Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 12:03 AM EDT

PDB ID	:	3G4S
Title	:	Co-crystal structure of Tiamulin bound to the large ribosomal subunit
Authors	:	Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2009-02-04
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

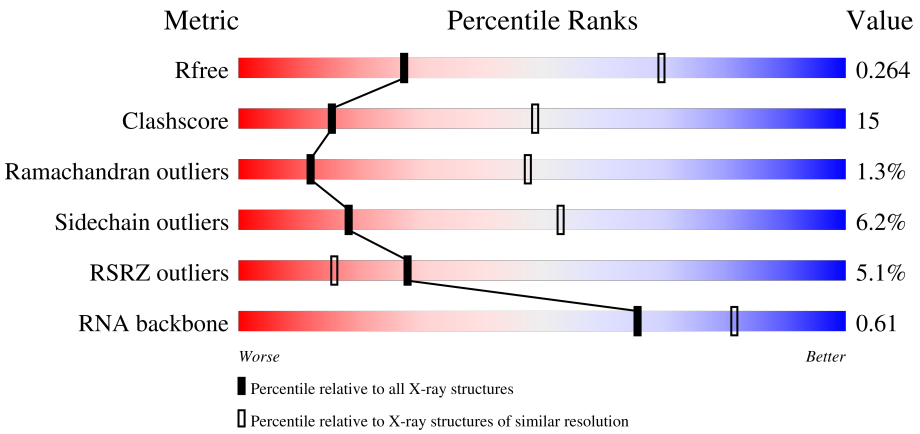
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 <=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	2923	34% 53% 7% 6%
2	A	237	4% 83% 16%
3	B	337	81% 17% •
4	C	246	% 82% 15% •

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Mol	Chain	Length	Quality of chain
5	D	177	21% 66% 12% 21%
6	E	172	2% 83% 16%
7	F	119	7% 85% 15%
8	G	348	2% 7% 92%
9	H	177	8% 74% 16% 10%
10	I	70	46% 86% 14%
11	J	142	87% 11%
12	K	132	2% 76% 23%
13	L	165	16% 74% 13% 12%
14	M	194	9% 80% 16%
15	N	186	7% 80% 19%
16	O	115	90% 9%
17	P	143	% 87% 13%
18	Q	95	4% 86% 13%
19	R	150	85% 14%
20	S	81	2% 86% 12%
21	T	119	8% 86% 13%
22	U	53	2% 85% 15%
23	V	65	5% 89% 11%
24	W	154	% 81% 18%
25	X	82	7% 84% 15%
26	Y	142	% 89% 10%
27	Z	73	73% 71% 26%
28	1	56	79% 21%
29	2	50	8% 74% 18% 8%

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Mol	Chain	Length	Quality of chain
30	3	92	86% 78% 15% 7%
31	9	122	25% 64% 11%

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	MG	0	8081	-	-	-	X
32	MG	0	8090	-	-	-	X
34	NA	0	8505	-	-	-	X
34	NA	0	8506	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8509	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	0	8568	-	-	-	X
36	SR	0	8922	-	-	-	X
36	SR	0	8947	-	-	-	X
36	SR	0	8994	-	-	-	X
36	SR	0	8997	-	-	-	X
36	SR	0	8998	-	-	-	X
36	SR	B	8987	-	-	-	X
36	SR	J	8986	-	-	-	X

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 99167 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
			Total	C	N	O	P			
1	0	2754	59021	26349	10873	19054	2745	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2P.

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

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	246	1860	1130	345	384	1	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	172	1358	840	224	290	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

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

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	70	520	323	81	115	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	132	994	609	189	192	4	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	194	1559	943	333	282	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	P	143	1137	683	229	225	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	R	150	1150	713	209	224	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	81	642	389	111	139	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	U	53	411	244	75	87	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	V	65	500	304	94	101	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	W	154	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
			Total	C	N	O	S			
25	X	82	655	402	129	123	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	Y	142	1131	686	228	217	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Z	73	574	343	113	113	5	0	0	0

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

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

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

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

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

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

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
31	9	122	2599	1160	471	847	121	0	0	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
32	0	84	84	84	0	0
32	A	2	2	2	0	0
32	B	1	1	1	0	0
32	C	1	1	1	0	0
32	K	1	1	1	0	0
32	T	1	1	1	0	0
32	Y	1	1	1	0	0
32	2	1	1	1	0	0
32	9	1	1	1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	C	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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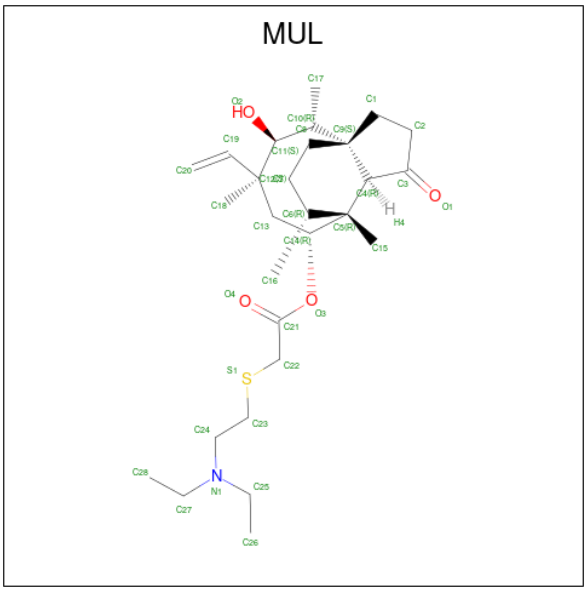
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	91	Total Sr 91 91	0	0
36	A	3	Total Sr 3 3	0	0
36	B	2	Total Sr 2 2	0	0
36	F	1	Total Sr 1 1	0	0
36	H	1	Total Sr 1 1	0	0
36	J	1	Total Sr 1 1	0	0
36	L	1	Total Sr 1 1	0	0
36	R	1	Total Sr 1 1	0	0
36	S	1	Total Sr 1 1	0	0
36	1	2	Total Sr 2 2	0	0
36	3	2	Total Sr 2 2	0	0
36	9	2	Total Sr 2 2	0	0

- Molecule 37 is TIAMULIN (three-letter code: MUL) (formula: $C_{28}H_{47}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
37	0	1	34	28	1	4	1	0	0

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
39	0	5940	5940	5940	0	0
39	A	125	125	125	0	0
39	B	140	140	140	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	C	158	Total O 158 158	0	0
39	D	45	Total O 45 45	0	0
39	E	42	Total O 42 42	0	0
39	F	26	Total O 26 26	0	0
39	G	18	Total O 18 18	0	0
39	H	70	Total O 70 70	0	0
39	I	4	Total O 4 4	0	0
39	J	47	Total O 47 47	0	0
39	K	58	Total O 58 58	0	0
39	L	94	Total O 94 94	0	0
39	M	132	Total O 132 132	0	0
39	N	55	Total O 55 55	0	0
39	O	43	Total O 43 43	0	0
39	P	59	Total O 59 59	0	0
39	Q	52	Total O 52 52	0	0
39	R	80	Total O 80 80	0	0
39	S	30	Total O 30 30	0	0
39	T	30	Total O 30 30	0	0
39	U	30	Total O 30 30	0	0
39	V	11	Total O 11 11	0	0
39	W	59	Total O 59 59	0	0

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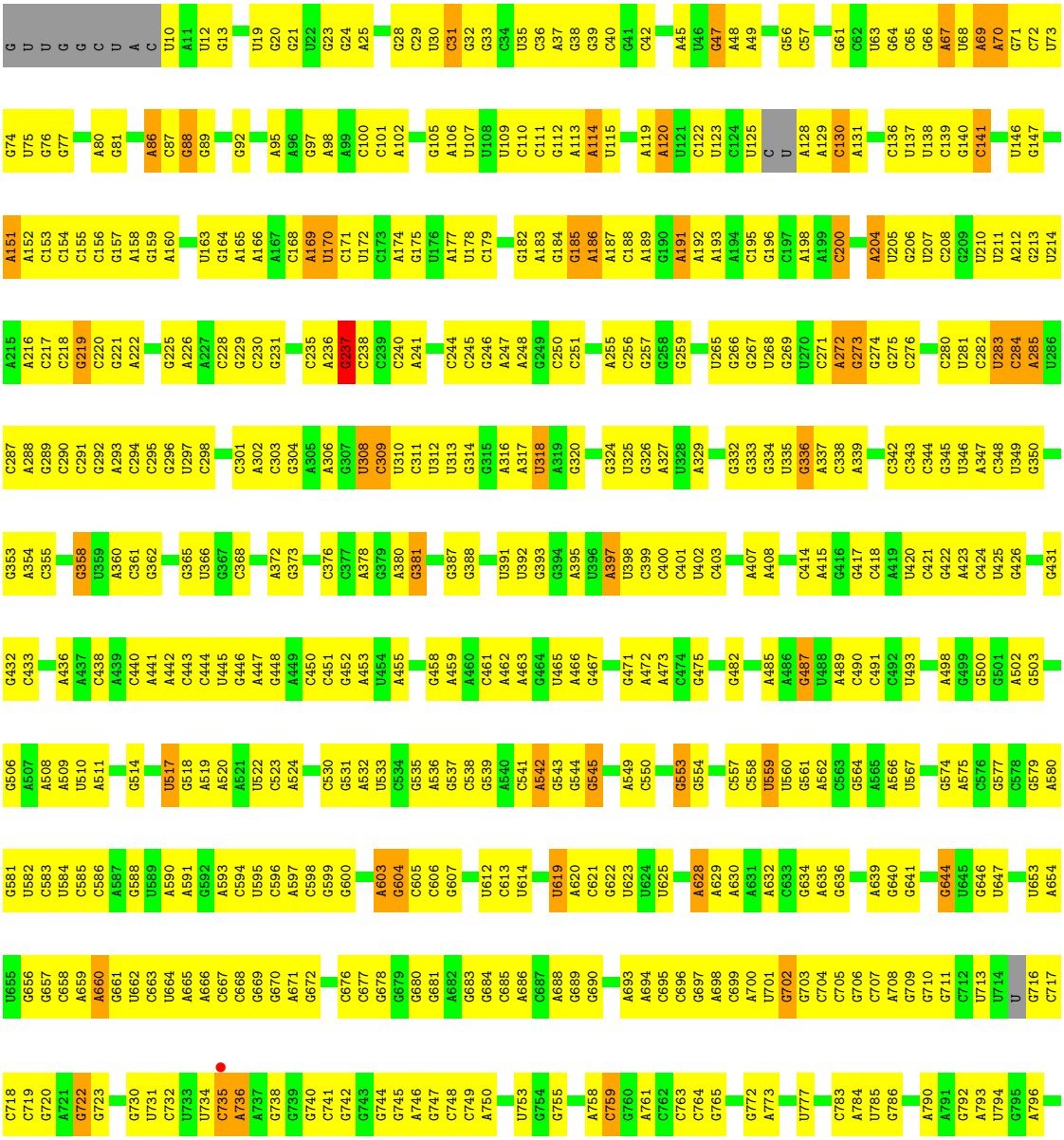
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	X	22	Total O 22 22	0	0
39	Y	105	Total O 105 105	0	0
39	Z	30	Total O 30 30	0	0
39	1	55	Total O 55 55	0	0
39	2	48	Total O 48 48	0	0
39	3	62	Total O 62 62	0	0
39	9	152	Total O 152 152	0	0

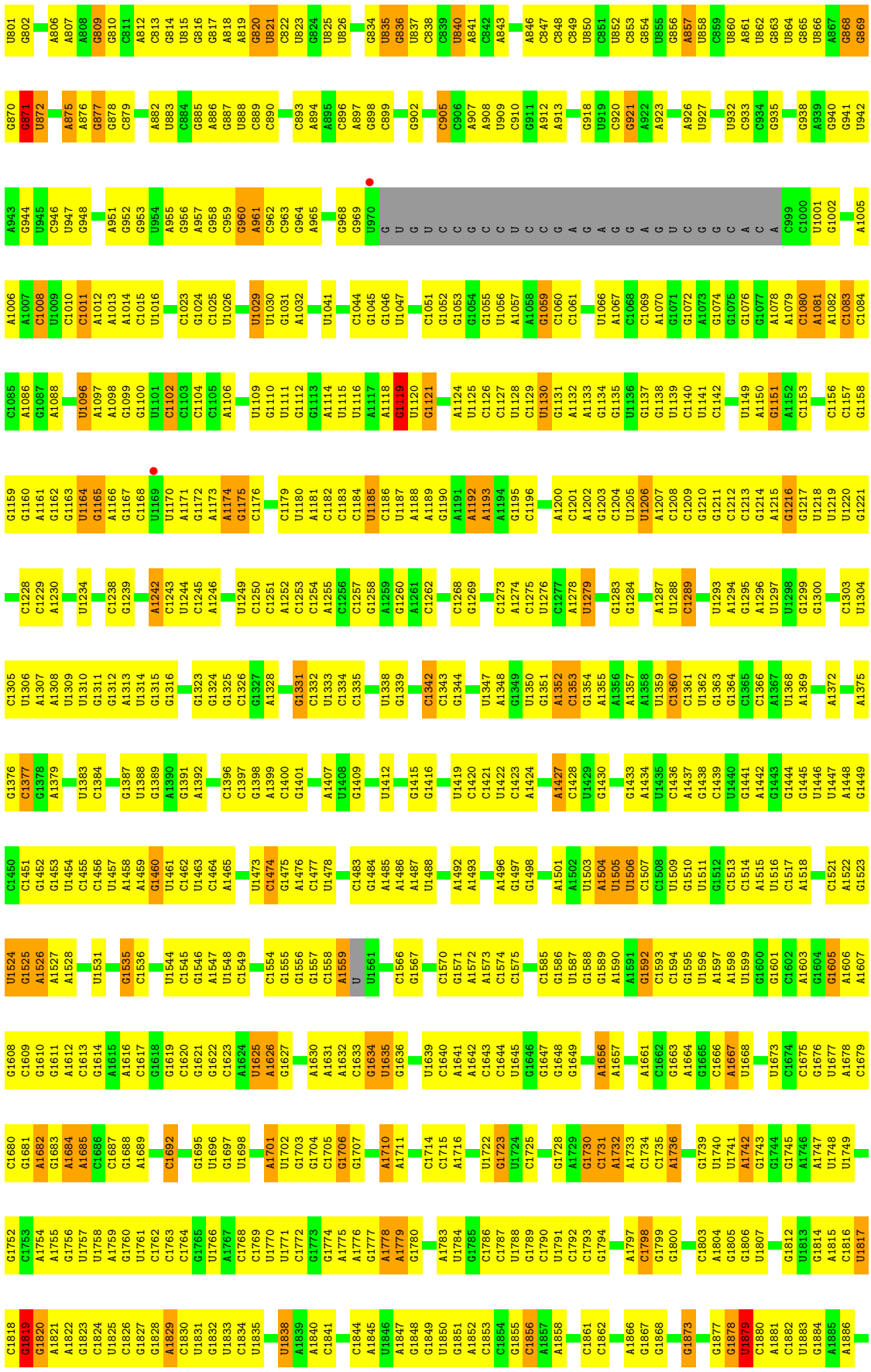
3 Residue-property plots (i)

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

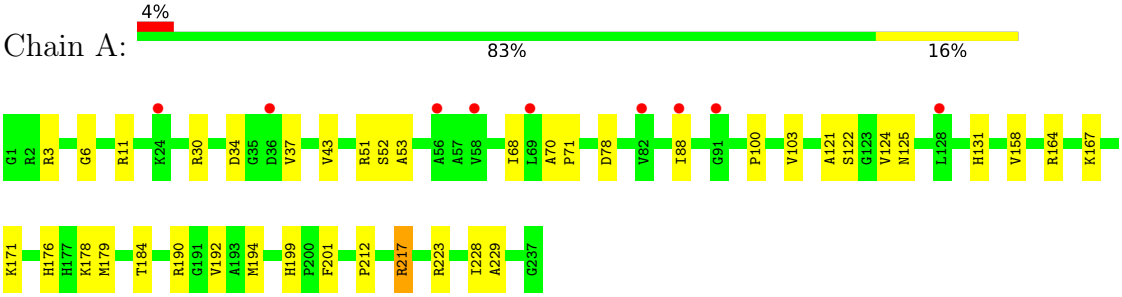
Chain 0:





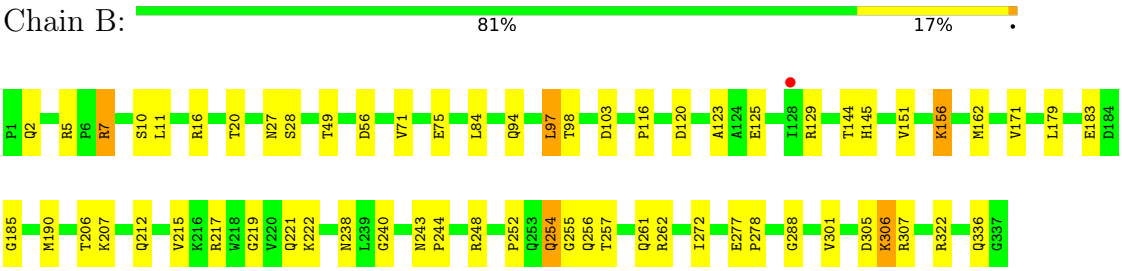
• Molecule 2: 50S ribosomal protein L2P

Chain A:



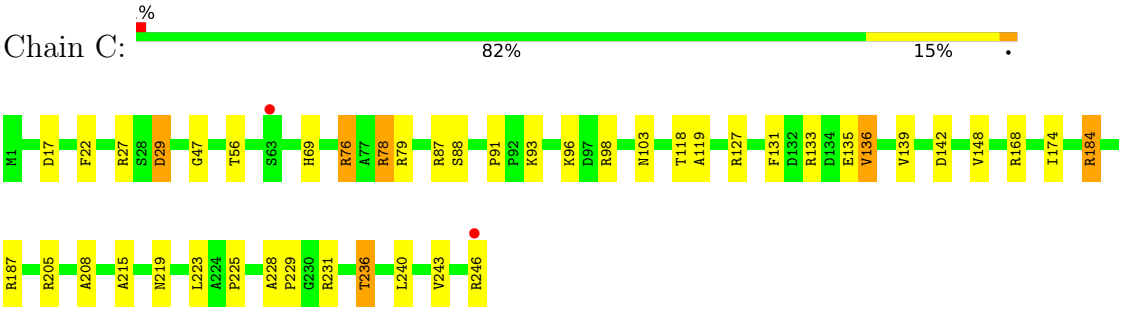
• Molecule 3: 50S ribosomal protein L3P

Chain B:



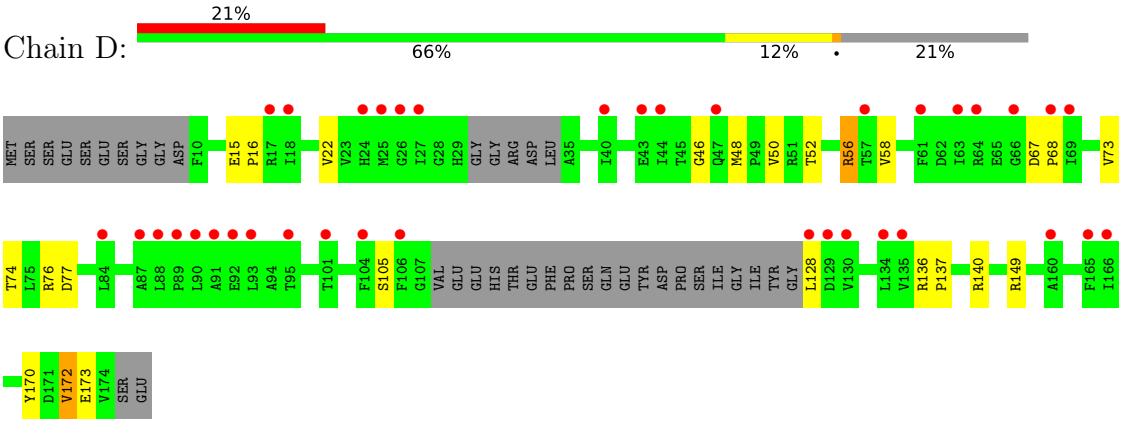
• Molecule 4: 50S ribosomal protein L4P

Chain C:



• Molecule 5: 50S ribosomal protein L5P

Chain D:



• Molecule 6: 50S ribosomal protein L6P

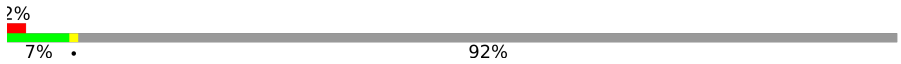
Chain E:

• Molecule 7: 50S ribosomal protein L7Ae

Chain F:

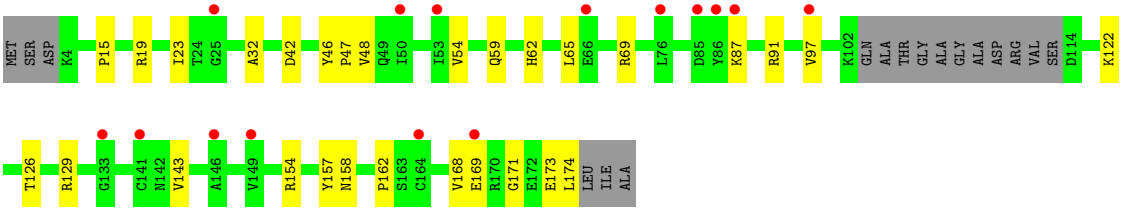
• Molecule 8: 50S ribosomal protein L10

Chain G:



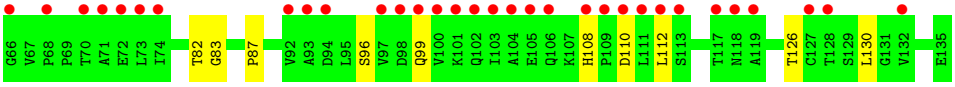
• Molecule 9: 50S ribosomal protein L10e

Chain H:



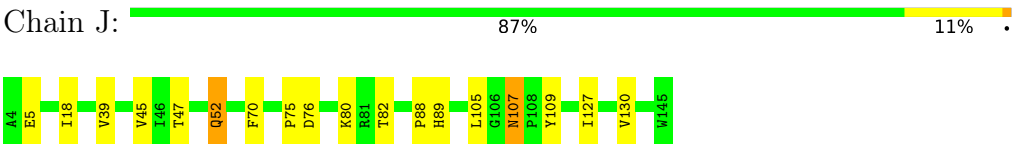
• Molecule 10: 50S ribosomal protein L11P

Chain I:



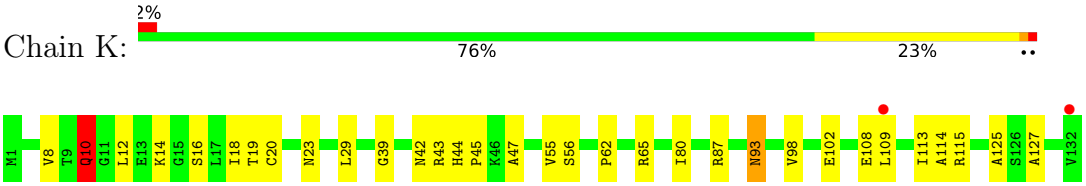
• Molecule 11: 50S ribosomal protein L13P

Chain J:



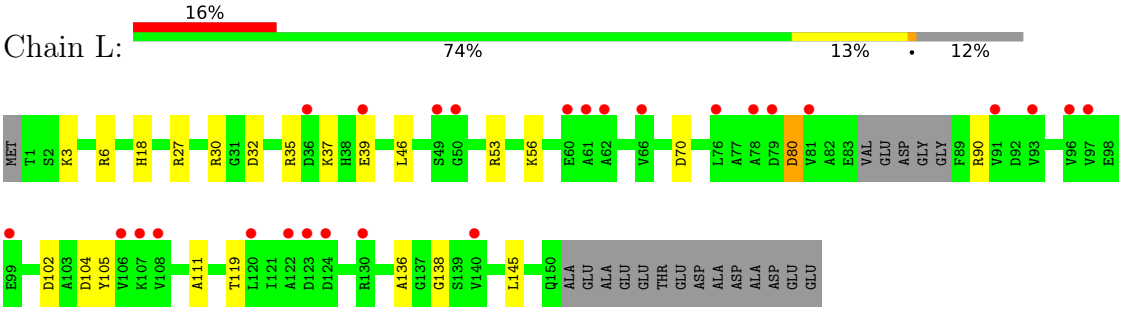
• Molecule 12: 50S ribosomal protein L14P

Chain K:



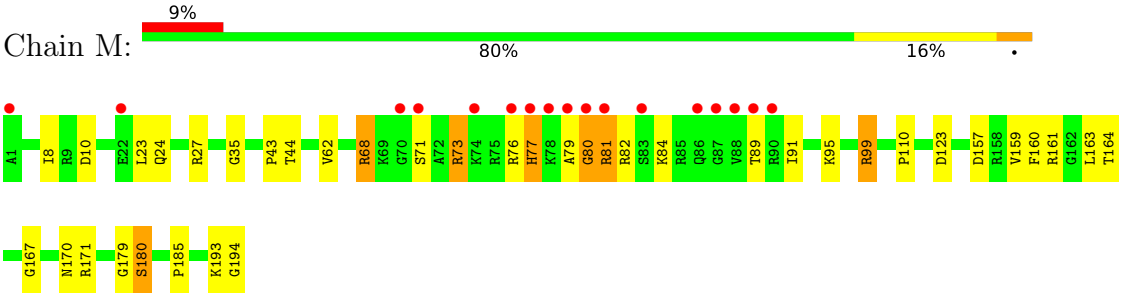
• Molecule 13: 50S ribosomal protein L15P

Chain L:



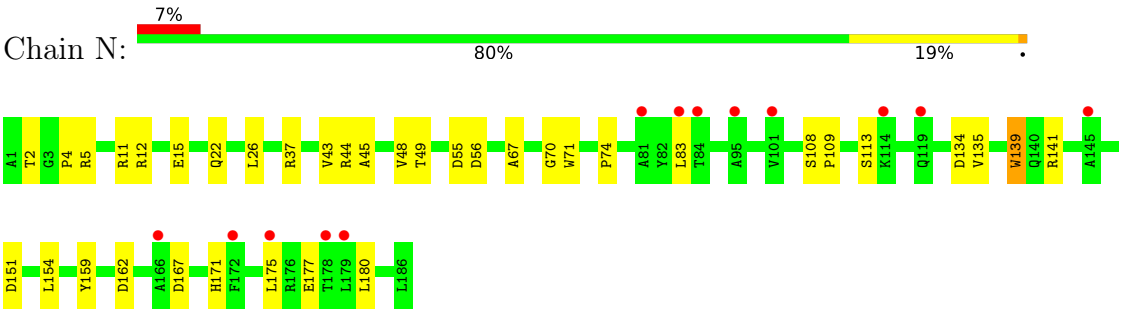
• Molecule 14: 50S ribosomal protein L15e

Chain M:



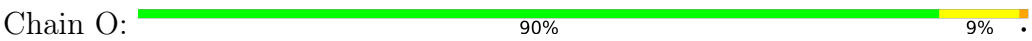
• Molecule 15: 50S ribosomal protein L18P

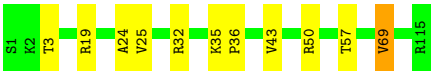
Chain N:



• Molecule 16: 50S ribosomal protein L18e

Chain O:



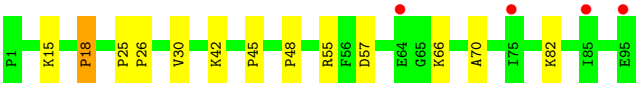


• Molecule 17: 50S ribosomal protein L19e

Chain P:

• Molecule 18: 50S ribosomal protein L21e

Chain Q:

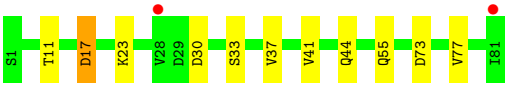


• Molecule 19: 50S ribosomal protein L22P

Chain R:

• Molecule 20: 50S ribosomal protein L23P

Chain S:



• Molecule 21: 50S ribosomal protein L24P

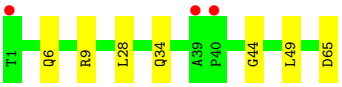
Chain T:

• Molecule 22: 50S ribosomal protein L24e

Chain U:

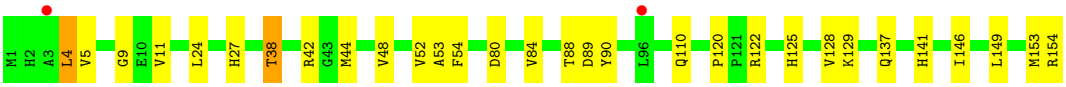
• Molecule 23: 50S ribosomal protein L29P

Chain V: 5% 89% 11%



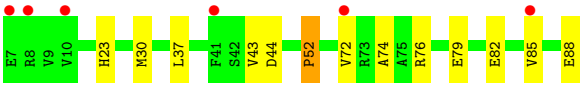
• Molecule 24: 50S ribosomal protein L30P

Chain W: % 81% 18%



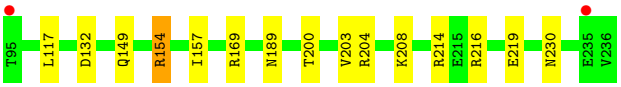
• Molecule 25: 50S ribosomal protein L31e

Chain X: 7% 84% 15%



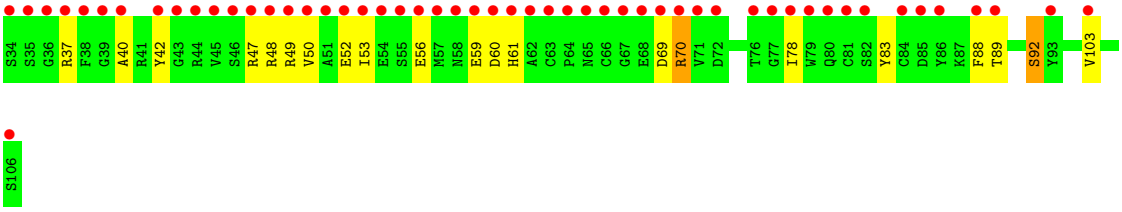
• Molecule 26: 50S ribosomal protein L32e

Chain Y: % 89% 10%



• Molecule 27: 50S ribosomal protein L37Ae

Chain Z: 73% 71% 26%

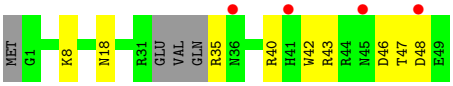


• Molecule 28: 50S ribosomal protein L37e

Chain 1: 79% 21%

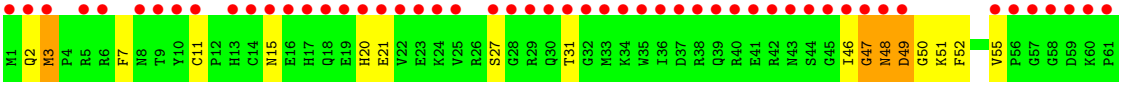
• Molecule 29: 50S ribosomal protein L39e

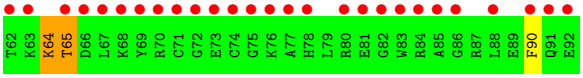
Chain 2: 8% 74% 18% 8%



- Molecule 30: 50S ribosomal protein L44E

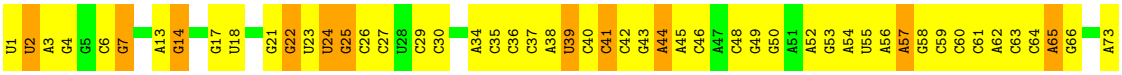
Chain 3:

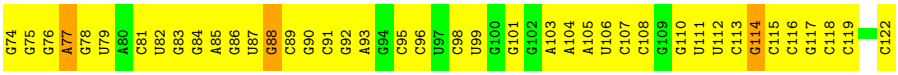




- Molecule 31: 5S ribosomal RNA

Chain 9:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 85.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 82.8 (85.66-2.41)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.290 0.199 , 0.264	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 119.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.47	0/65958	0.69	6/102869 (0.0%)
2	A	0.53	0/1787	0.77	0/2408
3	B	0.54	0/2690	0.77	1/3652 (0.0%)
4	C	0.56	0/1885	0.80	0/2552
5	D	0.70	0/1111	0.74	1/1498 (0.1%)
6	E	0.62	0/1383	0.71	0/1880
7	F	0.56	0/901	0.73	1/1224 (0.1%)
8	G	0.55	0/241	0.66	0/324
9	H	0.61	0/1302	0.78	0/1743
10	I	0.63	0/527	0.66	0/716
11	J	0.63	0/1136	0.75	0/1530
12	K	0.51	0/1004	0.78	0/1351
13	L	0.56	0/1130	0.77	0/1509
14	M	0.55	0/1583	0.79	1/2116 (0.0%)
15	N	0.60	0/1474	0.79	0/1999
16	O	0.52	0/874	0.77	0/1181
17	P	0.56	0/1148	0.69	0/1528
18	Q	0.53	0/749	0.74	0/1005
19	R	0.58	0/1173	0.74	0/1578
20	S	0.56	0/649	0.70	0/875
21	T	0.50	0/958	0.76	1/1289 (0.1%)
22	U	0.65	0/418	0.72	0/562
23	V	0.49	0/503	0.70	0/675
24	W	0.54	0/1219	0.78	0/1655
25	X	0.53	0/665	0.74	0/895
26	Y	0.55	0/1147	0.76	0/1536
27	Z	0.74	0/585	0.84	0/781
28	1	0.62	0/438	0.77	0/578
29	2	0.46	0/401	0.74	0/529
30	3	0.78	0/771	0.81	0/1024
31	9	0.38	0/2904	0.68	0/4526
All	All	0.50	0/98714	0.71	11/147588 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	25
24	W	0	1
All	All	0	26

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1504	A	N9-C1'-C2'	6.64	122.64	114.00
1	0	237	G	N9-C1'-C2'	-6.25	105.12	112.00
3	B	84	LEU	CA-CB-CG	5.84	128.74	115.30
1	0	871	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	0	820	G	N9-C1'-C2'	5.65	121.34	114.00
7	F	118	LEU	CA-CB-CG	5.64	128.28	115.30
1	0	2726	U	N1-C1'-C2'	5.45	121.09	114.00
5	D	170	TYR	N-CA-C	5.31	125.34	111.00
21	T	52	ARG	N-CA-C	5.24	125.14	111.00
1	0	755	G	O4'-C4'-C3'	-5.17	98.83	104.00
14	M	80	GLY	N-CA-C	5.08	125.79	113.10

