL:HG12	24:W:116:LEU:HD13	2.04	0.40
26:Y:177:LYS:HD3	26:Y:181:GLY:O	2.22	0.40
1:0:243:A:H2	1:0:274:G:N3	2.19	0.40
1:0:260:C:C4	1:0:261:A:C5	3.10	0.40
1:0:474:C:O3'	5:C:73:LEU:HD21	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:517:U:H2'	1:0:518:G:H5'	2.03	0.40
1:0:559:U:C6	1:0:559:U:C4'	3.04	0.40
1:0:705:C:O2	1:0:705:C:C2'	2.70	0.40
1:0:1006:A:N1	1:0:2311:A:H1'	2.37	0.40
1:0:1087:G:H4'	1:0:1088:A:OP1	2.22	0.40
1:0:1180:U:O2'	31:I:92:PRO:HD2	2.21	0.40
1:0:1189:A:C3'	38:0:7666:HOH:O	2.62	0.40
1:0:1308:A:O4'	5:C:226:GLY:HA3	2.21	0.40
1:0:1309:U:H2'	1:0:1310:U:O4'	2.21	0.40
1:0:1705:C:P	17:P:59:ARG:HH12	2.45	0.40
1:0:1741:U:H3'	38:0:9763:HOH:O	2.20	0.40
1:0:2673:U:C4	1:0:2674:G:C6	3.10	0.40
2:9:3110:G:C2'	2:9:3111:U:H5'	2.51	0.40
38:9:466:HOH:O	18:Q:25:PRO:HB3	2.21	0.40
5:C:175:LYS:HD2	5:C:187:ARG:HB3	2.04	0.40
6:D:64:ARG:HB3	6:D:67:ASP:OD2	2.22	0.40
12:K:62:PRO:HG3	12:K:65:ARG:NH2	2.37	0.40
16:O:14:LEU:HB3	16:O:26:TRP:O	2.21	0.40
16:O:45:LEU:CD1	16:O:88:LYS:HD2	2.51	0.40
1:0:160:A:C4	1:0:177:A:C2	3.09	0.40
1:0:245:C:H2'	1:0:246:G:H5'	2.04	0.40
1:0:820:G:H5'	1:0:821:U:C5'	2.51	0.40
1:0:1329:A:H5''	38:0:3790:HOH:O	2.20	0.40
1:0:1334:C:H2'	1:0:1335:C:H6	1.86	0.40
1:0:1453:G:H2'	1:0:1454:U:O4'	2.22	0.40
1:0:1544:U:H2'	1:0:1545:C:H6	1.87	0.40
1:0:1617:C:C4	1:0:1643:C:H4'	2.57	0.40
1:0:2739:A:C6	1:0:2740:G:C5	3.09	0.40
7:E:6:GLU:HA	7:E:46:THR:HG22	2.03	0.40
14:M:28:GLN:HA	14:M:31:TRP:HB2	2.03	0.40
17:P:40:VAL:O	17:P:44:VAL:HG23	2.22	0.40
23:V:39:ALA:O	23:V:41:GLU:N	2.51	0.40
25:X:8:ARG:NH1	38:X:2479:HOH:O	2.49	0.40
27:Z:49:ARG:NH2	27:Z:52:THR:HA	2.37	0.40
29:2:49:GLU:HB2	38:2:131:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	212 (90%)	21 (9%)	2 (1%)	14	41
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	10	34
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	16	44
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	5	20
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	21	51
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	4	17
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	6	23
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	30
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100	100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	5	20
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	18	48
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	11	36
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	41
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	9	32
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	9	32
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	14	41

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP
15	N	184	ILE
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
6	D	27	ILE
6	D	137	PRO
6	D	173	GLU
8	F	44	SER
24	W	49	ASN
3	A	37	VAL
15	N	139	TRP
27	Z	42	CYS
5	C	79	ARG
10	H	16	ARG
10	H	168	ALA
17	P	117	SER
25	X	70	ILE
4	B	2	GLN
5	C	8	LEU
8	F	64	PRO
21	T	44	ALA
24	W	77	ALA
4	B	306	LYS
7	E	44	GLY
11	J	89	HIS
18	Q	18	PRO
27	Z	43	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	170 (95%)	9 (5%)	22	53
4	B	282/283 (100%)	266 (94%)	16 (6%)	18	49
5	C	193/193 (100%)	175 (91%)	18 (9%)	8	27
6	D	117/148 (79%)	114 (97%)	3 (3%)	40	73
7	E	152/156 (97%)	146 (96%)	6 (4%)	28	63
8	F	93/94 (99%)	89 (96%)	4 (4%)	26	60
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	128 (97%)	4 (3%)	36	70
11	J	118/121 (98%)	110 (93%)	8 (7%)	14	42
12	K	106/106 (100%)	103 (97%)	3 (3%)	38	72
13	L	113/127 (89%)	108 (96%)	5 (4%)	25	59
14	M	158/158 (100%)	150 (95%)	8 (5%)	21	53
15	N	149/150 (99%)	144 (97%)	5 (3%)	32	66
16	O	93/94 (99%)	90 (97%)	3 (3%)	34	68
17	P	113/117 (97%)	109 (96%)	4 (4%)	32	66
18	Q	79/80 (99%)	76 (96%)	3 (4%)	29	64
19	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
20	S	71/74 (96%)	68 (96%)	3 (4%)	26	60
21	T	105/106 (99%)	101 (96%)	4 (4%)	29	64
22	U	44/52 (85%)	43 (98%)	1 (2%)	44	76
23	V	51/57 (90%)	50 (98%)	1 (2%)	48	78
24	W	130/130 (100%)	124 (95%)	6 (5%)	24	57
25	X	66/74 (89%)	62 (94%)	4 (6%)	17	46
26	Y	120/196 (61%)	114 (95%)	6 (5%)	22	53
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	45 (98%)	1 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	2	42/46 (91%)	40 (95%)	2 (5%)	23	55
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	74
31	I	58/129 (45%)	56 (97%)	2 (3%)	32	66
All	All	3093/3602 (86%)	2958 (96%)	135 (4%)	25	59

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	36	ASP
3	A	69	LEU
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	56	ASP
4	B	97	LEU
4	B	98	THR
4	B	149	ASP
4	B	162	MET
4	B	175	LEU
4	B	195	ARG
4	B	251	VAL
4	B	254	GLN
4	B	257	THR
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	67	GLN
5	C	73	LEU
5	C	76	ARG
5	C	91	PRO
5	C	94	THR
5	C	115	LEU
5	C	136	VAL