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1096	U	Sidechain
1	0	1119	G	Sidechain
1	0	1458	A	Sidechain
1	0	1635	U	Sidechain
1	0	1696	U	Sidechain
1	0	1706	G	Sidechain
1	0	1736	A	Sidechain
1	0	1817	U	Sidechain
1	0	1819	G	Sidechain
1	0	1878	G	Sidechain
1	0	1879	U	Sidechain
1	0	2492	U	Sidechain
1	0	2631	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2782	G	Sidechain
1	0	436	A	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	49	A	Sidechain
1	0	493	U	Sidechain
1	0	517	U	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	753	U	Sidechain
1	0	864	U	Sidechain
24	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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	1915	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	37	0
4	C	1860	0	1813	32	0
5	D	1094	0	1085	12	0
6	E	1358	0	1266	12	0
7	F	890	0	843	7	0
8	G	240	0	231	1	0
9	H	1282	0	1292	12	0
10	I	520	0	500	6	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	20	0
13	L	1118	0	1076	13	0
14	M	1559	0	1573	32	0
15	N	1445	0	1401	20	0
16	O	865	0	873	9	0
17	P	1137	0	1123	17	0
18	Q	735	0	729	9	0
19	R	1150	0	1122	15	0
20	S	642	0	605	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	T	950	0	924	13	0
22	U	411	0	368	3	0
23	V	500	0	511	3	0
24	W	1196	0	1137	25	0
25	X	655	0	653	6	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	15	0
28	1	431	0	426	8	0
29	2	396	0	413	6	0
30	3	755	0	732	16	0
31	9	2599	0	1325	113	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	91	0	0	0	0
36	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	34	0	47	17	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5940	0	0	278	0
39	1	55	0	0	0	0
39	2	48	0	0	1	0
39	3	62	0	0	1	0
39	9	152	0	0	12	0
39	A	125	0	0	3	0
39	B	140	0	0	2	0
39	C	158	0	0	3	0
39	D	45	0	0	1	0
39	E	42	0	0	0	0
39	F	26	0	0	2	0
39	G	18	0	0	0	0
39	H	70	0	0	1	0
39	I	4	0	0	0	0
39	J	47	0	0	1	0
39	K	58	0	0	0	0
39	L	94	0	0	4	0
39	M	132	0	0	1	0
39	N	55	0	0	1	0
39	O	43	0	0	1	0
39	P	59	0	0	0	0
39	Q	52	0	0	0	0
39	R	80	0	0	0	0
39	S	30	0	0	1	0
39	T	30	0	0	0	0
39	U	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	V	11	0	0	0	0
39	W	59	0	0	0	0
39	X	22	0	0	0	0
39	Y	105	0	0	1	0
39	Z	30	0	0	2	0
All	All	99167	0	59972	2229	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 (2229) 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:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5"	1.27	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08
31:9:56:A:H2'	31:9:57:A:H5"	1.33	1.07
1:0:2717:C:C2'	1:0:2718:C:H5"	1.86	1.06
1:0:541:C:H2'	1:0:542:A:H5"	1.45	0.98
31:9:76:G:H3'	31:9:77:A:H5"	1.44	0.98
1:0:506:G:H22	1:0:509:A:H5"	1.28	0.97
31:9:92:G:H2'	31:9:93:A:C8	2.00	0.96
1:0:910:C:H3'	39:0:5899:HOH:O	1.71	0.91
1:0:1205:U:H2'	1:0:1206:U:H5'	1.52	0.91
1:0:1166:A:H61	1:0:1180:U:H3	1.15	0.90
31:9:73:A:H61	31:9:108:C:H42	1.19	0.90
1:0:541:C:C2'	1:0:542:A:H5"	1.99	0.90
1:0:1778:A:H2'	1:0:1779:A:H5'	1.53	0.89
1:0:500:G:H21	19:R:98:ASN:HD21	1.20	0.89
12:K:18:ILE:HG22	12:K:93:ASN:HD22	1.38	0.88
1:0:1973:A:H2'	1:0:1974:G:O4'	1.72	0.88
1:0:821:U:H3'	39:0:8403:HOH:O	1.73	0.88
1:0:1667:A:H8	1:0:1667:A:H5'	1.37	0.87
1:0:506:G:H22	1:0:509:A:C5'	1.87	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.75	0.86
1:0:2415:A:H2'	1:0:2416:G:H5'	1.57	0.86
1:0:1762:C:H2'	1:0:1763:C:H6	1.41	0.85
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.85
1:0:1474:C:H6	1:0:1474:C:H5'	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H4'	1:0:1702:U:H5"	1.57	0.84
1:0:1455:C:H2'	1:0:1455:C:O2	1.78	0.84
1:0:101:C:H2'	1:0:102:A:H8	1.43	0.84
1:0:2469:A:H1'	39:0:7426:HOH:O	1.77	0.84
1:0:195:C:H2'	1:0:196:G:H5'	1.59	0.84
1:0:2073:G:H5"	39:0:8459:HOH:O	1.75	0.84
1:0:2502:C:H2'	1:0:2503:A:H5'	1.60	0.84
1:0:545:G:H5'	1:0:545:G:H8	1.41	0.83
1:0:1585:C:H2'	1:0:1586:G:H8	1.42	0.83
1:0:1125:U:H2'	1:0:1126:C:H5'	1.61	0.83
1:0:681:G:N3	1:0:681:G:H5'	1.93	0.83
1:0:1544:U:H2'	1:0:1545:C:H6	1.44	0.83
1:0:1165:G:H1'	1:0:1174:A:H1'	1.60	0.82
1:0:2764:C:H2'	1:0:2765:C:H6	1.45	0.82
1:0:2716:G:H5"	3:B:206:THR:HG21	1.62	0.82
1:0:101:C:H2'	1:0:102:A:C8	2.14	0.81
14:M:24:GLN:NE2	14:M:27:ARG:HH11	1.77	0.81
1:0:213:G:H22	1:0:225:G:H2'	1.45	0.81
1:0:2472:C:O2'	1:0:2634:G:H4'	1.80	0.81
15:N:141:ARG:NH2	31:9:48:C:H4'	1.96	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
1:0:154:C:H2'	1:0:155:C:H6	1.46	0.81
1:0:557:C:H42	1:0:600:G:H1	1.29	0.81
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.44	0.81
15:N:37:ARG:NH1	31:9:6:C:H5"	1.96	0.81
1:0:663:C:H5"	4:C:103:ASN:HD22	1.44	0.80
37:0:9101:MUL:C21	37:0:9101:MUL:H163	2.11	0.80
1:0:1800:G:H1'	17:P:88:GLN:NE2	1.97	0.80
1:0:2088:C:H2'	1:0:2089:A:H8	1.47	0.79
1:0:2102:G:H2'	39:0:7719:HOH:O	1.82	0.79
1:0:2703:A:H2'	1:0:2704:C:H6	1.45	0.79
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.79
1:0:870:G:H2'	1:0:871:G:H5"	1.65	0.79
1:0:559:U:H6	1:0:559:U:H5'	1.48	0.79
1:0:156:C:H5"	14:M:171:ARG:HD3	1.64	0.78
1:0:2502:C:C2'	1:0:2503:A:H5'	2.13	0.78
1:0:1447:U:H3'	1:0:1506:U:O2	1.83	0.78
1:0:1585:C:H2'	1:0:1586:G:C8	2.17	0.78
31:9:56:A:C2'	31:9:57:A:H5"	2.11	0.78
1:0:1300:G:H1'	39:0:3448:HOH:O	1.82	0.78
1:0:1596:U:H2'	1:0:1598:A:OP2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:110:C:H1'	39:0:6248:HOH:O	1.83	0.78
1:0:2505:G:O2'	1:0:2506:A:H5'	1.84	0.78
1:0:625:U:H5"	1:0:1044:C:N4	1.98	0.78
1:0:663:C:H5"	4:C:103:ASN:ND2	1.98	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.11	0.77
1:0:2816:A:H5"	1:0:2817:G:H5'	1.64	0.77
1:0:541:C:H2'	1:0:542:A:C5'	2.15	0.77
31:9:24:U:H3'	31:9:25:G:H5'	1.65	0.77
1:0:2712:G:H5'	39:0:4183:HOH:O	1.85	0.77
1:0:2264:A:H4'	39:0:4146:HOH:O	1.85	0.77
1:0:2248:C:H2'	1:0:2249:G:H8	1.47	0.77
14:M:24:GLN:HE21	14:M:27:ARG:HH11	1.29	0.77
1:0:213:G:N2	1:0:225:G:H2'	2.00	0.76
1:0:447:A:O2'	1:0:448:G:H5'	1.85	0.76
17:P:115:SER:H	17:P:118:GLN:HE21	1.32	0.76
1:0:308:U:H2'	21:T:52:ARG:NH2	1.99	0.76
1:0:2289:G:O2'	1:0:2290:U:H5'	1.86	0.76
1:0:694:A:H2'	1:0:695:C:H5'	1.67	0.76
31:9:92:G:H2'	31:9:93:A:H8	1.49	0.76
1:0:1372:A:H3'	39:0:6923:HOH:O	1.86	0.76
37:0:9101:MUL:H10	37:0:9101:MUL:H14	1.68	0.76
1:0:2270:G:H4'	2:A:223:ARG:HH12	1.49	0.75
1:0:1160:G:H5'	1:0:1161:A:C5'	2.12	0.75
1:0:659:A:H5"	39:O:6799:HOH:O	1.86	0.75
1:0:1444:G:O2'	1:0:1445:G:H5'	1.86	0.75
1:0:2466:G:H5"	39:0:8275:HOH:O	1.85	0.75
1:0:1167:G:H1	1:0:1179:C:H42	1.35	0.75
1:0:1171:A:H2'	1:0:1172:G:H5'	1.67	0.75
1:0:2371:G:H5'	39:0:3898:HOH:O	1.87	0.75
1:0:170:U:H5'	30:3:48:ASN:HD22	1.51	0.75
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.51	0.75
1:0:542:A:H5'	1:0:542:A:H8	1.52	0.74
1:0:1116:U:O2'	1:0:1118:A:H2	1.67	0.74
1:0:2326:C:H2'	1:0:2327:A:H8	1.52	0.74
1:0:188:C:H5"	14:M:163:LEU:HD21	1.69	0.74
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.53	0.74
1:0:2059:U:H2'	1:0:2060:A:H8	1.52	0.74
1:0:424:C:H2'	1:0:425:U:H6	1.53	0.73
1:0:1485:A:H1'	39:0:3502:HOH:O	1.88	0.73
1:0:2253:G:H2'	1:0:2254:G:H8	1.53	0.73
1:0:1351:G:H3'	39:0:4782:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1692:C:H3'	39:0:8632:HOH:O	1.88	0.73
12:K:10:GLN:NE2	12:K:10:GLN:H	1.86	0.73
31:9:29:C:H2'	31:9:30:C:H5'	1.70	0.73
1:0:146:U:O2'	1:0:147:G:H5'	1.89	0.73
1:0:1829:A:H2'	1:0:1830:C:H5'	1.71	0.73
1:0:1132:A:N6	1:0:1229:C:H2'	2.04	0.73
1:0:2326:C:H2'	1:0:2327:A:C8	2.24	0.73
1:0:2372:A:H2'	1:0:2373:U:H6	1.54	0.73
1:0:21:G:H4'	19:R:2:ILE:HG22	1.71	0.73
1:0:1701:A:H5'	39:0:5659:HOH:O	1.88	0.73
1:0:625:U:H3'	39:0:7470:HOH:O	1.87	0.72
1:0:2534:C:H1'	39:0:8122:HOH:O	1.87	0.72
1:0:136:C:H2'	1:0:137:U:O4'	1.89	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.90	0.72
1:0:327:A:H4'	1:0:329:A:C8	2.25	0.72
1:0:2426:G:H5'	39:0:3025:HOH:O	1.89	0.72
1:0:2616:G:H1'	39:0:8273:HOH:O	1.90	0.72
1:0:561:G:H2'	1:0:562:A:H8	1.55	0.72
39:D:3839:HOH:O	31:9:58:G:H1'	1.90	0.72
1:0:92:G:H4'	23:V:44:GLY:HA3	1.72	0.71
1:0:381:G:H5"	39:0:2945:HOH:O	1.91	0.71
1:0:905:C:H3'	39:0:4139:HOH:O	1.89	0.71
1:0:1159:G:H2'	1:0:1160:G:O4'	1.90	0.71
1:0:1377:C:H5'	1:0:1377:C:H6	1.55	0.71
1:0:290:C:H1'	39:0:5406:HOH:O	1.89	0.71
1:0:1118:A:C8	1:0:1118:A:H3'	2.25	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
1:0:12:U:H2'	1:0:13:G:H5'	1.70	0.71
1:0:1165:G:H21	1:0:1173:A:H5"	1.54	0.71
1:0:2637:A:H4'	39:0:3790:HOH:O	1.90	0.71
1:0:1303:C:O2	1:0:1353:C:H1'	1.90	0.71
1:0:282:C:H1'	1:0:368:C:N4	2.06	0.71
1:0:2269:C:H2'	1:0:2270:G:O4'	1.91	0.71
1:0:870:G:C2'	1:0:871:G:H5"	2.21	0.70
1:0:1883:U:H5"	1:0:2013:G:OP2	1.90	0.70
1:0:2059:U:H2'	1:0:2060:A:C8	2.26	0.70
1:0:1451:C:H5'	1:0:1505:U:C5	2.26	0.70
27:Z:60:ASP:HB3	27:Z:69:ASP:HB3	1.73	0.70
31:9:24:U:H3'	31:9:25:G:C5'	2.20	0.70
1:0:1673:U:H4'	39:S:1504:HOH:O	1.90	0.70
1:0:2271:G:H5'	39:0:3548:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1741:U:H5'	1:0:1742:A:OP1	1.91	0.70
1:0:2758:G:H2'	1:0:2759:C:C6	2.26	0.70
1:0:282:C:O2'	1:0:283:U:H5'	1.90	0.70
1:0:671:A:O2'	1:0:672:G:H2'	1.92	0.70
1:0:2312:G:H2'	1:0:2313:C:H5'	1.73	0.70
1:0:2710:U:H1'	39:0:7520:HOH:O	1.92	0.70
1:0:1873:G:H3'	39:0:4169:HOH:O	1.91	0.70
1:0:2461:U:O2	1:0:2466:G:H1'	1.91	0.70
1:0:221:G:H5"	39:0:4894:HOH:O	1.91	0.70
1:0:1130:U:H2'	1:0:1131:G:O4'	1.92	0.69
1:0:2758:G:H2'	1:0:2759:C:H6	1.56	0.69
1:0:432:G:H5"	39:0:6484:HOH:O	1.92	0.69
31:9:39:U:H3'	31:9:40:C:C5'	2.22	0.69
1:0:1347:U:H2'	1:0:1348:A:C8	2.26	0.69
1:0:2050:G:H5"	19:R:80:TYR:O	1.91	0.69
1:0:1205:U:C2'	1:0:1206:U:H5'	2.22	0.69
1:0:1682:A:O2'	1:0:1683:G:H5"	1.93	0.69
1:0:2563:U:HO2'	1:0:2564:G:H8	1.40	0.69
1:0:73:U:H2'	1:0:74:G:C8	2.28	0.69
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.69
1:0:1186:C:H42	1:0:1190:G:H22	1.39	0.69
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.69
1:0:1189:A:H3'	39:0:7609:HOH:O	1.92	0.69
1:0:1856:C:H5'	1:0:1858:A:O4'	1.92	0.68
1:0:1790:C:H2'	1:0:1791:U:C6	2.28	0.68
1:0:1278:A:H4'	1:0:1279:U:C4	2.28	0.68
1:0:137:U:H2'	1:0:139:C:C5	2.29	0.68
1:0:2584:G:H4'	39:0:6824:HOH:O	1.92	0.68
1:0:399:C:H5'	14:M:179:GLY:O	1.93	0.68
1:0:1793:C:O2	1:0:1793:C:H2'	1.92	0.68
1:0:2894:C:O2'	1:0:2895:C:H5'	1.94	0.68
1:0:1838:U:O2'	1:0:2644:C:H5'	1.92	0.68
12:K:10:GLN:H	12:K:10:GLN:HE21	1.39	0.68
1:0:191:A:H2'	1:0:237:G:O6	1.93	0.68
1:0:2726:U:H5"	1:0:2749:U:H3	1.59	0.68
1:0:2812:A:H2	1:0:2814:A:H62	1.41	0.68
1:0:1120:U:H5"	1:0:1120:U:C6	2.29	0.68
1:0:2430:A:H4'	13:L:46:LEU:O	1.94	0.68
1:0:558:C:C2'	1:0:559:U:H5"	2.24	0.68
1:0:1589:G:H22	1:0:1605:G:H1'	1.58	0.68
1:0:1097:A:H5"	24:W:125:HIS:NE2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1574:C:H2'	1:0:1575:C:H6	1.58	0.67
1:0:500:G:N2	19:R:98:ASN:HD21	1.92	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.41	0.67
1:0:2416:G:H2'	1:0:2417:C:C6	2.29	0.67
31:9:114:G:H2'	31:9:115:C:C6	2.29	0.67
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.76	0.67
1:0:1882:C:OP1	2:A:192:VAL:HG23	1.94	0.67
1:0:2372:A:H2'	1:0:2373:U:C6	2.28	0.67
1:0:119:A:H2'	1:0:120:A:H5"	1.77	0.67
1:0:2332:A:H5'	5:D:56:ARG:HH22	1.58	0.67
1:0:169:A:H1'	30:3:48:ASN:ND2	2.09	0.67
1:0:1126:C:O5'	1:0:1126:C:H6	1.77	0.67
13:L:27:ARG:HH21	13:L:30:ARG:HE	1.42	0.67
1:0:2365:G:H4'	18:Q:45:PRO:O	1.95	0.67
1:0:2787:C:H5	39:0:3383:HOH:O	1.77	0.67
1:0:1829:A:H61	27:Z:42:TYR:HA	1.59	0.67
1:0:318:U:H5'	1:0:339:A:C2	2.29	0.66
1:0:1544:U:H2'	1:0:1545:C:C6	2.28	0.66
1:0:2032:U:H2'	1:0:2033:G:H5"	1.76	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:2712:G:H1'	39:0:5039:HOH:O	1.95	0.66
1:0:171:C:H3'	39:0:5555:HOH:O	1.94	0.66
31:9:52:A:H2'	31:9:53:G:O4'	1.95	0.66
1:0:622:G:O2'	1:0:623:U:H5'	1.95	0.66
1:0:713:U:O5'	1:0:713:U:H6	1.79	0.66
1:0:1047:U:H5'	39:0:5458:HOH:O	1.94	0.66
1:0:1667:A:H5'	1:0:1667:A:C8	2.26	0.66
1:0:1268:C:O2'	1:0:1269:G:H5'	1.96	0.66
1:0:2498:C:O2'	1:0:2499:U:H5'	1.96	0.66
1:0:848:C:H5'	39:0:7034:HOH:O	1.95	0.66
1:0:1209:C:H2'	1:0:1210:G:H8	1.59	0.66
1:0:1589:G:N2	1:0:1605:G:H1'	2.10	0.66
1:0:2433:A:H8	1:0:2433:A:O5'	1.79	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.77	0.66
9:H:59:GLN:NE2	9:H:129:ARG:HE	1.94	0.66
1:0:2904:U:H2'	1:0:2905:A:H8	1.61	0.66
1:0:183:A:H1'	14:M:161:ARG:NH1	2.11	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
15:N:141:ARG:HH21	31:9:48:C:H4'	1.61	0.66
1:0:683:G:H5"	39:0:4020:HOH:O	1.95	0.66
1:0:2296:C:H2'	1:0:2297:U:C6	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:886:A:H1'	39:0:3891:HOH:O	1.95	0.65
1:0:1679:C:H5'	39:0:4044:HOH:O	1.95	0.65
1:0:1743:G:H1'	39:0:3739:HOH:O	1.96	0.65
31:9:34:A:H2'	31:9:35:C:O4'	1.95	0.65
1:0:2488:A:H1'	39:0:3221:HOH:O	1.96	0.65
1:0:1181:A:H2'	1:0:1182:C:H5'	1.76	0.65
1:0:1412:U:O4	1:0:1681:G:H2'	1.97	0.65
1:0:1165:G:O3'	1:0:1174:A:H4'	1.96	0.65
1:0:316:A:N3	1:0:336:G:O2'	2.29	0.65
1:0:1762:C:H2'	1:0:1763:C:C6	2.28	0.65
1:0:2088:C:H2'	1:0:2089:A:C8	2.32	0.65
1:0:2415:A:C2'	1:0:2416:G:H5'	2.25	0.65
1:0:338:C:H3'	39:0:8434:HOH:O	1.96	0.65
1:0:1114:A:O2'	1:0:1115:U:H5'	1.96	0.65
1:0:1735:C:O2'	1:0:1736:A:H5'	1.96	0.65
31:9:3:A:N6	31:9:22:G:H1'	2.11	0.65
1:0:431:G:H5'	39:0:7692:HOH:O	1.97	0.65
1:0:545:G:H5'	1:0:545:G:C8	2.29	0.64
1:0:1728:G:H1'	39:0:5467:HOH:O	1.96	0.64
1:0:2010:A:H2'	39:0:5197:HOH:O	1.97	0.64
1:0:2486:A:H2	37:0:9101:MUL:H221	1.63	0.64
1:0:200:C:H2'	39:0:7991:HOH:O	1.97	0.64
1:0:450:C:OP1	4:C:184:ARG:NH2	2.31	0.64
1:0:1626:A:H2'	1:0:1627:G:O4'	1.98	0.64
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.64
35:0:8812:CL:CL	39:0:4058:HOH:O	2.50	0.64
14:M:79:ALA:HB3	14:M:81:ARG:HH12	1.63	0.64
31:9:104:A:O2'	31:9:105:A:H5'	1.97	0.64
1:0:702:G:O2'	1:0:703:G:H5'	1.97	0.64
1:0:932:U:O2'	1:0:1296:A:H1'	1.97	0.64
1:0:1015:C:H2'	1:0:1016:U:H6	1.61	0.64
1:0:2769:C:H2'	1:0:2770:G:O4'	1.98	0.64
1:0:558:C:H2'	1:0:559:U:H5"	1.79	0.64
1:0:1307:A:H2'	1:0:1308:A:C8	2.33	0.64
1:0:2748:G:H2'	39:0:7410:HOH:O	1.98	0.64
1:0:1559:A:H1'	39:0:5067:HOH:O	1.97	0.64
1:0:1308:A:H4'	4:C:225:PRO:O	1.98	0.64
1:0:1483:C:O2'	1:0:1484:G:H5'	1.98	0.64
1:0:1595:G:O2'	1:0:1596:U:H5'	1.98	0.64
1:0:1921:A:O2'	1:0:1922:A:H5'	1.97	0.64
1:0:1139:U:H2'	1:0:1140:C:C6	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2524:G:H21	1:0:2526:C:N4	1.96	0.64
1:0:2898:G:H4'	3:B:288:GLY:HA2	1.80	0.64
1:0:73:U:H2'	1:0:74:G:H8	1.61	0.64
1:0:1184:C:H1'	39:0:7308:HOH:O	1.98	0.64
1:0:837:U:H4'	39:0:7940:HOH:O	1.98	0.63
1:0:1115:U:H2'	1:0:1116:U:H6	1.63	0.63
1:0:1276:U:H3'	16:O:19:ARG:HH11	1.63	0.63
1:0:1771:U:H1'	27:Z:47:ARG:HH21	1.62	0.63
4:C:127:ARG:NH2	4:C:225:PRO:HG2	2.12	0.63
1:0:444:C:H1'	39:0:8745:HOH:O	1.97	0.63
1:0:2032:U:H5"	39:0:6193:HOH:O	1.98	0.63
1:0:2320:U:H2'	30:3:2:GLN:O	1.98	0.63
1:0:2526:C:O2'	1:0:2527:U:H5'	1.98	0.63
1:0:506:G:N2	1:0:509:A:H5"	2.08	0.63
1:0:958:G:H4'	31:9:105:A:H4'	1.80	0.63
1:0:1181:A:C2'	1:0:1182:C:H5'	2.27	0.63
1:0:1307:A:H2'	1:0:1308:A:H8	1.63	0.63
1:0:2819:C:H4'	3:B:97:LEU:O	1.98	0.63
31:9:98:C:H2'	31:9:99:U:H6	1.62	0.63
1:0:1061:C:H3'	39:0:4002:HOH:O	1.99	0.63
1:0:2472:C:H3'	39:0:8235:HOH:O	1.98	0.63
1:0:2740:G:H2'	1:0:2741:A:O4'	1.99	0.63
3:B:7:ARG:HH12	3:B:11:LEU:HD22	1.63	0.63
1:0:1593:C:H2'	1:0:1594:C:H6	1.64	0.63
1:0:2332:A:H3'	1:0:2333:G:H8	1.64	0.63
1:0:432:G:H2'	1:0:433:C:H6	1.62	0.63
1:0:1523:G:H2'	1:0:1524:U:C6	2.34	0.63
1:0:1183:C:H2'	39:0:5603:HOH:O	1.98	0.63
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.46	0.63
1:0:2256:G:H2'	1:0:2257:G:H5'	1.81	0.62
14:M:43:PRO:HG3	14:M:62:VAL:HG21	1.81	0.62
1:0:1127:C:H2'	1:0:1128:U:H5'	1.81	0.62
1:0:2714:U:H2'	1:0:2715:G:H8	1.64	0.62
1:0:221:G:H2'	1:0:222:A:C8	2.33	0.62
1:0:451:C:O2'	1:0:452:G:H5'	1.99	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.63	0.62
1:0:1204:C:H2'	1:0:1205:U:O4'	1.99	0.62
1:0:2607:U:OP2	3:B:243:ASN:HB2	1.99	0.62
1:0:219:G:H5'	1:0:220:C:H5"	1.82	0.62
1:0:1220:U:H2'	1:0:1221:G:H8	1.64	0.62
1:0:109:U:O2	1:0:109:U:H2'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:935:G:H4'	39:0:7674:HOH:O	1.98	0.62
1:0:1805:G:O2'	1:0:1806:G:H5'	1.99	0.62
1:0:1931:A:H2'	1:0:1932:G:H5'	1.81	0.62
1:0:2314:G:O2'	1:0:2315:C:H5'	2.00	0.62
37:0:9101:MUL:H201	37:0:9101:MUL:H263	1.81	0.62
31:9:84:G:H2'	31:9:85:A:H8	1.64	0.62
1:0:1139:U:H2'	1:0:1140:C:H6	1.63	0.62
1:0:69:A:H5'	1:0:69:A:C8	2.35	0.62
1:0:1125:U:C2'	1:0:1126:C:H5'	2.29	0.62
1:0:1211:G:O2'	1:0:1212:C:H5'	1.99	0.62
1:0:1554:C:H1'	1:0:1632:A:H1'	1.82	0.62
1:0:2433:A:H2	1:0:2458:U:H3	1.46	0.62
1:0:2769:C:C2'	1:0:2770:G:H5'	2.30	0.62
1:0:2887:G:H2'	1:0:2888:U:C6	2.34	0.62
1:0:1162:G:H1'	10:I:112:LEU:HD11	1.80	0.62
1:0:1213:C:O2'	1:0:1214:G:H5'	2.00	0.62
14:M:77:HIS:HD2	14:M:81:ARG:H	1.47	0.62
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.82	0.61
1:0:646:G:H2'	1:0:647:U:C6	2.35	0.61
1:0:1008:C:H5"	9:H:19:ARG:HH12	1.63	0.61
1:0:2896:A:N3	1:0:2896:A:H2'	2.15	0.61
1:0:812:A:H2'	1:0:813:C:C6	2.36	0.61
1:0:1391:G:H2'	1:0:1392:A:H5'	1.81	0.61
1:0:1474:C:H5'	1:0:1474:C:C6	2.30	0.61
1:0:857:A:H4'	2:A:176:HIS:CD2	2.35	0.61
1:0:907:A:H2'	1:0:908:A:H8	1.65	0.61
1:0:1333:U:H2'	1:0:1334:C:H6	1.65	0.61
1:0:2781:U:H1'	6:E:139:GLU:OE2	2.00	0.61
21:T:41:ARG:HH21	21:T:67:LEU:HD21	1.64	0.61
31:9:39:U:H3	31:9:42:C:H5"	1.64	0.61
1:0:106:A:O2'	1:0:107:U:H5'	2.00	0.61
1:0:178:U:H2'	1:0:179:C:H6	1.66	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.61
1:0:2373:U:H1'	39:0:3565:HOH:O	2.01	0.61
1:0:183:A:C2	1:0:184:G:C4	2.88	0.61
1:0:1014:A:H5"	31:9:101:G:O2'	1.99	0.61
1:0:1051:C:H2'	1:0:1052:G:O4'	2.00	0.61
1:0:1347:U:H2'	1:0:1348:A:H8	1.63	0.61
1:0:2295:G:N3	1:0:2361:A:H2	1.97	0.61
1:0:2627:G:H5'	39:0:3864:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:27:ARG:HH22	14:M:44:THR:HG23	1.65	0.61
1:0:2426:G:H1'	39:0:5391:HOH:O	2.00	0.61
1:0:852:U:H3'	39:0:8226:HOH:O	1.99	0.61
1:0:1202:A:H2'	1:0:1203:G:O4'	2.01	0.61
1:0:1279:U:O2	1:0:1279:U:H2'	1.98	0.61
1:0:2041:G:O2'	1:0:2042:U:H5'	2.00	0.61
1:0:2486:A:C2	37:0:9101:MUL:H221	2.36	0.61
31:9:105:A:H2'	31:9:106:U:O4'	2.01	0.61
31:9:13:A:O2'	31:9:14:G:H5"	2.01	0.61
1:0:146:U:C2'	1:0:147:G:H5'	2.31	0.60
1:0:195:C:C2'	1:0:196:G:H5'	2.31	0.60
1:0:312:U:O2'	1:0:313:U:H5'	2.01	0.60
1:0:2248:C:H3'	39:0:4476:HOH:O	2.00	0.60
7:F:30:LYS:HB2	7:F:97:ALA:HB3	1.83	0.60
1:0:185:G:O3'	1:0:186:A:H4'	2.00	0.60
1:0:287:C:H42	1:0:365:G:H1	1.49	0.60
1:0:327:A:H4'	1:0:329:A:N7	2.15	0.60
1:0:1398:G:H2'	1:0:1399:A:H8	1.64	0.60
1:0:1516:U:H2'	1:0:1517:C:O4'	2.01	0.60
1:0:2548:C:H5'	3:B:252:PRO:HD2	1.83	0.60
1:0:1761:U:H5'	17:P:81:LYS:O	2.01	0.60
1:0:2122:C:H1'	14:M:76:ARG:HH21	1.66	0.60
5:D:76:ARG:NH2	31:9:44:A:H1'	2.15	0.60
37:0:9101:MUL:H271	37:0:9101:MUL:S1	2.42	0.60
1:0:854:G:H8	39:0:8680:HOH:O	1.82	0.60
1:0:2714:U:H2'	1:0:2715:G:C8	2.36	0.60
31:9:116:C:O2'	31:9:117:G:H5'	2.01	0.60
1:0:542:A:H5'	1:0:542:A:C8	2.35	0.60
1:0:1590:A:H1'	1:0:1606:A:C2	2.36	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.60
1:0:2385:G:H2'	1:0:2386:U:C6	2.37	0.60
1:0:1641:A:H2'	1:0:1642:A:O4'	2.01	0.60
1:0:1916:C:H2'	1:0:1917:G:H8	1.65	0.60
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.83	0.60
1:0:24:G:N2	1:0:518:G:H1'	2.17	0.60
1:0:280:C:H2'	1:0:281:U:O4'	2.02	0.60
1:0:333:G:O2'	1:0:334:G:H5'	2.02	0.60
1:0:2032:U:H2'	1:0:2033:G:C5'	2.31	0.60
1:0:2065:C:H4'	39:0:7923:HOH:O	2.01	0.60
1:0:1299:G:N7	13:L:6:ARG:NH1	2.49	0.60
1:0:2769:C:O2'	1:0:2770:G:H5'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:630:A:H3'	39:0:5239:HOH:O	2.01	0.60
1:0:1398:G:H2'	1:0:1399:A:C8	2.36	0.60
1:0:1455:C:O2	1:0:1455:C:C2'	2.50	0.60
1:0:1255:A:H3'	39:0:6875:HOH:O	2.02	0.59
1:0:2248:C:H2'	1:0:2249:G:C8	2.34	0.59
1:0:2296:C:H2'	1:0:2297:U:H6	1.67	0.59
31:9:56:A:H2'	31:9:57:A:C5'	2.22	0.59
1:0:1276:U:H3'	16:O:19:ARG:NH1	2.18	0.59
1:0:105:G:O2'	1:0:106:A:H5'	2.02	0.59
1:0:1711:A:H3'	39:0:5721:HOH:O	2.02	0.59
12:K:23:ASN:ND2	12:K:108:GLU:H	2.00	0.59
1:0:69:A:H5'	1:0:69:A:H8	1.66	0.59
1:0:557:C:N4	1:0:600:G:H1	1.99	0.59
1:0:1119:G:H5'	11:J:52:GLN:NE2	2.17	0.59
1:0:1313:A:H5'	26:Y:208:LYS:O	2.01	0.59
1:0:1806:G:C6	1:0:1807:U:N3	2.70	0.59
1:0:308:U:H5'	1:0:309:C:OP1	2.03	0.59
1:0:1632:A:H2'	1:0:1633:C:H5'	1.83	0.59
1:0:2270:G:H4'	2:A:223:ARG:NH1	2.17	0.59
1:0:2324:G:H1'	39:0:5418:HOH:O	2.02	0.59
1:0:2402:A:H8	1:0:2402:A:O5'	1.86	0.59
1:0:2502:C:H2'	1:0:2503:A:C5'	2.33	0.59
1:0:595:U:H2'	1:0:596:C:H6	1.68	0.59
1:0:2828:G:O5'	1:0:2828:G:H8	1.85	0.59
1:0:790:A:H1'	1:0:1710:A:H2'	1.85	0.59
1:0:820:G:H5'	1:0:821:U:H5'	1.83	0.59
1:0:2345:A:H3'	1:0:2346:C:C5	2.37	0.59
1:0:1167:G:H2'	1:0:1168:C:C6	2.38	0.59
1:0:1797:A:H4'	1:0:1798:C:C5	2.38	0.59
31:9:37:C:O2'	31:9:38:A:H5'	2.03	0.59
31:9:39:U:H1'	31:9:44:A:H61	1.68	0.59
1:0:244:C:H6	1:0:244:C:O5'	1.85	0.59
1:0:1015:C:H2'	1:0:1016:U:C6	2.38	0.59
1:0:2783:A:H3'	39:0:4201:HOH:O	2.02	0.59
27:Z:59:GLU:HG2	27:Z:60:ASP:H	1.68	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.58
1:0:871:G:C8	1:0:871:G:C5'	2.77	0.58
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.35	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.69	0.58
1:0:2332:A:H3'	1:0:2333:G:C8	2.38	0.58
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.58
1:0:29:C:O2'	1:0:30:U:H5'	2.03	0.58
1:0:553:G:H2'	1:0:554:G:H5'	1.86	0.58
1:0:1666:C:H2'	1:0:1667:A:C8	2.39	0.58
1:0:1803:C:H2'	1:0:1804:A:C8	2.37	0.58
1:0:1921:A:H2'	1:0:1922:A:O4'	2.03	0.58
1:0:1055:G:N2	1:0:1057:A:H3'	2.18	0.58
1:0:1889:C:O2'	1:0:1890:U:H5'	2.03	0.58
1:0:1931:A:C2'	1:0:1932:G:H5'	2.34	0.58
1:0:2433:A:H1'	39:0:7055:HOH:O	2.03	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
1:0:2531:U:H4'	39:0:5083:HOH:O	2.04	0.58
1:0:2748:G:H5'	39:0:7410:HOH:O	2.04	0.58
22:U:49:LEU:HD12	39:U:3805:HOH:O	2.02	0.58
1:0:164:G:H3'	39:0:8274:HOH:O	2.03	0.58
1:0:1375:A:H2'	1:0:1376:G:H5'	1.86	0.58
1:0:1504:A:H4'	1:0:1506:U:C5	2.39	0.58
1:0:2410:G:H1'	39:0:7571:HOH:O	2.03	0.58
1:0:2768:A:H2'	1:0:2769:C:C6	2.39	0.58
1:0:2831:C:H2'	1:0:2832:C:O4'	2.03	0.58
1:0:306:A:P	21:T:38:ARG:HH21	2.27	0.58
1:0:822:C:O2	1:0:822:C:H2'	2.03	0.57
1:0:1163:G:OP2	1:0:1164:U:H3'	2.04	0.57
1:0:1769:C:O2'	1:0:1770:U:H5'	2.02	0.57
1:0:1787:C:O2'	1:0:1788:U:H5'	2.04	0.57