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Mol	Chain	Res	Type
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	237	GLU
5	C	240	LEU
5	C	243	VAL
6	D	50	VAL
6	D	61	PHE
6	D	149	ARG
7	E	7	ILE
7	E	16	ASP
7	E	68	HIS
7	E	86	VAL
7	E	102	VAL
7	E	126	ILE
8	F	12	LEU
8	F	24	ARG
8	F	46	GLU
8	F	103	GLU
10	H	62	LEU
10	H	84	LYS
10	H	119	LYS
10	H	154	TYR
11	J	46	ILE
11	J	74	ARG
11	J	93	ARG
11	J	120	SER
11	J	127	ILE
11	J	130	VAL
11	J	131	THR
11	J	132	LEU
12	K	10	GLN
12	K	98	VAL
12	K	132	VAL
13	L	35	ARG
13	L	43	HIS
13	L	99	GLU
13	L	101	ASP

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Mol	Chain	Res	Type
13	L	140	VAL
14	M	10	ASP
14	M	46	LEU
14	M	75	ARG
14	M	81	ARG
14	M	93	ARG
14	M	99	ARG
14	M	116	ASN
14	M	164	THR
15	N	26	LEU
15	N	49	THR
15	N	127	LEU
15	N	138	ASP
15	N	152	GLU
16	O	36	PRO
16	O	43	VAL
16	O	98	LEU
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	11	ARG
18	Q	18	PRO
18	Q	95	GLU
19	R	13	THR
19	R	39	THR
19	R	82	GLU
19	R	143	VAL
20	S	10	VAL
20	S	57	THR
20	S	72	ASP
21	T	39	ASN
21	T	48	VAL
21	T	96	VAL
21	T	117	ASP
22	U	47	ARG
23	V	12	THR
24	W	26	ILE
24	W	35	VAL
24	W	73	LEU
24	W	142	ASP
24	W	146	ILE

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Mol	Chain	Res	Type
24	W	151	GLU
25	X	15	ARG
25	X	52	PRO
25	X	72	VAL
25	X	82	GLU
26	Y	154	ARG
26	Y	172	THR
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
26	Y	235	GLU
28	1	47	ASP
29	2	18	ASN
29	2	31	ARG
30	3	22	VAL
30	3	65	THR
31	I	87	THR
31	I	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	5	GLN
3	A	47	HIS
3	A	125	ASN
3	A	199	HIS
3	A	218	ASN
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	230	GLN
4	B	238	ASN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	39	GLN
5	C	67	GLN
5	C	129	HIS
5	C	163	HIS
6	D	47	GLN
6	D	85	GLN
6	D	103	ASN

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Mol	Chain	Res	Type
7	E	74	HIS
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	46	GLN
10	H	56	GLN
10	H	59	HIS
10	H	128	GLN
10	H	170	ASN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
13	L	18	HIS
13	L	41	HIS
13	L	116	HIS
14	M	24	GLN
14	M	58	GLN
14	M	170	ASN
15	N	21	HIS
15	N	22	GLN
15	N	93	GLN
15	N	107	ASN
16	O	100	GLN
17	P	50	GLN
17	P	73	HIS
17	P	89	ASN
17	P	118	GLN
18	Q	40	HIS
19	R	22	GLN
19	R	61	GLN
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	122	GLN
20	S	9	HIS
20	S	53	ASN
20	S	55	GLN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN

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Mol	Chain	Res	Type
23	V	4	HIS
23	V	60	GLN
24	W	12	ASN
24	W	27	HIS
24	W	28	HIS
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
25	X	36	HIS
26	Y	119	GLN
26	Y	134	HIS
26	Y	149	GLN
26	Y	188	HIS
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	16	ASN
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	20	HIS
30	3	48	ASN
31	I	93	GLN
31	I	123	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	249 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	267 (9%)	34 (1%)

All (267) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C

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Mol	Chain	Res	Type
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G

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Mol	Chain	Res	Type
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	645	U
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	885	G
1	0	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	1003	U

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Mol	Chain	Res	Type
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
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	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1216	G
1	0	1232	A
1	0	1233	A
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C
1	0	1474	C

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Mol	Chain	Res	Type
1	0	1475	G
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1668	U
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	1732	A
1	0	1742	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A

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Mol	Chain	Res	Type
1	0	1979	G
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	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	2362	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	2468	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U

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Mol	Chain	Res	Type
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
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	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U

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Mol	Chain	Res	Type
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1165	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1506	U
1	0	1563	G
1	0	1667	A
1	0	1685	A
1	0	1942	A

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Mol	Chain	Res	Type
1	0	2313	C
1	0	2361	A
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	19,22,23	0.32	0	25,31,34	0.43	0
1	OMG	0	2588	1	23,26,27	0.33	0	32,38,41	0.42	0
1	UR3	0	2619	1	19,22,23	0.49	0	26,32,35	0.75	1 (3%)
1	1MA	0	628	1	21,25,26	0.70	1 (4%)	30,37,40	0.71	1 (3%)
1	PSU	0	2621	1	18,21,22	1.57	2 (11%)	21,30,33	1.42	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
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.21	1.43	1.36
1	0	2621	PSU	C6-C5	2.83	1.38	1.35
1	0	628	1MA	C6-N6	2.35	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.68	120.66	118.17
1	0	2621	PSU	C6-N1-C2	-3.16	119.75	122.69
1	0	2621	PSU	O2-C2-N1	2.98	125.86	122.79
1	0	2619	UR3	C4-N3-C2	2.83	126.86	124.58
1	0	628	1MA	N1-C2-N3	2.66	129.16	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 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	$\# Z > 2$
32	13T	0	9000	-	42,43,43	2.00	10 (23%)	51,63,63	1.83	9 (17%)

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
32	13T	0	9000	-	-	16/73/81/81	0/1/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	13T	C18-C19	6.97	1.56	1.47
32	0	9000	13T	C10-C9	4.13	1.57	1.50
32	0	9000	13T	O5-C5	3.42	1.26	1.21
32	0	9000	13T	O2-C1	3.31	1.29	1.21
32	0	9000	13T	O7-C11	3.13	1.26	1.21
32	0	9000	13T	C9-C8	3.00	1.40	1.33
32	0	9000	13T	C27-C10	2.59	1.57	1.54
32	0	9000	13T	C26-C8	2.29	1.54	1.50
32	0	9000	13T	C29-C16	2.22	1.55	1.52
32	0	9000	13T	O1-C1	2.07	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	13T	C18-O11-C19	8.03	65.36	60.81
32	0	9000	13T	O11-C18-C19	-4.35	56.62	59.38
32	0	9000	13T	O4-C3-C4	4.13	115.61	105.83
32	0	9000	13T	O11-C19-C18	-2.66	58.01	59.82
32	0	9000	13T	C27-C10-C9	2.51	113.14	110.73
32	0	9000	13T	C7-C6-C5	-2.21	106.74	109.48
32	0	9000	13T	O1-C1-O2	2.17	128.12	124.14
32	0	9000	13T	C19-C20-C21	-2.15	108.45	114.18
32	0	9000	13T	C12-C11-C10	2.00	120.31	117.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