1:0:2016:U:H2'	1:0:2017:U:O4'	2.04	0.57
1:0:2507:G:H2'	1:0:2510:C:N4	2.19	0.57
1:0:735:C:N4	30:3:15:ASN:HD21	2.03	0.57
1:0:1057:A:H1'	1:0:2492:U:O2'	2.04	0.57
1:0:1421:C:H2'	1:0:1422:U:H6	1.68	0.57
1:0:1309:U:O2'	1:0:1310:U:H5'	2.04	0.57
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.20	0.57
1:0:1477:C:H5'	1:0:1868:G:H5'	1.86	0.57
1:0:2312:G:C2'	1:0:2313:C:H5'	2.34	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
1:0:2691:A:OP1	1:0:2691:A:H8	1.86	0.57
9:H:32:ALA:H	9:H:69:ARG:HH12	1.51	0.57
1:0:664:U:O2'	1:0:665:A:H5'	2.04	0.57
1:0:872:U:H3'	39:0:3723:HOH:O	2.05	0.57
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.15	0.57
1:0:2005:G:O2'	1:0:2008:U:OP2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:236:A:H4'	1:0:237:G:H5'	1.86	0.57
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.57
1:0:2241:C:O2'	1:0:2242:U:H5'	2.04	0.57
1:0:2385:G:H2'	1:0:2386:U:H6	1.68	0.57
1:0:2449:G:H2'	1:0:2450:C:C6	2.40	0.57
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.40	0.57
24:W:52:VAL:HG22	24:W:53:ALA:H	1.69	0.57
1:0:67:A:N1	1:0:109:U:H1'	2.19	0.57
1:0:73:U:O2'	1:0:74:G:H5'	2.04	0.57
1:0:152:A:H1'	1:0:440:C:O2'	2.05	0.57
1:0:705:C:H3'	1:0:706:G:H8	1.69	0.57
1:0:1634:G:H2'	1:0:1635:U:C6	2.39	0.57
1:0:2054:A:H4'	19:R:135:ALA:O	2.05	0.57
1:0:2378:U:H4'	39:0:3392:HOH:O	2.04	0.57
1:0:2777:G:H1'	39:0:6143:HOH:O	2.04	0.57
1:0:111:C:H2'	1:0:112:G:O4'	2.05	0.57
1:0:581:G:O2'	1:0:582:U:H5'	2.05	0.57
1:0:790:A:H8	39:0:5403:HOH:O	1.87	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.18	0.57
1:0:39:G:C2	1:0:444:C:C2	2.93	0.57
1:0:343:C:H2'	1:0:344:C:H6	1.69	0.57
1:0:1829:A:C2'	1:0:1830:C:H5'	2.34	0.57
1:0:2336:G:H1	1:0:2348:C:H42	1.53	0.57
1:0:2505:G:C2'	1:0:2506:A:H5'	2.35	0.57
1:0:2904:U:H2'	1:0:2905:A:C8	2.40	0.57
1:0:152:A:O2'	1:0:153:C:H5'	2.05	0.57
1:0:2673:U:C4	1:0:2674:G:C6	2.93	0.57
1:0:2735:U:H2'	1:0:2736:U:C6	2.39	0.57
1:0:566:A:H2'	1:0:567:U:H5'	1.86	0.56
1:0:1106:A:O5'	1:0:1106:A:H8	1.87	0.56
1:0:2241:C:H2'	1:0:2242:U:C6	2.40	0.56
1:0:2533:C:H5'	1:0:2533:C:C6	2.35	0.56
4:C:139:VAL:HG13	39:C:6251:HOH:O	2.04	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
1:0:1383:U:H2'	1:0:1384:C:C6	2.40	0.56
1:0:1477:C:H5'	1:0:1868:G:C5'	2.35	0.56
1:0:1617:C:C5	1:0:1643:C:H4'	2.40	0.56
1:0:1697:G:H1'	39:0:7038:HOH:O	2.06	0.56
1:0:1894:C:N4	1:0:1939:U:H2'	2.20	0.56
1:0:2388:C:O2'	1:0:2389:U:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.41	0.56
1:0:2689:A:H2'	1:0:2690:U:H5'	1.86	0.56
1:0:10:U:O4	1:0:532:A:OP2	2.22	0.56
1:0:348:C:H2'	1:0:349:U:H6	1.69	0.56
1:0:619:U:H3'	39:0:7549:HOH:O	2.05	0.56
1:0:1165:G:H21	1:0:1173:A:C5'	2.17	0.56
1:0:1175:G:O2'	1:0:1193:A:H2'	2.05	0.56
1:0:1555:G:H4'	1:0:1630:A:H2	1.70	0.56
1:0:2432:C:H4'	39:0:5597:HOH:O	2.05	0.56
1:0:2500:C:O2'	1:0:2501:G:H5'	2.05	0.56
1:0:2820:A:H2'	1:0:2821:C:O4'	2.05	0.56
1:0:182:G:H5'	39:0:4102:HOH:O	2.04	0.56
1:0:345:G:N2	1:0:346:U:H1'	2.21	0.56
1:0:1081:A:H5"	39:0:7126:HOH:O	2.05	0.56
3:B:179:LEU:O	3:B:183:GLU:HG2	2.06	0.56
31:9:29:C:C2'	31:9:30:C:H5'	2.35	0.56
31:9:82:U:H5"	39:9:123:HOH:O	2.05	0.56
1:0:12:U:C2'	1:0:13:G:H5'	2.35	0.56
1:0:95:A:H5"	1:0:97:G:O4'	2.06	0.56
1:0:221:G:H2'	1:0:222:A:H8	1.71	0.56
1:0:814:G:N2	1:0:815:U:H1'	2.21	0.56
1:0:1163:G:H5'	10:I:110:ASP:O	2.06	0.56
3:B:7:ARG:NH2	3:B:11:LEU:HD13	2.21	0.56
1:0:25:A:O2'	1:0:640:G:H5'	2.05	0.56
1:0:814:G:H2'	1:0:815:U:C6	2.41	0.56
1:0:1759:A:N3	1:0:1818:C:H2'	2.21	0.56
1:0:1877:G:H5"	39:0:6762:HOH:O	2.05	0.56
1:0:171:C:O2'	1:0:172:U:H5'	2.06	0.56
1:0:2439:C:H5'	39:0:4534:HOH:O	2.06	0.56
31:9:104:A:C2'	31:9:105:A:H5'	2.35	0.56
1:0:154:C:O2'	1:0:155:C:H5'	2.06	0.56
1:0:1369:A:H5'	39:0:7798:HOH:O	2.06	0.56
20:S:33:SER:O	20:S:37:VAL:HG23	2.06	0.56
1:0:636:G:H5'	1:0:2059:U:OP2	2.06	0.56
1:0:834:G:H3'	1:0:835:U:H4'	1.87	0.56
1:0:2751:C:H3'	39:0:7028:HOH:O	2.05	0.56
15:N:159:TYR:HE1	31:9:50:G:H5"	1.70	0.56
1:0:738:G:N2	1:0:2384:U:H4'	2.21	0.55
1:0:1099:G:H2'	1:0:1100:G:O4'	2.05	0.55
1:0:1167:G:H1	1:0:1179:C:N4	2.03	0.55
1:0:1242:A:H5'	11:J:82:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1554:C:C1'	1:0:1632:A:H1'	2.36	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
1:0:2831:C:C2'	1:0:2832:C:H5'	2.36	0.55
14:M:159:VAL:HG12	35:M:8818:CL:CL	2.43	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.41	0.55
1:0:2256:G:C2'	1:0:2257:G:H5'	2.36	0.55
7:F:77:VAL:HG21	7:F:83:LEU:HD13	1.88	0.55
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.55
1:0:68:U:O2'	1:0:69:A:H5"	2.07	0.55
1:0:189:A:OP1	14:M:171:ARG:NH2	2.38	0.55
1:0:226:A:H1'	1:0:393:G:N7	2.21	0.55
1:0:2768:A:H2'	1:0:2769:C:H6	1.72	0.55
1:0:2781:U:O2'	1:0:2782:G:H5'	2.06	0.55
1:0:2906:A:H5'	1:0:2907:C:O4'	2.06	0.55
5:D:140:ARG:HB3	31:9:29:C:H5"	1.89	0.55
1:0:290:C:O2'	1:0:291:C:H5'	2.06	0.55
1:0:338:C:H4'	4:C:174:ILE:CD1	2.36	0.55
1:0:414:C:O2'	1:0:415:A:H5'	2.07	0.55
1:0:612:U:H2'	1:0:613:C:C6	2.41	0.55
1:0:1030:U:H5'	39:0:3468:HOH:O	2.05	0.55
1:0:1119:G:N2	1:0:1246:A:C2	2.74	0.55
1:0:1420:C:H2'	1:0:1420:C:O2	2.07	0.55
1:0:2716:G:H5'	3:B:262:ARG:HG3	1.88	0.55
1:0:2782:G:O6	1:0:2790:C:H5"	2.06	0.55
1:0:696:C:H2'	1:0:697:G:O4'	2.06	0.55
1:0:897:A:H2'	1:0:899:C:C5	2.42	0.55
1:0:1441:G:H1'	39:0:7717:HOH:O	2.06	0.55
1:0:1784:U:O2'	1:0:1812:G:H2'	2.06	0.55
1:0:2397:G:H2'	1:0:2398:A:H8	1.72	0.55
1:0:2465:A:H1'	39:0:3104:HOH:O	2.05	0.55
1:0:2868:C:H1'	39:0:6832:HOH:O	2.07	0.55
1:0:128:A:C8	1:0:128:A:H3'	2.41	0.55
1:0:355:C:H1'	39:0:3088:HOH:O	2.06	0.55
1:0:1816:C:H6	1:0:1816:C:O5'	1.89	0.55
1:0:2274:A:O2'	1:0:2275:G:H5'	2.07	0.55
1:0:2506:A:O2'	1:0:2507:G:C8	2.56	0.55
12:K:23:ASN:HD21	12:K:108:GLU:H	1.54	0.55
19:R:66:VAL:HG22	19:R:79:ARG:NH1	2.22	0.55
1:0:159:G:H1	1:0:175:G:HO2'	1.53	0.55
1:0:466:A:H2'	1:0:467:G:O4'	2.06	0.55
1:0:517:U:H2'	1:0:518:G:H5'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:849:C:H2'	1:0:850:U:O4'	2.07	0.55
1:0:962:C:H2'	1:0:963:C:H5'	1.87	0.55
1:0:1850:U:H2'	1:0:1851:G:H8	1.71	0.55
1:0:414:C:H2'	1:0:415:A:O4'	2.06	0.55
1:0:1745:G:H22	1:0:2033:G:H5'	1.71	0.55
1:0:2071:C:H5'	39:0:4847:HOH:O	2.07	0.55
1:0:2764:C:H2'	1:0:2765:C:C6	2.33	0.55
1:0:125:U:H2'	39:0:8398:HOH:O	2.07	0.55
1:0:819:A:H5'	27:Z:37:ARG:HD2	1.89	0.55
1:0:1159:G:H21	1:0:1189:A:H8	1.55	0.55
1:0:2431:C:H2'	1:0:2432:C:O4'	2.07	0.55
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.21	0.55
1:0:1189:A:H1'	1:0:1209:C:O4'	2.07	0.55
1:0:2072:G:H3'	1:0:2073:G:C5'	2.37	0.55
1:0:2654:C:O2'	1:0:2655:U:H5'	2.07	0.55
14:M:27:ARG:NH2	14:M:44:THR:HG23	2.21	0.55
31:9:61:C:H2'	31:9:62:A:H8	1.72	0.55
1:0:35:U:O2'	1:0:36:C:H5'	2.07	0.54
1:0:1167:G:H3'	39:0:7346:HOH:O	2.07	0.54
1:0:1835:U:H5	1:0:1840:A:N7	2.06	0.54
1:0:1928:C:H2'	1:0:1929:G:O4'	2.07	0.54
39:0:4183:HOH:O	12:K:39:GLY:HA2	2.07	0.54
6:E:137:ASP:O	6:E:141:VAL:HG23	2.06	0.54
15:N:11:ARG:HD3	31:9:114:G:O6	2.08	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:250:C:H2'	1:0:251:C:H6	1.73	0.54
1:0:312:U:C2	1:0:320:G:N2	2.75	0.54
1:0:420:U:H3	1:0:2447:A:H61	1.56	0.54
1:0:676:C:O2'	4:C:219:ASN:ND2	2.33	0.54
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.89	0.54
1:0:1166:A:P	1:0:1174:A:H4'	2.46	0.54
1:0:1333:U:H2'	1:0:1334:C:C6	2.41	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.07	0.54
1:0:313:U:C2'	1:0:314:G:H5'	2.37	0.54
1:0:1120:U:H5"	1:0:1120:U:H6	1.73	0.54
1:0:2321:A:H2	1:0:2378:U:H3	1.51	0.54
1:0:2506:A:HO2'	1:0:2507:G:H8	1.49	0.54
1:0:590:A:H2'	1:0:591:A:O4'	2.08	0.54
1:0:1016:U:H1'	39:0:8289:HOH:O	2.06	0.54
1:0:2422:U:H5'	39:0:5459:HOH:O	2.08	0.54
1:0:2781:U:C2'	1:0:2782:G:H5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.88	0.54
1:0:816:G:C6	1:0:817:G:N1	2.75	0.54
1:0:1586:G:H1'	39:0:6211:HOH:O	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.90	0.54
1:0:1730:G:C5'	1:0:1731:C:H6	2.20	0.54
1:0:1803:C:H2'	1:0:1804:A:H8	1.72	0.54
1:0:1925:G:O2'	1:0:1926:G:H5'	2.08	0.54
1:0:2042:U:H2'	1:0:2043:U:C6	2.42	0.54
1:0:2819:C:H2'	1:0:2820:A:H8	1.72	0.54
31:9:76:G:C3'	31:9:77:A:H5"	2.29	0.54
1:0:722:G:H2'	1:0:723:G:H5'	1.88	0.54
1:0:1328:A:OP1	26:Y:169:ARG:HD2	2.08	0.54
1:0:1387:G:H21	17:P:1:THR:N	2.04	0.54
1:0:1510:G:H2'	1:0:1511:U:O4'	2.08	0.54
1:0:1571:G:C2'	1:0:1626:A:H61	2.21	0.54
1:0:2027:U:O2'	1:0:2028:U:H5'	2.07	0.54
1:0:2349:G:H2'	1:0:2350:G:H8	1.72	0.54
1:0:2908:A:H2'	1:0:2909:G:O4'	2.06	0.54
1:0:420:U:H1'	39:0:5263:HOH:O	2.07	0.54
1:0:491:C:N3	1:0:502:A:C2	2.75	0.54
1:0:814:G:C2	1:0:815:U:C2	2.95	0.54
1:0:920:C:H4'	1:0:921:G:C2	2.42	0.54
1:0:1747:A:C6	1:0:2035:C:O2	2.61	0.54
1:0:2537:G:H5"	1:0:2538:A:H5"	1.89	0.54
1:0:1099:G:P	24:W:129:LYS:HE3	2.48	0.54
1:0:1631:A:H2'	1:0:1632:A:C8	2.43	0.54
1:0:2607:U:OP1	1:0:2609:G:H4'	2.07	0.54
1:0:2661:U:H3	1:0:2812:A:H62	1.55	0.54
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.89	0.54
31:9:73:A:H2'	31:9:74:G:C8	2.43	0.54
1:0:814:G:H4'	39:0:7058:HOH:O	2.08	0.54
1:0:847:C:H4'	39:0:8386:HOH:O	2.08	0.54
1:0:1461:U:H2'	1:0:1462:C:C6	2.43	0.54
1:0:2439:C:H2'	1:0:2440:C:H6	1.73	0.54
1:0:2474:A:N7	1:0:2621:PSU:H4'	2.23	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	0.54
1:0:293:A:H2'	1:0:294:C:H6	1.73	0.54
1:0:2502:C:H4'	9:H:158:ASN:ND2	2.23	0.54
1:0:2726:U:H5"	1:0:2749:U:N3	2.22	0.54
1:0:2898:G:O2'	1:0:2899:A:H5'	2.06	0.54
31:9:95:C:H2'	31:9:96:C:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:310:U:H2'	1:0:311:C:C6	2.43	0.53
1:0:440:C:H2'	1:0:441:A:C8	2.43	0.53
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.53
1:0:2404:G:H5"	39:0:8706:HOH:O	2.07	0.53
31:9:76:G:O5'	31:9:76:G:H8	1.91	0.53
1:0:272:A:H5'	1:0:273:G:OP2	2.07	0.53
1:0:667:C:H2'	1:0:668:C:H6	1.72	0.53
1:0:698:A:H5"	13:L:111:ALA:HB2	1.90	0.53
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.53
1:0:907:A:H2'	1:0:908:A:C8	2.43	0.53
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.53
1:0:1244:U:H4'	1:0:1246:A:O4'	2.08	0.53
1:0:1570:C:H2'	1:0:1571:G:O4'	2.08	0.53
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.53
1:0:2511:A:H2'	1:0:2512:U:O4'	2.08	0.53
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.39	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.89	0.53
1:0:42:C:OP2	1:0:185:G:H2'	2.08	0.53
1:0:1353:C:H3'	39:0:8238:HOH:O	2.08	0.53
27:Z:48:ARG:O	27:Z:52:GLU:HB2	2.09	0.53
1:0:31:C:O2'	1:0:32:G:H5'	2.08	0.53
1:0:1438:G:H1'	29:2:42:TRP:HZ2	1.73	0.53
1:0:1829:A:H5"	39:0:6825:HOH:O	2.08	0.53
37:0:9101:MUL:H163	37:0:9101:MUL:O3	2.09	0.53
18:Q:26:PRO:O	18:Q:30:VAL:HG23	2.07	0.53
1:0:869:G:H1'	39:0:7658:HOH:O	2.09	0.53
1:0:1352:A:H4'	1:0:1353:C:OP1	2.08	0.53
1:0:1950:G:H2'	1:0:1951:G:H8	1.74	0.53
1:0:1976:G:H1'	1:0:2005:G:N2	2.23	0.53
1:0:2508:C:H2'	39:0:6319:HOH:O	2.08	0.53
1:0:2809:G:H2'	1:0:2810:G:O4'	2.07	0.53
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.53
1:0:1166:A:N6	1:0:1180:U:H3	1.97	0.53
1:0:1427:A:O2'	1:0:1428:C:H5'	2.08	0.53
1:0:1430:G:N2	39:0:7999:HOH:O	2.41	0.53
4:C:142:ASP:OD1	4:C:236:THR:HG23	2.09	0.53
1:0:23:G:H1'	1:0:520:A:N6	2.22	0.53