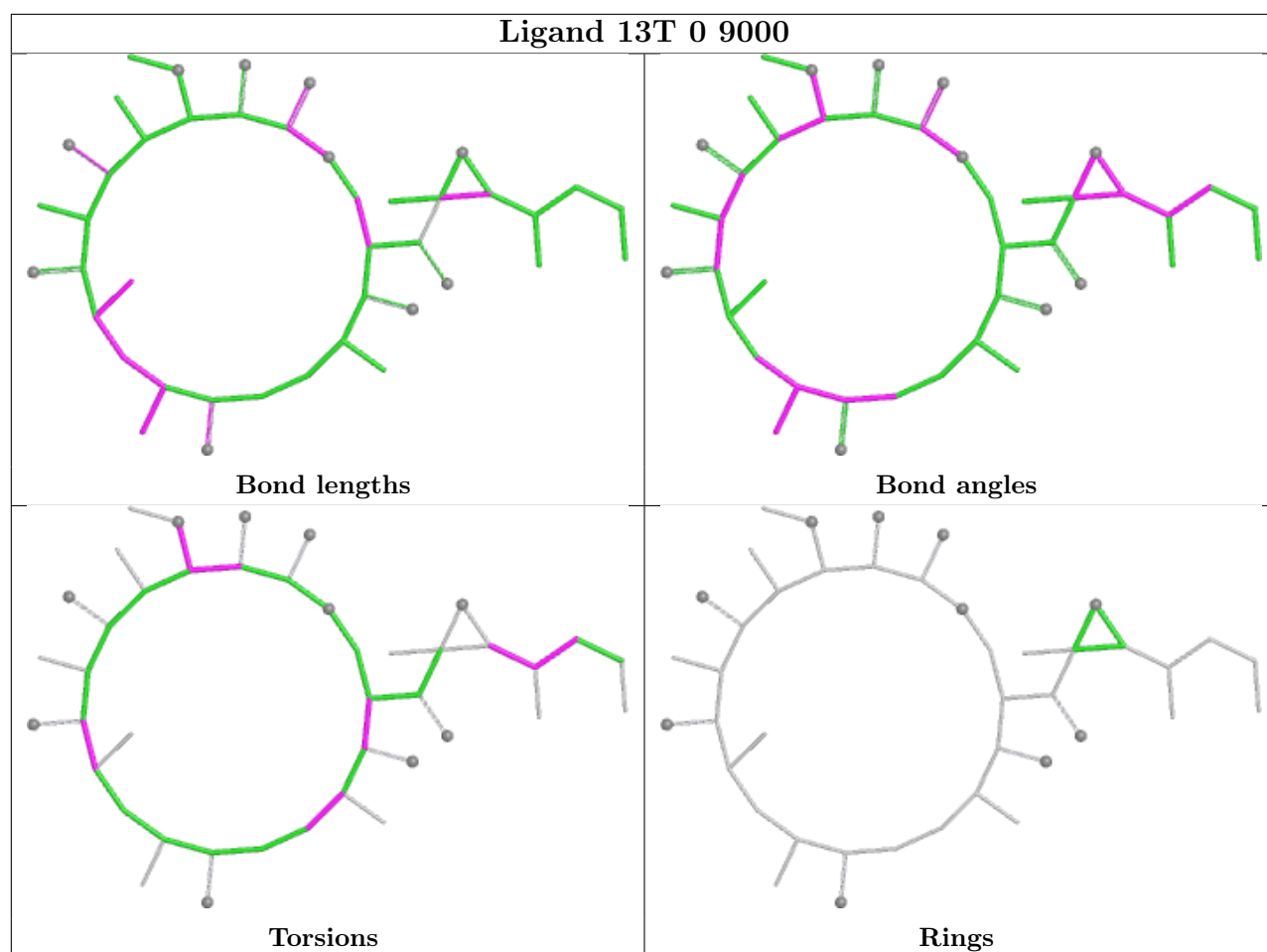
Mol	Chain	Res	Type	Atoms
32	0	9000	13T	C2-C3-O4-C32
32	0	9000	13T	C1-C2-C3-O4
32	0	9000	13T	O6-C7-C8-C9
32	0	9000	13T	O6-C7-C8-C26
32	0	9000	13T	C6-C7-C8-C9
32	0	9000	13T	C6-C7-C8-C26
32	0	9000	13T	C18-C19-C20-C21
32	0	9000	13T	O11-C19-C20-C21
32	0	9000	13T	O11-C19-C20-C31
32	0	9000	13T	C14-C15-C16-C29
32	0	9000	13T	O9-C15-C16-C17
32	0	9000	13T	C14-C15-C16-C17
32	0	9000	13T	O9-C15-C16-C29
32	0	9000	13T	C12-C13-C14-C15
32	0	9000	13T	C31-C20-C21-C22
32	0	9000	13T	C18-C19-C20-C31

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	13T	24	0

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%)	0.13	26 (0%) 81 75	23, 50, 93, 150	0
2	9	122/122 (100%)	0.15	3 (2%) 58 48	43, 69, 91, 151	0
3	A	237/240 (98%)	0.67	11 (4%) 37 29	32, 55, 86, 105	0
4	B	337/338 (99%)	0.90	24 (7%) 22 17	33, 60, 82, 90	0
5	C	246/246 (100%)	0.53	6 (2%) 59 50	30, 50, 73, 82	0
6	D	140/177 (79%)	1.73	50 (35%) 1 0	63, 103, 124, 130	0
7	E	172/178 (96%)	0.94	15 (8%) 16 13	55, 73, 90, 96	0
8	F	119/120 (99%)	0.84	8 (6%) 24 19	57, 74, 96, 106	0
9	G	29/348 (8%)	1.11	3 (10%) 12 10	81, 94, 103, 103	0
10	H	160/171 (93%)	0.70	5 (3%) 51 42	52, 67, 93, 100	0
11	J	142/145 (97%)	0.77	10 (7%) 22 18	45, 56, 74, 94	0
12	K	132/132 (100%)	0.72	2 (1%) 72 64	41, 54, 75, 81	0
13	L	145/165 (87%)	0.90	13 (8%) 15 13	32, 71, 107, 118	0
14	M	194/194 (100%)	0.45	4 (2%) 63 54	36, 47, 60, 64	0
15	N	186/187 (99%)	0.94	21 (11%) 10 9	50, 67, 110, 119	0
16	O	115/116 (99%)	0.67	3 (2%) 57 48	44, 59, 71, 76	0
17	P	143/149 (95%)	0.97	11 (7%) 19 16	46, 60, 70, 75	0
18	Q	95/96 (98%)	0.49	3 (3%) 50 41	43, 52, 64, 72	0
19	R	150/155 (96%)	0.54	4 (2%) 56 47	38, 50, 68, 73	0
20	S	81/85 (95%)	0.79	8 (9%) 13 11	52, 65, 81, 85	0
21	T	119/120 (99%)	0.75	3 (2%) 58 48	47, 62, 83, 96	0
22	U	53/66 (80%)	0.88	5 (9%) 14 12	51, 61, 75, 81	0
23	V	65/71 (91%)	1.21	12 (18%) 3 3	59, 79, 109, 114	0
24	W	154/154 (100%)	0.55	4 (2%) 57 48	42, 56, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	1.25	13 (15%) 5 4	52, 64, 87, 97	0
26	Y	142/241 (58%)	0.54	3 (2%) 63 54	30, 51, 70, 86	0
27	Z	73/73 (100%)	1.01	11 (15%) 5 4	58, 69, 80, 94	0
28	1	56/57 (98%)	0.21	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	1.16	10 (21%) 2 2	41, 69, 90, 99	0
30	3	92/92 (100%)	0.50	3 (3%) 49 40	42, 60, 71, 82	0
31	I	70/161 (43%)	2.38	37 (52%) 0 0	109, 119, 135, 135	0
All	All	6646/7463 (89%)	0.52	331 (4%) 34 27	23, 57, 100, 151	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	6.5
25	X	88	GLU	6.4
6	D	10	PHE	6.2
15	N	166	ALA	6.2
4	B	1	PRO	6.0
31	I	133	THR	6.0
31	I	79	ILE	5.7
31	I	109	ALA	5.4
31	I	75	THR	5.4
23	V	43	PRO	5.4
31	I	118	SER	5.3
6	D	63	ILE	5.2
25	X	85	VAL	5.0
27	Z	11	SER	4.9
27	Z	22	SER	4.8
31	I	76	ALA	4.8
23	V	39	ALA	4.7
13	L	97	VAL	4.7
6	D	18	ILE	4.6
15	N	154	LEU	4.4
1	0	10	U	4.2
13	L	100	ALA	4.2
6	D	57	THR	4.1
23	V	2	VAL	4.1
29	2	49	GLU	4.1
15	N	168	LEU	4.1
6	D	55	LYS	4.1
31	I	88	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
31	I	139	ILE	3.9
17	P	58	SER	3.9
31	I	137	VAL	3.9
6	D	90	LEU	3.9
23	V	40	PRO	3.8
15	N	158	LEU	3.8
13	L	99	GLU	3.8
7	E	45	ASP	3.8
1	0	2637	A	3.7
13	L	102	ASP	3.7
25	X	65	ASN	3.7
31	I	90	GLY	3.7
31	I	96	PHE	3.7
6	D	174	VAL	3.6
6	D	134	LEU	3.6
26	Y	235	GLU	3.6
31	I	129	VAL	3.6
6	D	107	GLY	3.6
25	X	84	ILE	3.5
6	D	150	SER	3.5
31	I	138	THR	3.4
26	Y	108	ASP	3.4
13	L	146	GLY	3.4
13	L	60	GLU	3.3
31	I	113	HIS	3.3
29	2	38	LYS	3.3
31	I	78	LEU	3.3
31	I	93	GLN	3.3
6	D	66	GLY	3.3
31	I	121	LEU	3.3
3	A	211	LYS	3.2
25	X	87	ALA	3.2
11	J	70	PHE	3.2
25	X	83	ALA	3.2
31	I	105	VAL	3.2
11	J	92	GLN	3.2
22	U	52	THR	3.2
9	G	12	ILE	3.2
31	I	135	LEU	3.2
3	A	36	ASP	3.1
17	P	18	LYS	3.1
2	9	3002	U	3.1