1:0:139:C:H4'	1:0:140:G:O5'	2.09	0.53
1:0:381:G:H2'	39:0:6358:HOH:O	2.08	0.53
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.08	0.53
1:0:1167:G:H4'	10:I:130:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:C2'	1:0:1172:G:H5'	2.39	0.53
1:0:1311:G:H5"	39:0:5005:HOH:O	2.06	0.53
1:0:1342:C:H2'	1:0:1343:C:H5'	1.90	0.53
1:0:1398:G:O2'	1:0:1399:A:H5'	2.09	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.09	0.53
1:0:1574:C:H2'	1:0:1575:C:C6	2.41	0.53
1:0:1758:U:H6	1:0:1758:U:O5'	1.92	0.53
1:0:2294:C:H42	1:0:2314:G:H1	1.55	0.53
1:0:2433:A:H2'	1:0:2434:A:C8	2.44	0.53
1:0:2474:A:H4'	1:0:2475:C:O5'	2.08	0.53
1:0:2486:A:H3'	39:0:3735:HOH:O	2.08	0.53
1:0:318:U:H5'	1:0:339:A:C4	2.43	0.53
1:0:710:G:OP1	16:O:24:ALA:HB3	2.09	0.53
1:0:1081:A:C6	1:0:1082:A:N1	2.76	0.53
1:0:1817:U:O2	17:P:81:LYS:NZ	2.32	0.53
1:0:1981:A:H3'	39:0:6149:HOH:O	2.09	0.53
1:0:2586:U:H3	1:0:2592:G:H22	1.55	0.53
1:0:2617:G:H4'	39:0:3214:HOH:O	2.08	0.53
24:W:24:LEU:HD21	24:W:44:MET:SD	2.48	0.53
1:0:228:C:H2'	1:0:229:G:H5'	1.89	0.53
1:0:2387:U:H2'	1:0:2388:C:C6	2.43	0.53
1:0:2742:G:H5'	39:0:5015:HOH:O	2.07	0.53
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.53
1:0:303:C:O2'	1:0:304:G:H5'	2.09	0.53
1:0:561:G:H2'	1:0:562:A:C8	2.41	0.53
1:0:1666:C:H2'	1:0:1667:A:H8	1.72	0.53
1:0:2240:U:O2'	1:0:2241:C:H5'	2.09	0.53
1:0:2250:G:H2'	1:0:2251:G:O4'	2.08	0.53
1:0:2563:U:O2'	1:0:2564:G:H8	1.92	0.53
1:0:523:C:O2'	1:0:524:A:H5'	2.09	0.52
1:0:734:U:H2'	1:0:736:A:OP2	2.09	0.52
1:0:2241:C:H2'	1:0:2242:U:H6	1.74	0.52
1:0:1363:G:H1'	39:0:4378:HOH:O	2.08	0.52
1:0:1741:U:C4	1:0:2033:G:C8	2.98	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.38	0.52
1:0:2026:C:O2'	1:0:2027:U:H5'	2.10	0.52
1:0:2089:A:O2'	1:0:2090:G:H5'	2.10	0.52
1:0:380:A:H2'	39:0:6974:HOH:O	2.09	0.52
1:0:482:G:H4'	1:0:508:A:N1	2.25	0.52
1:0:1011:C:H3'	1:0:1012:A:C8	2.44	0.52
1:0:1460:G:H5'	39:0:3232:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:72:C:H5'	39:0:5110:HOH:O	2.09	0.52
1:0:640:G:O2'	1:0:641:G:H5'	2.08	0.52
1:0:656:G:H2'	1:0:657:G:H8	1.75	0.52
1:0:912:A:C4	1:0:1294:A:C2	2.97	0.52
1:0:1438:G:H1'	29:2:42:TRP:CZ2	2.45	0.52
1:0:1886:A:H4'	39:Z:395:HOH:O	2.08	0.52
1:0:2018:A:H2	27:Z:40:ALA:O	1.93	0.52
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.42	0.52
31:9:39:U:N3	31:9:42:C:H5"	2.24	0.52
1:0:705:C:O2	1:0:705:C:H2'	2.10	0.52
1:0:960:G:N3	1:0:960:G:H2'	2.23	0.52
1:0:1363:G:H2'	1:0:1364:G:C8	2.44	0.52
1:0:1970:G:H1'	39:0:8299:HOH:O	2.08	0.52
1:0:157:G:H4'	14:M:95:LYS:HE2	1.91	0.52
1:0:628:1MA:HM11	39:0:3514:HOH:O	2.10	0.52
1:0:809:G:H2'	1:0:810:G:C8	2.45	0.52
1:0:875:A:C2	2:A:194:MET:SD	3.03	0.52
1:0:955:A:H2'	1:0:956:G:O4'	2.10	0.52
1:0:1436:C:O2'	1:0:1437:A:H5'	2.10	0.52
1:0:2345:A:H3'	1:0:2346:C:C6	2.44	0.52
1:0:2548:C:H5"	39:0:5919:HOH:O	2.09	0.52
3:B:7:ARG:NH1	3:B:11:LEU:HD22	2.24	0.52
1:0:660:A:N6	1:0:746:A:O4'	2.42	0.52
1:0:710:G:H2'	1:0:711:G:H8	1.74	0.52
1:0:1181:A:H2'	1:0:1182:C:C5'	2.40	0.52
1:0:1359:U:C5	1:0:2101:A:C8	2.98	0.52
1:0:1461:U:H2'	1:0:1462:C:H6	1.75	0.52
1:0:2790:C:H5'	39:0:8847:HOH:O	2.08	0.52
1:0:39:G:H2'	1:0:40:C:O4'	2.09	0.52
1:0:210:U:O2'	1:0:211:U:H5'	2.10	0.52
1:0:226:A:H1'	1:0:393:G:C5	2.44	0.52
1:0:968:G:H2'	1:0:969:G:H8	1.75	0.52
1:0:1130:U:H5'	39:0:7596:HOH:O	2.10	0.52
1:0:1166:A:H1'	1:0:1192:A:C2	2.45	0.52
1:0:1400:C:O2'	1:0:1401:G:H5'	2.08	0.52
1:0:1634:G:H2'	1:0:1635:U:H6	1.75	0.52
1:0:1688:G:C6	1:0:1692:C:C6	2.98	0.52
1:0:2121:G:H5"	39:0:9100:HOH:O	2.10	0.52
1:0:2269:C:O2'	1:0:2270:G:H5'	2.10	0.52
1:0:2718:C:H3'	39:0:6906:HOH:O	2.10	0.52
1:0:640:G:C6	1:0:641:G:N7	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1011:C:H3'	1:0:1012:A:H8	1.74	0.52
1:0:2703:A:H2'	1:0:2704:C:C6	2.37	0.52
31:9:29:C:H2'	31:9:30:C:C5'	2.39	0.52
31:9:119:C:H4'	39:9:2285:HOH:O	2.08	0.52
1:0:39:G:O2'	1:0:40:C:H5'	2.10	0.52
1:0:183:A:H1'	14:M:161:ARG:HH11	1.75	0.52
1:0:653:U:H2'	1:0:654:A:C8	2.45	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.39	0.52
1:0:1705:C:P	17:P:59:ARG:HH12	2.33	0.52
1:0:2392:C:H4'	18:Q:55:ARG:HH11	1.75	0.52
1:0:2851:G:O2'	1:0:2852:A:H5'	2.10	0.52
14:M:99:ARG:HE	14:M:170:ASN:HD22	1.57	0.52
1:0:282:C:H1'	1:0:368:C:H42	1.75	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.75	0.51
1:0:289:G:O2'	1:0:290:C:H5'	2.10	0.51
1:0:685:C:O2	1:0:748:C:H4'	2.11	0.51
1:0:947:U:O2'	1:0:948:G:H5'	2.10	0.51
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.51
31:9:7:G:H5'	39:9:5071:HOH:O	2.09	0.51
1:0:422:G:O2'	1:0:423:A:H5'	2.10	0.51
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	0.51
1:0:1573:A:H2'	1:0:1574:C:O4'	2.09	0.51
1:0:1736:A:H1'	39:0:7468:HOH:O	2.10	0.51
12:K:18:ILE:HG22	12:K:93:ASN:ND2	2.18	0.51
31:9:86:G:C2	31:9:88:G:C8	2.98	0.51
1:0:301:C:O2'	1:0:302:A:H5'	2.10	0.51
1:0:1137:G:H1'	39:0:8578:HOH:O	2.10	0.51
31:9:98:C:H2'	31:9:99:U:C6	2.43	0.51
1:0:593:A:H1'	39:0:8441:HOH:O	2.10	0.51
1:0:968:G:H2'	1:0:969:G:C8	2.45	0.51
1:0:1023:C:O2'	1:0:1024:G:H5'	2.11	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.51
1:0:2897:C:O2'	1:0:2898:G:H5'	2.11	0.51
21:T:41:ARG:NH1	21:T:42:VAL:O	2.44	0.51
31:9:3:A:C8	31:9:26:C:N3	2.78	0.51
1:0:45:A:H5"	1:0:47:G:H5'	1.92	0.51
1:0:120:A:H2'	1:0:120:A:N3	2.26	0.51
1:0:441:A:H1'	1:0:442:A:N7	2.25	0.51
1:0:1044:C:H5"	39:0:2991:HOH:O	2.10	0.51
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1445:G:N2	1:0:1678:A:H1'	2.26	0.51
1:0:1706:G:C5	1:0:1707:G:C6	2.99	0.51
1:0:1928:C:C4	1:0:1929:G:N7	2.78	0.51
1:0:2586:U:H3	1:0:2592:G:H1	1.58	0.51
1:0:2851:G:H2'	1:0:2902:A:H61	1.76	0.51
2:A:199:HIS:HD2	2:A:201:PHE:H	1.57	0.51
1:0:772:G:H2'	1:0:773:A:O4'	2.11	0.51
1:0:2065:C:O2'	1:0:2066:C:H5'	2.10	0.51
1:0:2481:G:H3'	39:0:3932:HOH:O	2.10	0.51
1:0:2748:G:H1'	39:0:7865:HOH:O	2.10	0.51
1:0:2909:G:O2'	1:0:2910:A:H5'	2.11	0.51
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.93	0.51
31:9:81:C:O2'	31:9:82:U:H5'	2.11	0.51
1:0:47:G:H1'	1:0:114:A:N1	2.24	0.51
1:0:706:G:N2	1:0:707:C:H41	2.09	0.51
1:0:1069:C:H4'	1:0:1081:A:O2'	2.10	0.51
1:0:1332:C:H2'	1:0:1333:U:H6	1.75	0.51
1:0:2499:U:H2'	1:0:2500:C:C6	2.46	0.51
1:0:2821:C:H4'	3:B:116:PRO:HG3	1.91	0.51
2:A:167:LYS:HE3	27:Z:50:VAL:HG13	1.93	0.51
13:L:138:GLY:HA3	39:L:4360:HOH:O	2.11	0.51
24:W:80:ASP:O	24:W:84:VAL:HG23	2.11	0.51
31:9:84:G:H4'	39:9:4718:HOH:O	2.11	0.51
1:0:567:U:O5'	1:0:567:U:H6	1.92	0.51
1:0:677:C:H4'	4:C:246:ARG:HH12	1.75	0.51
1:0:870:G:H2'	1:0:871:G:C5'	2.40	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.78	0.51
1:0:1844:C:O5'	1:0:1844:C:H6	1.93	0.51
1:0:1931:A:H2'	1:0:1932:G:C5'	2.40	0.51
1:0:2061:C:H2'	1:0:2062:A:H5'	1.93	0.51
37:0:9101:MUL:H11A	39:0:3722:HOH:O	2.11	0.51
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.51
1:0:821:U:H5"	39:0:6706:HOH:O	2.10	0.51
1:0:1289:C:H3'	39:0:5826:HOH:O	2.10	0.51
1:0:1363:G:P	4:C:76:ARG:HH22	2.34	0.51
1:0:2061:C:C2'	1:0:2062:A:H5'	2.41	0.51
1:0:2830:U:O2'	1:0:2831:C:H5'	2.11	0.51
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.93	0.51
1:0:10:U:C4	1:0:532:A:C8	2.99	0.51
1:0:74:G:H5'	23:V:9:ARG:HH22	1.76	0.51
1:0:100:C:H4'	21:T:16:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:694:A:C2'	1:0:695:C:H5'	2.39	0.51
1:0:876:A:H2'	1:0:877:G:H5'	1.91	0.51
1:0:1359:U:C5	1:0:2101:A:H8	2.29	0.51
1:0:1427:A:C2'	1:0:1428:C:H5'	2.41	0.51
6:E:7:ILE:HG23	6:E:45:ASP:O	2.11	0.51
1:0:716:G:C6	1:0:717:C:N4	2.80	0.50
1:0:745:G:H4'	39:0:4576:HOH:O	2.10	0.50
1:0:1133:A:H2'	1:0:1134:G:O4'	2.11	0.50
1:0:1192:A:H3'	1:0:1193:A:H5'	1.93	0.50
1:0:1820:G:H2'	1:0:1821:A:H8	1.76	0.50
1:0:1878:G:H5'	39:0:3014:HOH:O	2.11	0.50
1:0:1891:G:H1'	1:0:1972:U:O2	2.11	0.50
1:0:1904:A:C2	1:0:1905:U:H1'	2.46	0.50
1:0:2798:G:H3'	39:0:3048:HOH:O	2.11	0.50
5:D:48:MET:O	31:9:41:C:H4'	2.10	0.50
30:3:3:MET:O	30:3:90:PHE:HA	2.11	0.50
31:9:118:C:O5'	31:9:118:C:H6	1.94	0.50
1:0:301:C:H42	1:0:350:G:H1	1.58	0.50
1:0:398:U:O3'	14:M:179:GLY:HA3	2.11	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
1:0:1598:A:C2	1:0:1599:U:C2	2.99	0.50
1:0:1678:A:C5	1:0:1679:C:C5	2.99	0.50
1:0:2838:A:O2'	1:0:2839:C:H5'	2.12	0.50
5:D:22:VAL:HG22	5:D:74:THR:HG22	1.93	0.50
31:9:59:C:O5'	31:9:59:C:H6	1.93	0.50
31:9:114:G:H2'	31:9:115:C:H6	1.72	0.50
1:0:447:A:OP1	21:T:2:LYS:HG2	2.10	0.50
1:0:710:G:O2'	1:0:711:G:H5'	2.10	0.50
1:0:1507:C:H4'	39:0:8231:HOH:O	2.10	0.50
1:0:1942:A:H2'	1:0:1943:C:H6	1.76	0.50
1:0:2295:G:N3	1:0:2361:A:C2	2.79	0.50
31:9:99:U:H5'	39:9:5904:HOH:O	2.11	0.50
1:0:219:G:C5'	1:0:220:C:H5"	2.40	0.50
1:0:685:C:O2'	1:0:748:C:OP1	2.23	0.50
1:0:894:A:OP2	39:0:3250:HOH:O	2.19	0.50
1:0:1331:G:O2'	1:0:1332:C:H5'	2.12	0.50
1:0:1680:C:H2'	1:0:1681:G:O4'	2.11	0.50
1:0:1766:U:H4'	39:0:9080:HOH:O	2.11	0.50
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.94	0.50
1:0:2750:G:H2'	1:0:2751:C:C6	2.47	0.50
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:574:G:O2'	1:0:575:A:H5'	2.11	0.50
1:0:2869:G:H2'	1:0:2870:C:C6	2.46	0.50
1:0:313:U:O2'	1:0:314:G:H5'	2.10	0.50
1:0:690:G:H1'	1:0:731:U:O2'	2.12	0.50
1:0:1305:C:O2'	1:0:1306:U:H5'	2.12	0.50
1:0:1496:A:H5'	1:0:1572:A:H1'	1.93	0.50
1:0:2819:C:H2'	1:0:2820:A:C8	2.46	0.50
1:0:796:A:H5'	39:0:5974:HOH:O	2.11	0.50
1:0:962:C:H1'	15:N:5:ARG:NH2	2.27	0.50
1:0:1647:G:O2'	1:0:1648:G:H5'	2.12	0.50
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.50
4:C:56:THR:HG21	4:C:78:ARG:HB3	1.92	0.50
31:9:2:U:H4'	39:9:5321:HOH:O	2.11	0.50
1:0:229:G:O2'	1:0:230:C:H5'	2.12	0.50
1:0:292:G:H1'	1:0:360:A:N6	2.27	0.50
1:0:559:U:H6	1:0:559:U:C5'	2.23	0.50
1:0:843:A:C2	1:0:846:A:C8	3.00	0.50
1:0:1213:C:C2'	1:0:1214:G:H5'	2.42	0.50
1:0:1251:C:H2'	1:0:1252:A:O4'	2.12	0.50
1:0:1797:A:H5'	39:0:7113:HOH:O	2.12	0.50
1:0:1992:U:O2	1:0:1994:A:H8	1.95	0.50
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.09	0.50
26:Y:214:ARG:HH12	26:Y:230:ASN:ND2	2.09	0.50
1:0:530:C:H4'	1:0:612:U:H4'	1.94	0.50
1:0:639:A:H2'	1:0:640:G:C8	2.47	0.50
1:0:840:U:C2	1:0:2648:U:O4	2.65	0.50
1:0:1511:U:H4'	39:0:6890:HOH:O	2.11	0.50
1:0:2251:G:H2'	1:0:2252:A:H8	1.76	0.50
1:0:2484:U:H3'	39:0:3554:HOH:O	2.12	0.50
3:B:75:GLU:OE2	3:B:151:VAL:HG13	2.12	0.50
20:S:37:VAL:O	20:S:41:VAL:HG23	2.11	0.50
26:Y:216:ARG:HD3	39:Y:4408:HOH:O	2.12	0.50
31:9:78:G:H22	31:9:103:A:P	2.35	0.50
31:9:82:U:H2'	31:9:83:G:C8	2.47	0.50
1:0:553:G:H5'	39:0:8126:HOH:O	2.11	0.49
1:0:820:G:H3'	39:0:6706:HOH:O	2.12	0.49
1:0:876:A:C2'	1:0:877:G:H5'	2.41	0.49
1:0:1315:G:H3'	1:0:1316:G:H5'	1.93	0.49
1:0:1557:G:H2'	1:0:1558:C:O4'	2.11	0.49
1:0:2710:U:H6	1:0:2710:U:O5'	1.95	0.49
1:0:2837:U:H2'	39:0:6433:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:88:SER:HB3	4:C:91:PRO:HB3	1.95	0.49
14:M:79:ALA:HB3	14:M:81:ARG:NH1	2.26	0.49
1:0:137:U:H2'	1:0:139:C:H5	1.76	0.49
1:0:599:G:H2'	1:0:600:G:H8	1.77	0.49
1:0:1622:G:H2'	1:0:1623:C:H5'	1.94	0.49
1:0:2675:A:H1'	1:0:2813:A:C2	2.47	0.49
1:0:2831:C:O2'	1:0:2832:C:H5'	2.12	0.49
1:0:2862:G:H4'	3:B:336:GLN:O	2.12	0.49
1:0:2871:G:H2'	1:0:2872:U:C6	2.47	0.49