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Mol	Chain	Res	Type	RSRZ
19	R	55	GLN	3.1
17	P	92	GLU	3.1
7	E	53	GLU	3.1
15	N	163	PHE	3.0
15	N	165	ALA	3.0
3	A	31	LYS	3.0
14	M	1	ALA	3.0
4	B	5	ARG	3.0
31	I	89	SER	3.0
13	L	82	ALA	3.0
7	E	154	ILE	3.0
29	2	39	ARG	3.0
31	I	100	LEU	3.0
6	D	62	ASP	3.0
15	N	167	ASP	3.0
15	N	152	GLU	3.0
10	H	40	ALA	3.0
11	J	4	ALA	3.0
11	J	144	THR	3.0
13	L	105	TYR	2.9
6	D	59	GLY	2.9
6	D	35	ALA	2.9
1	0	1130	U	2.9
6	D	157	LEU	2.9
8	F	102	GLY	2.9
3	A	37	VAL	2.9
2	9	3001	U	2.9
4	B	108	GLU	2.9
31	I	72	VAL	2.9
6	D	22	VAL	2.8
17	P	62	ALA	2.8
25	X	74	ALA	2.8
6	D	128	LEU	2.8
27	Z	21	VAL	2.8
6	D	69	ILE	2.8
29	2	37	HIS	2.8
23	V	45	ARG	2.8
6	D	106	PHE	2.8
15	N	1	ALA	2.8
13	L	148	GLU	2.8
7	E	97	VAL	2.8
25	X	23	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	101	THR	2.8
5	C	180	SER	2.8
7	E	172	PRO	2.8
1	0	272	A	2.7
5	C	61	PHE	2.7
12	K	58	THR	2.7
13	L	55	GLN	2.7
7	E	6	GLU	2.7
9	G	71	LEU	2.7
20	S	81	ILE	2.7
1	0	1172	G	2.7
6	D	17	ARG	2.7
17	P	116	SER	2.7
30	3	35	TRP	2.7
6	D	11	HIS	2.7
6	D	153	THR	2.7
22	U	51	TRP	2.7
4	B	303	GLY	2.7
7	E	100	ASP	2.7
3	A	32	VAL	2.7
23	V	41	GLU	2.7
8	F	17	LEU	2.7
9	G	26	MET	2.6
6	D	139	TYR	2.6
29	2	35	ARG	2.6
15	N	169	PRO	2.6
27	Z	34	ASN	2.6
6	D	53	LYS	2.6
31	I	102	VAL	2.6
1	0	1171	A	2.6
21	T	118	SER	2.6
11	J	47	THR	2.6
7	E	108	LEU	2.6
30	3	41	GLU	2.6
7	E	10	ASP	2.6
7	E	160	ARG	2.6
31	I	131	THR	2.6
16	O	1	SER	2.6
6	D	56	ARG	2.6
3	A	237	GLY	2.6
31	I	117	LEU	2.6
6	D	135	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
10	H	111	ASP	2.6
15	N	160	SER	2.5
5	C	245	GLU	2.5
23	V	36	ALA	2.5
25	X	71	ARG	2.5
5	C	63	SER	2.5
18	Q	17	LYS	2.5
21	T	10	SER	2.5
4	B	70	PRO	2.5
4	B	155	PRO	2.5
6	D	68	PRO	2.5
1	0	1161	A	2.5
20	S	12	GLU	2.5
27	Z	20	ARG	2.5
6	D	154	LYS	2.5
23	V	38	GLY	2.5
1	0	960	G	2.5
1	0	1951	G	2.5
6	D	54	ALA	2.5
20	S	21	GLN	2.5
31	I	106	LYS	2.5
7	E	87	PHE	2.5
21	T	13	ARG	2.5
1	0	87	C	2.5
25	X	66	THR	2.5
1	0	497	A	2.5
6	D	102	GLY	2.4
31	I	85	PHE	2.4
15	N	148	ALA	2.4
17	P	77	ALA	2.4
4	B	98	THR	2.4
4	B	119	HIS	2.4
3	A	27	LEU	2.4
13	L	145	LEU	2.4
19	R	73	ASP	2.4
15	N	43	VAL	2.4
1	0	1198	U	2.4
1	0	1561	U	2.4
6	D	104	PHE	2.4
20	S	74	ALA	2.4
12	K	44	LEU	2.4
1	0	2769	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	2748	G	2.4
4	B	4	SER	2.4
31	I	124	ALA	2.4
7	E	5	LEU	2.4
6	D	141	VAL	2.4
18	Q	65	GLY	2.4
27	Z	19	GLY	2.4
15	N	162	ASP	2.4
27	Z	24	ARG	2.4
27	Z	25	ARG	2.4
6	D	19	GLU	2.4
13	L	83	GLU	2.4
4	B	128	ILE	2.4
6	D	58	VAL	2.3
29	2	28	LYS	2.3
23	V	44	GLY	2.3
15	N	164	ASP	2.3
19	R	7	GLU	2.3
25	X	7	GLU	2.3
14	M	174	SER	2.3
20	S	2	TRP	2.3
4	B	144	THR	2.3
6	D	75	LEU	2.3
24	W	4	LEU	2.3
11	J	46	ILE	2.3
6	D	172	VAL	2.3
17	P	59	ARG	2.3
14	M	70	GLY	2.3
8	F	49	PHE	2.3
7	E	13	ALA	2.3
27	Z	10	ARG	2.3
4	B	57	GLU	2.3
8	F	16	ALA	2.3
15	N	145	ALA	2.3
17	P	143	ALA	2.3
4	B	21	SER	2.3
17	P	49	ILE	2.3
27	Z	18	TYR	2.3
8	F	1	PRO	2.3
1	0	2911	C	2.3
3	A	91	GLY	2.3
6	D	61	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	C	95	GLU	2.3
31	I	115	ASP	2.3
10	H	65	SER	2.3
17	P	117	SER	2.3
31	I	87	THR	2.3
3	A	82	VAL	2.3
4	B	278	PRO	2.3
7	E	65	PHE	2.2
23	V	35	ALA	2.2
4	B	80	ARG	2.2
4	B	208	GLY	2.2
15	N	161	GLY	2.2
31	I	116	LEU	2.2
31	I	140	GLU	2.2
1	0	1173	A	2.2
1	0	1199	A	2.2
1	0	2345	A	2.2
1	0	2664	A	2.2
15	N	119	GLN	2.2
4	B	118	ASP	2.2
25	X	10	VAL	2.2
1	0	1525	G	2.2
5	C	171	GLU	2.2
6	D	65	GLU	2.2
6	D	88	LEU	2.2
16	O	24	ALA	2.2
2	9	3024	U	2.2
4	B	319	ASP	2.2
6	D	130	VAL	2.2
31	I	128	VAL	2.2
6	D	105	SER	2.2
31	I	134	SER	2.2
4	B	117	GLU	2.2
11	J	49	ARG	2.2
29	2	31	ARG	2.2
20	S	77	VAL	2.2
31	I	97	VAL	2.2
1	0	31	C	2.2
6	D	165	PHE	2.2
3	A	67	LEU	2.2
15	N	186	LEU	2.2
6	D	37	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
11	J	127	ILE	2.1
4	B	318	ASN	2.1
30	3	8	ASN	2.1
8	F	91	VAL	2.1
10	H	140	VAL	2.1
31	I	95	ASP	2.1
1	0	514	G	2.1
23	V	37	GLY	2.1
1	0	1965	C	2.1
11	J	6	PHE	2.1
31	I	132	CYS	2.1
4	B	189	ALA	2.1
6	D	12	GLU	2.1
15	N	68	GLU	2.1
29	2	44	ARG	2.1
27	Z	26	VAL	2.1
6	D	131	THR	2.1
22	U	47	ARG	2.1
8	F	79	GLN	2.1
13	L	150	GLN	2.1
3	A	236	GLY	2.1
14	M	191	GLY	2.1
24	W	62	LEU	2.1
29	2	48	ASP	2.1
16	O	47	ARG	2.1
17	P	94	TRP	2.1
7	E	20	ILE	2.1
20	S	78	ALA	2.1
1	0	1177	A	2.1
4	B	82	VAL	2.1
4	B	296	LEU	2.1
6	D	83	PHE	2.1
8	F	37	THR	2.1
29	2	46	ASP	2.1
4	B	101	TRP	2.1
6	D	44	ILE	2.1
11	J	136	SER	2.0
20	S	4	VAL	2.0
24	W	45	VAL	2.0
26	Y	236	VAL	2.0
6	D	91	ALA	2.0
10	H	129	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
18	Q	20	ASP	2.0
24	W	16	ASP	2.0
19	R	15	LYS	2.0
25	X	72	VAL	2.0
1	0	298	C	2.0
6	D	166	ILE	2.0
22	U	11	THR	2.0
22	U	46	ALA	2.0
15	N	159	TYR	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
1	OMU	0	2587	21/22	0.94	0.11	38,39,40,41	0
1	UR3	0	2619	21/22	0.94	0.10	36,38,39,40	0
1	1MA	0	628	23/24	0.95	0.10	33,35,36,37	0
1	PSU	0	2621	20/21	0.95	0.09	30,32,39,40	0
1	OMG	0	2588	24/25	0.96	0.10	37,38,39,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	9	8551	1/1	0.55	0.22	92,92,92,92	0
35	NA	0	8584	1/1	0.56	0.23	90,90,90,90	0
35	NA	0	8560	1/1	0.60	0.30	60,60,60,60	0
35	NA	0	8571	1/1	0.60	0.27	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8050	1/1	0.70	0.15	74,74,74,74	0
33	MG	9	8095	1/1	0.70	0.18	77,77,77,77	0
35	NA	0	8510	1/1	0.72	0.16	45,45,45,45	0
35	NA	0	8569	1/1	0.73	0.32	64,64,64,64	0
35	NA	0	8577	1/1	0.74	0.31	81,81,81,81	0
35	NA	0	8557	1/1	0.75	0.14	45,45,45,45	0
33	MG	0	8024	1/1	0.76	0.73	65,65,65,65	0
35	NA	0	8582	1/1	0.76	0.20	85,85,85,85	0
35	NA	0	8502	1/1	0.76	0.17	57,57,57,57	0
35	NA	0	8559	1/1	0.76	0.25	53,53,53,53	0
35	NA	0	8538	1/1	0.78	0.10	55,55,55,55	0
33	MG	0	8082	1/1	0.79	0.23	84,84,84,84	0
35	NA	0	8585	1/1	0.79	0.32	65,65,65,65	0
35	NA	0	8511	1/1	0.79	0.14	56,56,56,56	0
35	NA	0	8534	1/1	0.80	0.15	40,40,40,40	0
35	NA	H	8522	1/1	0.80	0.42	77,77,77,77	0
35	NA	J	8546	1/1	0.80	0.14	39,39,39,39	0
35	NA	S	8512	1/1	0.80	0.29	57,57,57,57	0
35	NA	9	8583	1/1	0.81	0.23	73,73,73,73	0
33	MG	0	8104	1/1	0.81	0.20	78,78,78,78	0
36	CL	0	8816	1/1	0.81	0.23	69,69,69,69	0
33	MG	0	8046	1/1	0.82	0.09	56,56,56,56	0
35	NA	0	8508	1/1	0.82	0.18	58,58,58,58	0
35	NA	0	8540	1/1	0.82	0.19	50,50,50,50	0
35	NA	0	8524	1/1	0.82	0.17	48,48,48,48	0
35	NA	0	8528	1/1	0.82	0.18	54,54,54,54	0
35	NA	0	8532	1/1	0.82	0.17	44,44,44,44	0
35	NA	0	8507	1/1	0.83	0.16	69,69,69,69	0
35	NA	0	8563	1/1	0.83	0.23	68,68,68,68	0
35	NA	0	8564	1/1	0.83	0.16	49,49,49,49	0
35	NA	0	8516	1/1	0.83	0.17	49,49,49,49	0
35	NA	0	8529	1/1	0.83	0.14	68,68,68,68	0
33	MG	0	8051	1/1	0.84	0.10	56,56,56,56	0
33	MG	0	8102	1/1	0.84	0.09	50,50,50,50	0
35	NA	0	8566	1/1	0.84	0.08	48,48,48,48	0
32	13T	0	9000	42/42	0.85	0.20	58,67,73,74	0
35	NA	0	8565	1/1	0.85	0.30	47,47,47,47	0
33	MG	0	8070	1/1	0.85	0.08	43,43,43,43	0
35	NA	0	8562	1/1	0.85	0.27	70,70,70,70	0
36	CL	0	8815	1/1	0.85	0.22	89,89,89,89	0
33	MG	0	8072	1/1	0.85	0.08	57,57,57,57	0
36	CL	J	8802	1/1	0.85	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8579	1/1	0.86	0.23	65,65,65,65	0
33	MG	0	8096	1/1	0.86	0.11	48,48,48,48	0
33	MG	0	8093	1/1	0.86	0.08	61,61,61,61	0
35	NA	0	8520	1/1	0.86	0.12	36,36,36,36	0
33	MG	0	8113	1/1	0.87	0.08	44,44,44,44	0
33	MG	0	8103	1/1	0.87	0.22	78,78,78,78	0
36	CL	0	8822	1/1	0.87	0.41	90,90,90,90	0
35	NA	0	8568	1/1	0.87	0.40	87,87,87,87	0
35	NA	0	8544	1/1	0.88	0.09	29,29,29,29	0
35	NA	0	8552	1/1	0.88	0.36	68,68,68,68	0
35	NA	0	8509	1/1	0.88	0.09	48,48,48,48	0
35	NA	0	8573	1/1	0.88	0.07	56,56,56,56	0
33	MG	0	8041	1/1	0.88	0.11	68,68,68,68	0
36	CL	A	8809	1/1	0.88	0.23	82,82,82,82	0
35	NA	0	8541	1/1	0.88	0.06	46,46,46,46	0
33	MG	0	8108	1/1	0.89	0.12	77,77,77,77	0
35	NA	A	8545	1/1	0.89	0.12	61,61,61,61	0
34	K	0	8401	1/1	0.89	0.29	84,84,84,84	0
35	NA	0	8525	1/1	0.89	0.18	59,59,59,59	0
35	NA	0	8515	1/1	0.89	0.16	49,49,49,49	0
33	MG	0	8087	1/1	0.89	0.13	63,63,63,63	0
35	NA	0	8531	1/1	0.89	0.17	57,57,57,57	0
35	NA	0	8554	1/1	0.89	0.13	42,42,42,42	0
35	NA	0	8567	1/1	0.89	0.19	61,61,61,61	0
35	NA	0	8517	1/1	0.89	0.09	37,37,37,37	0
35	NA	0	8550	1/1	0.90	0.26	65,65,65,65	0
33	MG	0	8114	1/1	0.90	0.17	54,54,54,54	0
33	MG	0	8097	1/1	0.90	0.09	45,45,45,45	0
33	MG	0	8112	1/1	0.90	0.10	39,39,39,39	0
35	NA	0	8558	1/1	0.90	0.24	75,75,75,75	0
35	NA	R	8586	1/1	0.90	0.26	23,23,23,23	0
35	NA	0	8536	1/1	0.90	0.09	54,54,54,54	0
35	NA	0	8526	1/1	0.90	0.17	70,70,70,70	0
33	MG	0	8052	1/1	0.90	0.13	68,68,68,68	0
35	NA	0	8518	1/1	0.90	0.21	58,58,58,58	0
35	NA	0	8530	1/1	0.90	0.12	45,45,45,45	0
35	NA	0	8549	1/1	0.90	0.15	53,53,53,53	0
36	CL	Y	8817	1/1	0.90	0.12	70,70,70,70	0
37	CD	O	8705	1/1	0.90	0.29	186,186,186,186	0
33	MG	0	8117	1/1	0.91	0.08	34,34,34,34	0
35	NA	0	8506	1/1	0.91	0.20	49,49,49,49	0
35	NA	0	8572	1/1	0.91	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8089	1/1	0.91	0.14	62,62,62,62	0
35	NA	0	8513	1/1	0.91	0.09	72,72,72,72	0
35	NA	C	8504	1/1	0.91	0.06	35,35,35,35	0
36	CL	J	8801	1/1	0.91	0.12	58,58,58,58	0
33	MG	0	8092	1/1	0.91	0.17	72,72,72,72	0
35	NA	0	8539	1/1	0.91	0.10	40,40,40,40	0
35	NA	R	8537	1/1	0.91	0.14	45,45,45,45	0
35	NA	0	8561	1/1	0.92	0.10	50,50,50,50	0
36	CL	0	8812	1/1	0.92	0.11	49,49,49,49	0
33	MG	0	8115	1/1	0.92	0.09	45,45,45,45	0
35	NA	0	8533	1/1	0.92	0.09	39,39,39,39	0
35	NA	0	8556	1/1	0.92	0.22	61,61,61,61	0
35	NA	0	8575	1/1	0.92	0.35	72,72,72,72	0
33	MG	0	8043	1/1	0.92	0.08	47,47,47,47	0
35	NA	0	8535	1/1	0.92	0.16	54,54,54,54	0
36	CL	J	8821	1/1	0.92	0.16	77,77,77,77	0
33	MG	0	8084	1/1	0.92	0.09	58,58,58,58	0
33	MG	0	8080	1/1	0.92	0.08	39,39,39,39	0
33	MG	Y	8109	1/1	0.93	0.09	44,44,44,44	0