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.59	0.49
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	0.49
1:0:635:A:H2'	1:0:636:G:H5"	1.93	0.49
1:0:818:A:O2'	27:Z:37:ARG:HD3	2.13	0.49
1:0:1175:G:H2'	1:0:1176:C:C6	2.47	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.41	0.49
1:0:1357:A:H1'	39:0:8869:HOH:O	2.12	0.49
1:0:1441:G:H2'	1:0:1442:A:C8	2.46	0.49
1:0:1447:U:H5"	1:0:1677:U:C5	2.48	0.49
1:0:1571:G:H1'	1:0:1627:G:N2	2.27	0.49
1:0:1820:G:O2'	1:0:1821:A:H5'	2.12	0.49
31:9:78:G:HO2'	31:9:79:U:P	2.36	0.49
1:0:564:G:H1'	39:0:5694:HOH:O	2.12	0.49
1:0:849:C:O2'	1:0:850:U:H5'	2.12	0.49
1:0:1080:C:H4'	1:0:1081:A:OP1	2.13	0.49
1:0:1170:U:H1'	1:0:1172:G:N7	2.27	0.49
1:0:1400:C:C2'	1:0:1401:G:H5'	2.42	0.49
1:0:1798:C:OP2	1:0:1799:G:H5"	2.13	0.49
1:0:2291:A:C4	1:0:2309:C:H5'	2.47	0.49
1:0:2611:G:H5'	1:0:2613:G:N7	2.28	0.49
1:0:2729:C:O2'	1:0:2730:G:H5'	2.13	0.49
39:0:3007:HOH:O	2:A:212:PRO:HB2	2.12	0.49
31:9:55:U:H4'	31:9:56:A:H8	1.77	0.49
1:0:694:A:H2'	1:0:695:C:C5'	2.41	0.49
1:0:740:G:H2'	1:0:741:C:C6	2.46	0.49
1:0:1314:U:H5"	1:0:1316:G:O4'	2.11	0.49
1:0:2643:G:H5"	39:0:8628:HOH:O	2.13	0.49
1:0:2885:A:H2'	1:0:2886:C:C6	2.48	0.49
31:9:13:A:H5'	39:9:2295:HOH:O	2.13	0.49
1:0:28:G:H1'	39:0:3446:HOH:O	2.10	0.49
1:0:463:A:H5'	1:0:465:U:O4'	2.13	0.49
1:0:560:U:H2'	1:0:561:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1476:A:O2'	1:0:1868:G:H5'	2.13	0.49
1:0:1675:C:N4	39:0:8358:HOH:O	2.44	0.49
1:0:1786:C:H2'	1:0:1787:C:H6	1.78	0.49
1:0:1819:G:H2'	1:0:1820:G:C4'	2.42	0.49
1:0:2831:C:H2'	1:0:2832:C:C5'	2.43	0.49
1:0:24:G:H22	1:0:518:G:H1'	1.76	0.49
1:0:178:U:H2'	1:0:179:C:C6	2.46	0.49
1:0:1119:G:H8	11:J:52:GLN:HE22	1.58	0.49
1:0:1183:C:H42	1:0:1184:C:H41	1.60	0.49
1:0:1344:G:H1'	39:0:9105:HOH:O	2.13	0.49
1:0:1447:U:C3'	1:0:1506:U:O2	2.59	0.49
1:0:1936:C:H2'	1:0:1937:U:C6	2.48	0.49
1:0:2038:A:C2	1:0:2039:A:N7	2.81	0.49
1:0:2657:G:H4'	39:0:6216:HOH:O	2.11	0.49
1:0:2710:U:O2'	1:0:2711:U:H5'	2.13	0.49
3:B:305:ASP:O	3:B:306:LYS:HB2	2.12	0.49
31:9:81:C:C2'	31:9:82:U:H5'	2.42	0.49
1:0:23:G:H1'	1:0:520:A:H61	1.76	0.49
1:0:196:G:H2'	39:L:6170:HOH:O	2.11	0.49
1:0:1202:A:O2'	1:0:1203:G:H5'	2.13	0.49
1:0:1415:G:O2'	1:0:1416:G:H5'	2.12	0.49
1:0:1453:G:H2'	1:0:1454:U:O4'	2.12	0.49
1:0:2266:A:H2'	1:0:2267:G:C8	2.47	0.49
1:0:245:C:C5	1:0:246:G:C5	3.01	0.49
1:0:579:G:H2'	1:0:580:A:C8	2.47	0.49
1:0:677:C:H2'	1:0:678:G:H8	1.78	0.49
1:0:1046:G:C2	1:0:1069:C:C2	3.01	0.49
1:0:1464:C:O2'	1:0:1465:A:H5'	2.12	0.49
1:0:1473:U:O2'	1:0:1474:C:H5"	2.13	0.49
1:0:1775:A:H3'	1:0:1776:A:H2'	1.95	0.49
1:0:2444:U:H2'	1:0:2445:U:O4'	2.12	0.49
25:X:43:VAL:HG13	25:X:76:ARG:HH12	1.77	0.49
1:0:20:G:H21	19:R:117:HIS:HD2	1.60	0.49
1:0:40:C:O5'	1:0:40:C:H6	1.96	0.49
1:0:248:A:H3'	1:0:248:A:N3	2.27	0.49
1:0:820:G:N3	1:0:1831:U:H1'	2.28	0.49
1:0:1097:A:H5"	24:W:125:HIS:CE1	2.47	0.49
1:0:1293:U:H5'	26:Y:154:ARG:HH21	1.77	0.49
1:0:1548:U:O2'	1:0:1549:C:H5'	2.13	0.49
1:0:1619:G:C5	1:0:1620:C:C4	3.01	0.49
1:0:1664:A:H8	1:0:1664:A:OP1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1675:C:O2'	1:0:1676:G:H5'	2.13	0.49
1:0:1739:G:N2	1:0:2041:G:H1'	2.28	0.49
1:0:2552:C:N4	39:0:8668:HOH:O	2.46	0.49
1:0:2617:G:H5"	39:0:8605:HOH:O	2.12	0.49
1:0:2734:G:O2'	1:0:2735:U:H5'	2.13	0.49
1:0:2824:C:H5"	1:0:2825:C:H5'	1.95	0.49
31:9:89:C:O2'	31:9:90:G:H5'	2.12	0.49
1:0:559:U:H5'	1:0:559:U:C6	2.39	0.48
1:0:1076:G:H1'	39:0:3130:HOH:O	2.13	0.48
1:0:1118:A:H8	1:0:1119:G:H5"	1.78	0.48
1:0:1149:U:O5'	1:0:1151:G:H5'	2.13	0.48
1:0:1774:G:O2'	1:0:1775:A:H5'	2.13	0.48
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.48
1:0:2717:C:O2'	1:0:2718:C:H5"	2.09	0.48
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.48
1:0:169:A:H4'	39:0:5424:HOH:O	2.13	0.48
1:0:421:C:H4'	1:0:1919:A:C6	2.48	0.48
1:0:465:U:O5'	1:0:465:U:H6	1.96	0.48
1:0:812:A:H2'	1:0:813:C:H6	1.76	0.48
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.48
1:0:1701:A:H5"	1:0:1702:U:H3'	1.94	0.48
1:0:1806:G:C2	1:0:1807:U:O2	2.67	0.48
1:0:1841:C:OP2	1:0:2022:A:C8	2.66	0.48
24:W:122:ARG:HH12	24:W:154:ARG:H	1.61	0.48
31:9:107:C:H2'	31:9:108:C:C6	2.48	0.48
1:0:158:A:H2'	1:0:159:G:O4'	2.13	0.48
1:0:163:U:O3'	1:0:896:C:H4'	2.13	0.48
1:0:877:G:H1'	39:A:491:HOH:O	2.14	0.48
1:0:1162:G:H2'	1:0:1163:G:C8	2.48	0.48
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.13	0.48
1:0:2392:C:H4'	18:Q:55:ARG:NH1	2.28	0.48
37:0:9101:MUL:H152	37:0:9101:MUL:O1	2.14	0.48
15:N:12:ARG:NH2	31:9:6:C:C5	2.81	0.48
19:R:63:ASN:HD22	19:R:75:TRP:HZ2	1.60	0.48
1:0:19:U:H2'	1:0:20:G:O4'	2.13	0.48
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.48
1:0:1174:A:C5	1:0:1201:C:H4'	2.48	0.48
1:0:1449:G:H5'	39:0:7441:HOH:O	2.12	0.48
1:0:1497:G:H2'	1:0:1498:G:C8	2.48	0.48
1:0:1733:A:H4'	3:B:212:GLN:HA	1.96	0.48
1:0:2609:G:H22	3:B:238:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:39:U:H3'	31:9:40:C:H5"	1.96	0.48
1:0:332:G:H4'	21:T:2:LYS:O	2.12	0.48
1:0:579:G:H4'	39:0:6205:HOH:O	2.12	0.48
1:0:1824:C:O2'	1:0:1999:C:H4'	2.13	0.48
1:0:1878:G:O2'	1:0:1879:U:H6	1.96	0.48
1:0:1902:G:O2'	1:0:1903:U:H5'	2.14	0.48
1:0:2480:G:H3'	39:0:8898:HOH:O	2.13	0.48
1:0:42:C:O5'	1:0:185:G:H5"	2.13	0.48
1:0:553:G:C2'	1:0:554:G:H5'	2.43	0.48
1:0:1174:A:C6	1:0:1201:C:H4'	2.48	0.48
1:0:1621:G:H2'	1:0:1622:G:O4'	2.14	0.48
1:0:1666:C:O2'	1:0:1667:A:H5"	2.13	0.48
1:0:1741:U:O2'	1:0:2723:G:H4'	2.14	0.48
1:0:2052:U:H2'	1:0:2053:G:O4'	2.14	0.48
1:0:2695:C:H2'	1:0:2696:G:C8	2.49	0.48
1:0:822:C:C2	1:0:823:U:C5	3.02	0.48
1:0:1163:G:H1	1:0:1184:C:H42	1.62	0.48
1:0:1861:C:H4'	2:A:6:GLY:O	2.13	0.48
12:K:12:LEU:HB2	12:K:47:ALA:HB3	1.95	0.48
1:0:37:A:C2	1:0:446:G:C2	3.02	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.48	0.48
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.48
1:0:276:C:H42	1:0:373:G:H1	1.62	0.48
1:0:1200:A:H3'	39:0:4912:HOH:O	2.12	0.48
1:0:1635:U:H2'	1:0:1636:G:H8	1.79	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.14	0.48
1:0:2539:U:O2'	37:0:9101:MUL:H22	2.13	0.48
6:E:24:GLY:HA3	6:E:76:VAL:HB	1.96	0.48
1:0:700:A:H4'	16:O:50:ARG:HH21	1.79	0.48
1:0:1242:A:H5'	11:J:82:THR:CG2	2.43	0.48
1:0:1723:G:H2'	39:0:5194:HOH:O	2.14	0.48
1:0:1829:A:N6	27:Z:42:TYR:HA	2.28	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2443:C:H3'	39:0:8103:HOH:O	2.13	0.48
1:0:2743:A:H5"	1:0:2743:A:H8	1.79	0.48
12:K:55:VAL:HG12	12:K:56:SER:N	2.29	0.48
1:0:37:A:H2'	1:0:38:G:C8	2.48	0.48
1:0:76:G:O2'	1:0:77:G:H5'	2.13	0.48
1:0:247:A:C2	1:0:265:U:C2	3.02	0.48
1:0:314:G:N1	1:0:317:A:OP2	2.47	0.48
1:0:393:G:H5"	39:0:6051:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:444:C:H2'	1:0:445:U:C6	2.49	0.48
1:0:705:C:H3'	1:0:706:G:C8	2.48	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.48
1:0:964:G:H2'	1:0:965:A:O4'	2.14	0.48
1:0:1684:A:O2'	1:0:1685:A:H5"	2.14	0.48
1:0:1850:U:H2'	1:0:1851:G:C8	2.49	0.48
1:0:2502:C:O2'	1:0:2503:A:H5'	2.14	0.48
1:0:2768:A:O2'	1:0:2769:C:H5'	2.13	0.48
1:0:2780:C:C1'	6:E:143:GLN:HE21	2.23	0.48
12:K:113:ILE:HG22	12:K:114:ALA:N	2.28	0.48
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.47
1:0:269:G:O3'	1:0:274:G:H4'	2.14	0.47
1:0:447:A:C2'	1:0:448:G:H5'	2.44	0.47
1:0:566:A:C2'	1:0:567:U:H5'	2.44	0.47
1:0:731:U:H2'	1:0:732:C:C6	2.49	0.47
1:0:1372:A:C2	1:0:2054:A:C4	3.02	0.47
1:0:1391:G:N2	1:0:1434:A:H5"	2.29	0.47
1:0:1487:A:H5'	39:0:3526:HOH:O	2.14	0.47
1:0:1855:G:H4'	1:0:1856:C:O5'	2.12	0.47
1:0:2134:G:H2'	1:0:2135:A:H8	1.78	0.47
1:0:2270:G:H4'	2:A:223:ARG:HH22	1.79	0.47
1:0:2781:U:H2'	1:0:2782:G:H5'	1.96	0.47
1:0:2911:C:H2'	1:0:2912:C:C6	2.48	0.47
1:0:391:U:O2'	1:0:392:U:H5'	2.14	0.47
1:0:699:C:H2'	1:0:744:G:N3	2.29	0.47
1:0:809:G:H2'	1:0:810:G:H8	1.77	0.47
1:0:849:C:H2'	1:0:850:U:H6	1.78	0.47
1:0:962:C:N4	1:0:1005:A:H61	2.12	0.47
1:0:1387:G:C2	1:0:1396:C:O2	2.67	0.47
1:0:1415:G:C2'	1:0:1416:G:H5'	2.44	0.47
1:0:1711:A:H2	1:0:1817:U:HO2'	1.62	0.47
1:0:1730:G:H5'	1:0:1731:C:C6	2.49	0.47
1:0:2070:G:H2'	1:0:2072:G:OP1	2.15	0.47
1:0:2458:U:O3'	30:3:64:LYS:HB2	2.14	0.47
1:0:2639:G:O2'	1:0:2640:U:H5'	2.14	0.47
1:0:2734:G:H2'	1:0:2735:U:O4'	2.13	0.47
37:0:9101:MUL:H14	37:0:9101:MUL:C10	2.41	0.47
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.55	0.47
17:P:98:ILE:HD12	17:P:102:ARG:HE	1.79	0.47
1:0:128:A:C8	1:0:128:A:C3'	2.96	0.47
1:0:158:A:H5"	39:0:7993:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:290:C:C2'	1:0:291:C:H5'	2.44	0.47
1:0:656:G:H5'	16:O:3:THR:HB	1.96	0.47
1:0:719:C:N3	1:0:720:G:H1'	2.29	0.47
1:0:941:G:C5	1:0:942:U:C4	3.02	0.47
1:0:957:A:H2'	1:0:958:G:O4'	2.14	0.47
1:0:1448:A:O4'	1:0:1506:U:O4'	2.31	0.47
1:0:1497:G:H2'	1:0:1498:G:H8	1.78	0.47
1:0:1515:A:H2'	1:0:1516:U:C6	2.49	0.47
1:0:2032:U:C2'	1:0:2033:G:H5"	2.43	0.47
1:0:2057:U:O5'	1:0:2057:U:H6	1.96	0.47
1:0:2291:A:C8	1:0:2309:C:H5'	2.49	0.47
1:0:2517:A:H2'	1:0:2518:C:O4'	2.13	0.47
12:K:62:PRO:HG3	12:K:65:ARG:HH21	1.79	0.47
31:9:3:A:H2	31:9:21:G:N3	2.12	0.47
1:0:137:U:OP1	1:0:259:G:O2'	2.31	0.47
1:0:221:G:H5'	39:0:6026:HOH:O	2.12	0.47
1:0:325:U:O2	1:0:326:G:C8	2.67	0.47
1:0:825:U:H5"	1:0:826:U:OP1	2.13	0.47
1:0:1730:G:H2'	1:0:1730:G:N3	2.29	0.47
1:0:1763:C:O2'	1:0:1764:C:H5'	2.15	0.47
1:0:1792:C:N3	1:0:1793:C:H5	2.12	0.47
1:0:2038:A:H5"	3:B:222:LYS:HG3	1.96	0.47
1:0:2047:C:P	39:0:7641:HOH:O	2.73	0.47
1:0:2089:A:C2'	1:0:2090:G:H5'	2.45	0.47
1:0:2286:G:H1'	39:0:7013:HOH:O	2.13	0.47
1:0:2355:G:H5"	1:0:2356:A:OP2	2.14	0.47
1:0:2815:G:H4'	1:0:2816:A:OP2	2.13	0.47
31:9:49:G:H5"	39:9:4707:HOH:O	2.13	0.47
1:0:37:A:H2'	1:0:38:G:H8	1.78	0.47
1:0:392:U:H5"	14:M:193:LYS:HG2	1.96	0.47
1:0:640:G:C4	1:0:641:G:C8	3.03	0.47
1:0:683:G:O2'	1:0:684:G:H5'	2.15	0.47
1:0:730:G:O2'	1:0:731:U:H5'	2.15	0.47
1:0:894:A:H5"	39:0:7673:HOH:O	2.13	0.47
1:0:1217:G:C2	1:0:1218:U:C2	3.03	0.47
1:0:1324:G:H21	26:Y:204:ARG:NH2	2.13	0.47
1:0:1377:C:H5'	1:0:1377:C:C6	2.43	0.47
1:0:2633:A:H2'	1:0:2634:G:H5'	1.97	0.47
1:0:2780:C:H2'	1:0:2781:U:C6	2.49	0.47
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.96	0.47
1:0:168:C:O5'	1:0:168:C:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:238:C:H4'	1:0:287:C:OP1	2.15	0.47
1:0:387:G:C2'	1:0:388:G:H5'	2.45	0.47
1:0:1666:C:C2'	1:0:1667:A:H5'	2.44	0.47
1:0:1969:A:O2'	1:0:1970:G:H5'	2.15	0.47
1:0:2072:G:H5'	39:0:3339:HOH:O	2.13	0.47
1:0:2332:A:H5'	5:D:56:ARG:NH2	2.27	0.47
1:0:2554:U:H3'	39:0:6989:HOH:O	2.14	0.47
1:0:2642:G:C6	1:0:2643:G:C6	3.02	0.47
1:0:2862:G:C6	1:0:2895:C:N4	2.83	0.47
37:0:9101:MUL:H262	37:0:9101:MUL:H242	1.71	0.47
1:0:57:C:H42	1:0:89:G:H1	1.63	0.47
1:0:208:C:H3'	1:0:208:C:C6	2.49	0.47
1:0:397:A:N3	1:0:418:C:H5'	2.30	0.47
1:0:459:A:H4'	39:0:4567:HOH:O	2.14	0.47
1:0:523:C:H2'	1:0:524:A:C8	2.49	0.47
1:0:544:G:H2'	1:0:545:G:H5"	1.97	0.47
1:0:561:G:N3	1:0:562:A:C8	2.83	0.47
1:0:603:A:H4'	1:0:604:G:O5'	2.15	0.47
1:0:699:C:C2	1:0:744:G:C2	3.02	0.47
1:0:711:G:C2	1:0:718:C:C2	3.03	0.47
1:0:763:C:O2'	1:0:764:C:H5'	2.14	0.47
1:0:920:C:H5	1:0:2467:A:OP1	1.98	0.47