33	MG	0	8063	1/1	0.93	0.09	63,63,63,63	0
33	MG	0	8090	1/1	0.93	0.12	73,73,73,73	0
33	MG	0	8076	1/1	0.93	0.06	49,49,49,49	0
33	MG	0	8085	1/1	0.93	0.07	48,48,48,48	0
33	MG	0	8116	1/1	0.93	0.06	56,56,56,56	0
33	MG	0	8045	1/1	0.93	0.15	67,67,67,67	0
33	MG	0	8111	1/1	0.93	0.07	46,46,46,46	0
33	MG	B	8055	1/1	0.93	0.12	64,64,64,64	0
35	NA	M	8547	1/1	0.93	0.12	41,41,41,41	0
36	CL	R	8806	1/1	0.93	0.09	49,49,49,49	0
35	NA	Q	8548	1/1	0.93	0.06	46,46,46,46	0
35	NA	0	8555	1/1	0.93	0.18	85,85,85,85	0
36	CL	0	8803	1/1	0.94	0.12	56,56,56,56	0
36	CL	0	8805	1/1	0.94	0.10	71,71,71,71	0
35	NA	0	8570	1/1	0.94	0.34	65,65,65,65	0
36	CL	0	8813	1/1	0.94	0.08	54,54,54,54	0
36	CL	0	8814	1/1	0.94	0.13	57,57,57,57	0
33	MG	0	8044	1/1	0.94	0.06	55,55,55,55	0
33	MG	0	8047	1/1	0.94	0.12	57,57,57,57	0
35	NA	0	8527	1/1	0.94	0.17	61,61,61,61	0
33	MG	0	8057	1/1	0.94	0.06	41,41,41,41	0
33	MG	0	8049	1/1	0.94	0.13	36,36,36,36	0
33	MG	0	8067	1/1	0.94	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8581	1/1	0.94	0.05	42,42,42,42	0
33	MG	0	8094	1/1	0.94	0.12	59,59,59,59	0
33	MG	0	8040	1/1	0.94	0.09	53,53,53,53	0
33	MG	T	8073	1/1	0.94	0.14	57,57,57,57	0
33	MG	A	8065	1/1	0.95	0.09	45,45,45,45	0
33	MG	0	8075	1/1	0.95	0.07	56,56,56,56	0
33	MG	K	8069	1/1	0.95	0.06	51,51,51,51	0
33	MG	0	8071	1/1	0.95	0.06	50,50,50,50	0
33	MG	0	8100	1/1	0.95	0.06	42,42,42,42	0
33	MG	0	8110	1/1	0.95	0.08	53,53,53,53	0
35	NA	0	8542	1/1	0.95	0.16	15,15,15,15	0
36	CL	B	8819	1/1	0.95	0.15	53,53,53,53	0
34	K	0	8402	1/1	0.95	0.12	61,61,61,61	0
33	MG	0	8101	1/1	0.95	0.06	45,45,45,45	0
35	NA	0	8503	1/1	0.95	0.15	1,1,1,1	0
36	CL	L	8810	1/1	0.95	0.10	59,59,59,59	0
36	CL	N	8807	1/1	0.95	0.10	71,71,71,71	0
36	CL	O	8808	1/1	0.95	0.09	67,67,67,67	0
35	NA	0	8505	1/1	0.95	0.06	37,37,37,37	0
35	NA	0	8553	1/1	0.95	0.08	44,44,44,44	0
33	MG	0	8035	1/1	0.95	0.08	46,46,46,46	0
33	MG	3	8118	1/1	0.96	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.96	0.04	33,33,33,33	0
35	NA	0	8514	1/1	0.96	0.07	38,38,38,38	0
33	MG	0	8061	1/1	0.96	0.05	44,44,44,44	0
35	NA	0	8501	1/1	0.96	0.06	50,50,50,50	0
33	MG	0	8037	1/1	0.96	0.06	42,42,42,42	0
33	MG	0	8028	1/1	0.96	0.05	33,33,33,33	0
33	MG	0	8068	1/1	0.96	0.06	56,56,56,56	0
35	NA	0	8521	1/1	0.96	0.16	77,77,77,77	0
33	MG	0	8048	1/1	0.96	0.05	49,49,49,49	0
35	NA	0	8574	1/1	0.96	0.13	67,67,67,67	0
33	MG	0	8053	1/1	0.96	0.04	43,43,43,43	0
33	MG	0	8025	1/1	0.96	0.05	43,43,43,43	0
35	NA	0	8578	1/1	0.96	0.13	57,57,57,57	0
33	MG	0	8098	1/1	0.96	0.12	42,42,42,42	0
33	MG	0	8099	1/1	0.96	0.12	70,70,70,70	0
36	CL	3	8804	1/1	0.96	0.07	56,56,56,56	0
36	CL	0	8811	1/1	0.96	0.08	58,58,58,58	0
33	MG	0	8106	1/1	0.97	0.10	71,71,71,71	0
33	MG	0	8042	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8523	1/1	0.97	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8022	1/1	0.97	0.05	37,37,37,37	0
33	MG	0	8029	1/1	0.97	0.05	42,42,42,42	0
35	NA	0	8543	1/1	0.97	0.13	35,35,35,35	0
33	MG	0	8039	1/1	0.97	0.06	64,64,64,64	0
36	CL	Y	8820	1/1	0.97	0.05	44,44,44,44	0
33	MG	0	8031	1/1	0.97	0.06	30,30,30,30	0
33	MG	0	8033	1/1	0.97	0.06	38,38,38,38	0
37	CD	Z	8703	1/1	0.97	0.04	71,71,71,71	0
33	MG	0	8059	1/1	0.98	0.04	39,39,39,39	0
33	MG	0	8060	1/1	0.98	0.06	45,45,45,45	0
33	MG	0	8036	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8011	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8064	1/1	0.98	0.06	41,41,41,41	0
33	MG	0	8012	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8091	1/1	0.98	0.04	65,65,65,65	0
33	MG	0	8027	1/1	0.98	0.03	40,40,40,40	0
33	MG	0	8016	1/1	0.98	0.04	18,18,18,18	0
33	MG	0	8018	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8021	1/1	0.98	0.05	37,37,37,37	0
36	CL	M	8818	1/1	0.98	0.05	44,44,44,44	0
33	MG	0	8008	1/1	0.98	0.05	29,29,29,29	0
33	MG	0	8056	1/1	0.98	0.05	56,56,56,56	0
33	MG	0	8023	1/1	0.98	0.12	61,61,61,61	0
33	MG	A	8066	1/1	0.98	0.05	73,73,73,73	0
35	NA	0	8576	1/1	0.98	0.04	33,33,33,33	0
33	MG	0	8081	1/1	0.98	0.07	43,43,43,43	0
33	MG	0	8058	1/1	0.98	0.06	42,42,42,42	0
37	CD	U	8701	1/1	0.98	0.03	67,67,67,67	0
33	MG	0	8083	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8032	1/1	0.99	0.04	35,35,35,35	0
33	MG	0	8077	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8079	1/1	0.99	0.03	27,27,27,27	0
33	MG	0	8005	1/1	0.99	0.04	32,32,32,32	0
33	MG	0	8107	1/1	0.99	0.05	38,38,38,38	0
33	MG	0	8034	1/1	0.99	0.03	25,25,25,25	0
33	MG	0	8017	1/1	0.99	0.03	31,31,31,31	0
33	MG	0	8054	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8006	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8019	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8086	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8038	1/1	0.99	0.03	31,31,31,31	0
33	MG	0	8020	1/1	0.99	0.04	39,39,39,39	0

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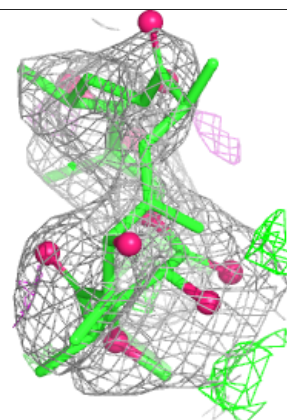
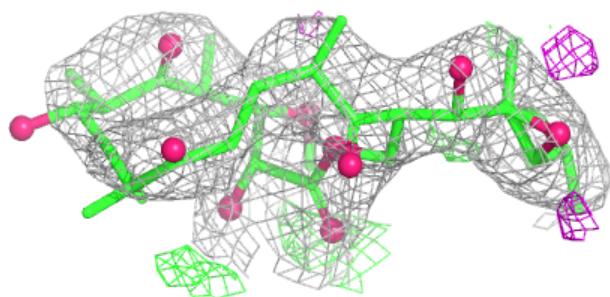
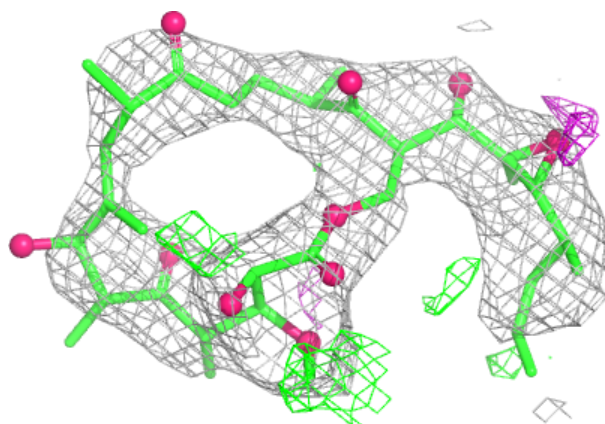
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8007	1/1	0.99	0.06	26,26,26,26	0
33	MG	0	8001	1/1	0.99	0.03	44,44,44,44	0
35	NA	0	8519	1/1	0.99	0.05	17,17,17,17	0
33	MG	0	8062	1/1	0.99	0.11	13,13,13,13	0
33	MG	0	8009	1/1	0.99	0.03	36,36,36,36	0
33	MG	0	8010	1/1	0.99	0.04	11,11,11,11	0
33	MG	0	8002	1/1	0.99	0.08	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	8004	1/1	0.99	0.04	37,37,37,37	0
33	MG	0	8013	1/1	0.99	0.07	38,38,38,38	0
33	MG	3	8078	1/1	0.99	0.02	16,16,16,16	0
33	MG	0	8014	1/1	0.99	0.05	41,41,41,41	0
35	NA	L	8580	1/1	0.99	0.10	1,1,1,1	0
33	MG	0	8074	1/1	0.99	0.02	30,30,30,30	0
33	MG	0	8015	1/1	0.99	0.03	35,35,35,35	0
37	CD	1	8702	1/1	0.99	0.05	65,65,65,65	0
37	CD	3	8704	1/1	0.99	0.03	65,65,65,65	0
33	MG	0	8003	1/1	1.00	0.02	36,36,36,36	0
33	MG	0	8030	1/1	1.00	0.04	35,35,35,35	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.

Electron density around 13T 0 9000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.