1:0:951:A:H5"	18:Q:42:LYS:HD3	1.97	0.47
1:0:1153:C:N3	1:0:2786:G:O6	2.47	0.47
1:0:1162:G:H2'	1:0:1163:G:H8	1.80	0.47
1:0:1220:U:H2'	1:0:1221:G:C8	2.47	0.47
1:0:1245:C:H3'	1:0:1245:C:H6	1.79	0.47
1:0:1351:G:H1'	39:0:3441:HOH:O	2.15	0.47
1:0:1656:A:H2'	1:0:1657:A:O4'	2.14	0.47
1:0:1851:G:H1'	39:0:3109:HOH:O	2.15	0.47
1:0:2035:C:O2'	1:0:2036:C:H5'	2.15	0.47
1:0:2081:A:H2'	1:0:2082:G:O4'	2.15	0.47
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.47
1:0:2093:G:H5"	39:0:7738:HOH:O	2.15	0.47
1:0:2119:C:O2'	1:0:2120:U:H5'	2.14	0.47
1:0:2253:G:H2'	1:0:2254:G:C8	2.40	0.47
1:0:2430:A:H2'	1:0:2431:C:C6	2.49	0.47
1:0:2499:U:H2'	1:0:2500:C:H6	1.80	0.47
1:0:2800:A:H5'	1:0:2801:A:OP2	2.15	0.47
1:0:2808:U:OP1	3:B:261:GLN:NE2	2.42	0.47
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:27:ARG:HG2	4:C:27:ARG:HH11	1.79	0.47
4:C:215:ALA:HB3	39:C:5535:HOH:O	2.15	0.47
6:E:91:PHE:HA	6:E:92:PRO:HD3	1.79	0.47
24:W:88:THR:HG22	24:W:89:ASP:H	1.79	0.47
31:9:35:C:H5"	39:9:4078:HOH:O	2.15	0.47
1:0:45:A:C5'	1:0:47:G:H5'	2.45	0.47
1:0:123:U:H1'	39:0:7179:HOH:O	2.14	0.47
1:0:216:A:O2'	1:0:217:C:H5'	2.15	0.47
1:0:292:G:O2'	1:0:360:A:N6	2.47	0.47
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.15	0.47
1:0:639:A:C6	1:0:640:G:C6	3.02	0.47
1:0:699:C:C6	1:0:744:G:N3	2.83	0.47
1:0:1119:G:C5	1:0:1243:C:C4	3.03	0.47
1:0:1566:C:H2'	1:0:1567:G:C8	2.50	0.47
1:0:1575:C:O2	1:0:1575:C:H2'	2.14	0.47
1:0:1776:A:C8	1:0:1778:A:O4'	2.67	0.47
1:0:1826:C:O2'	1:0:1827:G:H5'	2.15	0.47
1:0:2243:C:H5"	39:0:8382:HOH:O	2.15	0.47
1:0:2651:C:H2'	1:0:2652:U:O4'	2.14	0.47
12:K:8:VAL:HG13	12:K:80:ILE:HG22	1.97	0.47
30:3:51:LYS:HB2	39:3:1812:HOH:O	2.15	0.47
1:0:240:C:O2	1:0:240:C:H2'	2.14	0.47
1:0:837:U:H2'	1:0:838:C:O4'	2.15	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.15	0.47
1:0:2320:U:H3'	30:3:2:GLN:HB2	1.97	0.47
1:0:2547:C:H1'	39:B:342:HOH:O	2.13	0.47
1:0:2697:A:H2'	1:0:2698:G:O4'	2.15	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.96	0.47
31:9:58:G:H2'	31:9:59:C:O4'	2.15	0.47
31:9:82:U:H2'	31:9:83:G:H8	1.80	0.47
1:0:849:C:C5	1:0:850:U:C5	3.03	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
1:0:1098:A:O3'	24:W:129:LYS:HE3	2.15	0.47
1:0:1158:G:C2'	1:0:1159:G:H5'	2.45	0.47
1:0:1351:G:OP1	4:C:96:LYS:NZ	2.42	0.47
1:0:1363:G:H2'	1:0:1364:G:H8	1.80	0.47
1:0:1978:A:H5"	39:0:7843:HOH:O	2.14	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.32	0.47
1:0:2893:C:O2'	1:0:2894:C:H5'	2.15	0.47
2:A:70:ALA:HB1	27:Z:89:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:174:A:H4'	1:0:175:G:OP1	2.15	0.46
1:0:187:A:H5'	1:0:188:C:OP2	2.14	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:661:G:C6	1:0:662:U:C4	3.03	0.46
1:0:738:G:H21	1:0:2384:U:H4'	1.80	0.46
1:0:879:C:H3'	39:0:5621:HOH:O	2.14	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:1138:G:H4'	39:0:4849:HOH:O	2.15	0.46
1:0:1278:A:H4'	1:0:1279:U:N3	2.29	0.46
1:0:1444:G:C2'	1:0:1445:G:H5'	2.45	0.46
1:0:1477:C:H2'	1:0:1478:U:O4'	2.15	0.46
1:0:1518:A:H1'	39:0:8334:HOH:O	2.15	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.15	0.46
1:0:2569:A:H8	1:0:2569:A:O5'	1.97	0.46
1:0:2812:A:H1'	39:0:4957:HOH:O	2.15	0.46
31:9:45:A:C8	31:9:46:C:C5	3.03	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.14	0.46
1:0:154:C:H2'	1:0:155:C:C6	2.37	0.46
1:0:485:A:N3	1:0:487:G:H5"	2.30	0.46
1:0:1215:A:O3'	1:0:1216:G:C4'	2.63	0.46
1:0:1252:A:H4'	39:0:4164:HOH:O	2.14	0.46
1:0:1449:G:N3	1:0:1449:G:H2'	2.29	0.46
1:0:1477:C:O2'	1:0:1478:U:H5'	2.15	0.46
1:0:1616:A:H5"	1:0:1617:C:OP1	2.15	0.46
1:0:1883:U:H5'	1:0:2012:U:OP2	2.15	0.46
1:0:1920:C:H2'	1:0:1921:A:H5'	1.97	0.46
1:0:2070:G:H4'	39:0:2976:HOH:O	2.14	0.46
1:0:2088:C:H1'	1:0:2841:A:N1	2.30	0.46
1:0:2496:C:H1'	1:0:2527:U:N3	2.30	0.46
24:W:122:ARG:HH12	24:W:154:ARG:N	2.12	0.46
1:0:634:G:C2	1:0:635:A:C2	3.03	0.46
1:0:920:C:H4'	1:0:921:G:N3	2.29	0.46
1:0:1754:A:H2'	1:0:1755:A:O4'	2.16	0.46
1:0:1771:U:H4'	1:0:1772:C:OP2	2.15	0.46
1:0:1832:G:N2	1:0:1845:A:C4	2.83	0.46
1:0:2073:G:H2'	39:0:8459:HOH:O	2.16	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.51	0.46
1:0:2135:A:O4'	1:0:2243:C:N4	2.47	0.46
27:Z:56:GLU:O	27:Z:61:HIS:HE1	1.98	0.46
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.56	0.46
31:9:39:U:H1'	31:9:44:A:N6	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:287:C:N4	1:0:365:G:H1	2.10	0.46
1:0:544:G:C2'	1:0:545:G:H5"	2.45	0.46
1:0:689:G:O2'	1:0:742:G:H1'	2.15	0.46
1:0:722:G:C5	1:0:723:G:C8	3.03	0.46
1:0:862:U:H4'	39:0:7515:HOH:O	2.15	0.46
1:0:946:C:H6	1:0:946:C:O5'	1.99	0.46
1:0:1013:A:H5"	1:0:2302:A:N6	2.30	0.46
1:0:1215:A:O3'	1:0:1216:G:H4'	2.14	0.46
1:0:1455:C:O2	1:0:1456:C:C6	2.69	0.46
1:0:1639:U:H2'	1:0:1640:C:O5'	2.15	0.46
1:0:1977:U:OP1	1:0:1978:A:H5'	2.15	0.46
1:0:2134:G:O6	1:0:2258:A:H2'	2.15	0.46
1:0:2605:G:O2'	1:0:2606:G:H5'	2.14	0.46
10:I:96:SER:H	10:I:99:GLN:HB2	1.80	0.46
1:0:106:A:C2'	1:0:107:U:H5'	2.46	0.46
1:0:250:C:H2'	1:0:251:C:C6	2.50	0.46
1:0:445:U:O2'	1:0:446:G:H5'	2.16	0.46
1:0:853:C:H3'	39:0:3276:HOH:O	2.14	0.46
1:0:871:G:C6	1:0:872:U:N3	2.84	0.46
1:0:1132:A:H61	1:0:1229:C:H2'	1.79	0.46
1:0:1253:C:O2'	1:0:1254:C:H5'	2.16	0.46
1:0:1523:G:C5	1:0:1524:U:C4	3.03	0.46
1:0:2110:G:H4'	39:0:7642:HOH:O	2.15	0.46
1:0:2134:G:N2	1:0:2242:U:C2	2.83	0.46
1:0:2578:G:H5'	1:0:2578:G:C8	2.47	0.46
1:0:2668:G:H2'	1:0:2669:U:H6	1.79	0.46
1:0:2714:U:O3'	3:B:10:SER:HB2	2.14	0.46
1:0:2718:C:C2	1:0:2763:G:N2	2.84	0.46
1:0:2825:C:H4'	1:0:2826:G:O4'	2.16	0.46
1:0:353:G:H2'	1:0:354:A:C8	2.51	0.46
1:0:485:A:O2'	1:0:487:G:H5'	2.16	0.46
1:0:583:C:H2'	1:0:584:U:H6	1.80	0.46
1:0:763:C:H5"	39:0:3284:HOH:O	2.16	0.46
1:0:962:C:H2'	1:0:963:C:C5'	2.46	0.46
1:0:1556:G:O2'	1:0:1557:G:H5'	2.16	0.46
1:0:1769:C:C2'	1:0:1770:U:H5'	2.46	0.46
1:0:2416:G:H1'	39:0:5208:HOH:O	2.14	0.46
1:0:2745:C:H5"	39:0:5667:HOH:O	2.14	0.46
1:0:522:U:O2'	1:0:523:C:H5'	2.16	0.46
1:0:669:G:C4	1:0:670:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:677:C:H4'	4:C:246:ARG:NH1	2.30	0.46
1:0:1217:G:H2'	1:0:1218:U:C6	2.51	0.46
1:0:1463:U:H4'	39:0:6050:HOH:O	2.16	0.46
1:0:1684:A:H8	39:0:7816:HOH:O	1.98	0.46
1:0:1822:A:O2'	1:0:1823:G:H5'	2.16	0.46
1:0:2075:G:C6	1:0:2076:U:C4	3.04	0.46
1:0:2096:A:C8	1:0:2539:U:C2	3.03	0.46
1:0:2259:C:C5	1:0:2260:A:N7	2.84	0.46
1:0:2484:U:H4'	39:0:4578:HOH:O	2.16	0.46
1:0:2754:G:H2'	1:0:2755:G:O4'	2.16	0.46
1:0:2796:U:H1'	6:E:143:GLN:OE1	2.16	0.46
6:E:103:VAL:HG22	6:E:115:ARG:HB3	1.97	0.46
11:J:107:ASN:HD22	11:J:109:TYR:H	1.63	0.46
1:0:105:G:C2	1:0:106:A:C8	3.04	0.46
1:0:295:C:C2'	1:0:296:G:H5'	2.45	0.46
1:0:502:A:H2'	1:0:503:G:O4'	2.15	0.46
1:0:814:G:H2'	1:0:815:U:H6	1.81	0.46
1:0:1230:A:H8	1:0:1230:A:OP1	1.98	0.46
1:0:2338:G:H4'	5:D:105:SER:O	2.16	0.46
1:0:2403:C:H5'	39:0:5297:HOH:O	2.14	0.46
1:0:2791:U:H4'	1:0:2792:A:OP1	2.16	0.46
1:0:160:A:C4	1:0:177:A:C2	3.04	0.46
39:0:6068:HOH:O	31:9:83:G:H4'	2.14	0.46
2:A:125:ASN:HB3	2:A:158:VAL:HG12	1.98	0.46
8:G:64:ASN:HD22	8:G:64:ASN:N	2.14	0.46
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.96	0.46
1:0:230:C:H2'	1:0:231:G:H8	1.81	0.46
1:0:267:G:H2'	1:0:268:U:O4'	2.16	0.46
1:0:287:C:H2'	1:0:288:A:C8	2.51	0.46
1:0:295:C:O2'	1:0:296:G:H5'	2.16	0.46
1:0:707:C:C2	1:0:708:A:C8	3.04	0.46
1:0:1096:U:O2'	1:0:1097:A:H5'	2.16	0.46
1:0:1880:C:H2'	1:0:1881:A:O4'	2.16	0.46
1:0:2540:G:O2'	37:0:9101:MUL:H131	2.16	0.46
1:0:2775:A:C6	1:0:2799:A:C8	3.04	0.46
15:N:37:ARG:NH1	31:9:6:C:OP1	2.46	0.46
1:0:432:G:H2'	1:0:433:C:C6	2.47	0.45
1:0:606:C:O2'	1:0:607:G:H5'	2.16	0.45
1:0:676:C:HO2'	4:C:219:ASN:HD22	1.60	0.45
1:0:878:G:H4'	1:0:1835:U:H4'	1.96	0.45
1:0:893:C:H4'	1:0:894:A:OP1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1794:G:OP1	17:P:134:VAL:HG23	2.16	0.45
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.45
1:0:2732:U:H2'	1:0:2733:U:H6	1.80	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.16	0.45
1:0:207:U:H4'	1:0:438:C:O2	2.16	0.45
1:0:402:U:H2'	1:0:403:C:C6	2.51	0.45
1:0:820:G:H5'	1:0:821:U:C5'	2.47	0.45
1:0:1183:C:N3	1:0:1184:C:N4	2.64	0.45
1:0:1325:G:C2	1:0:1326:C:C6	3.04	0.45
1:0:1838:U:H3'	39:0:4588:HOH:O	2.15	0.45
1:0:2102:G:C6	37:0:9101:MUL:H173	2.51	0.45
1:0:2776:A:H2'	1:0:2777:G:H5'	1.98	0.45
13:L:80:ASP:HB3	13:L:90:ARG:HB3	1.98	0.45
29:2:35:ARG:N	39:2:3614:HOH:O	2.50	0.45
30:3:49:ASP:HB3	30:3:52:PHE:HB2	1.98	0.45
31:9:64:C:C2'	31:9:65:A:H5'	2.46	0.45
31:9:75:G:C2	31:9:107:C:N3	2.85	0.45
1:0:165:A:O2'	1:0:221:G:N2	2.48	0.45
1:0:585:C:H2'	1:0:586:C:C6	2.51	0.45
1:0:1476:A:O2'	1:0:1477:C:H5'	2.17	0.45
1:0:1594:C:O2'	1:0:1607:A:H4'	2.16	0.45
1:0:2598:U:O2	1:0:2600:A:C8	2.70	0.45
1:0:2695:C:H2'	1:0:2696:G:H8	1.82	0.45
7:F:67:ALA:HB1	7:F:72:VAL:O	2.17	0.45
1:0:156:C:H5"	14:M:171:ARG:CD	2.42	0.45
1:0:535:G:C5	1:0:2063:U:C4	3.04	0.45
1:0:1098:A:OP1	24:W:128:VAL:HG22	2.15	0.45
1:0:1368:U:O5'	1:0:1368:U:H6	2.00	0.45
1:0:1449:G:N3	1:0:1493:A:C2	2.84	0.45
1:0:1509:U:O2'	1:0:1510:G:H5'	2.16	0.45
1:0:1667:A:H2'	1:0:1668:U:C6	2.51	0.45
1:0:1740:U:O2	1:0:2724:U:H5"	2.16	0.45
1:0:2397:G:C5	1:0:2465:A:C6	3.05	0.45
1:0:2541:U:H4'	39:0:4427:HOH:O	2.16	0.45
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.34	0.45
1:0:883:U:C6	1:0:888:U:H5'	2.51	0.45
1:0:926:A:H4'	13:L:39:GLU:HG2	1.99	0.45
1:0:1141:U:O2'	1:0:1142:C:H5'	2.16	0.45
1:0:1180:U:H1'	10:I:87:PRO:HD2	1.97	0.45
1:0:1195:G:H2'	1:0:1196:C:O4'	2.16	0.45
1:0:1439:C:O5'	1:0:1439:C:H6	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2078:U:O2'	1:0:2079:G:H5'	2.16	0.45
1:0:2106:C:H2'	1:0:2107:U:C6	2.52	0.45
1:0:2297:U:O2'	1:0:2298:C:H5'	2.16	0.45
1:0:2388:C:H5"	18:Q:82:LYS:HG2	1.99	0.45
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.97	0.45
1:0:67:A:H5"	1:0:69:A:C8	2.52	0.45
1:0:247:A:H2'	39:0:8624:HOH:O	2.15	0.45
1:0:255:A:C5	1:0:256:C:C4	3.04	0.45
1:0:266:G:C2	1:0:267:G:C8	3.05	0.45
1:0:421:C:H4'	1:0:1919:A:C5	2.51	0.45
1:0:517:U:C2'	1:0:518:G:H5'	2.47	0.45
1:0:544:G:H2'	1:0:545:G:C5'	2.47	0.45
1:0:558:C:O2'	1:0:559:U:H5"	2.17	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.52	0.45
1:0:876:A:H2'	1:0:876:A:N3	2.30	0.45
1:0:1052:G:H2'	1:0:1052:G:N3	2.32	0.45
1:0:1220:U:H4'	9:H:174:LEU:HD21	1.98	0.45
1:0:1877:G:OP1	2:A:164:ARG:NH2	2.49	0.45
1:0:1909:A:H4'	39:0:8156:HOH:O	2.16	0.45
1:0:2270:G:H2'	39:0:4485:HOH:O	2.16	0.45
1:0:2444:U:H2'	1:0:2445:U:H6	1.81	0.45
1:0:2673:U:H4'	3:B:94:GLN:O	2.17	0.45
1:0:2689:A:C2'	1:0:2690:U:H5'	2.45	0.45
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.16	0.45
15:N:159:TYR:CE1	31:9:50:G:H5"	2.49	0.45
1:0:29:C:H5'	1:0:1342:C:OP1	2.16	0.45
1:0:293:A:H2'	1:0:294:C:C6	2.51	0.45
1:0:329:A:H5'	1:0:347:A:C1'	2.47	0.45
1:0:333:G:N1	1:0:344:C:C4	2.85	0.45
1:0:443:C:H2'	1:0:444:C:C6	2.52	0.45
1:0:1156:C:O2'	1:0:1157:C:H5'	2.17	0.45
1:0:1447:U:OP1	1:0:1506:U:N3	2.41	0.45
1:0:1919:A:H4'	39:0:3679:HOH:O	2.17	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.82	0.45
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.99	0.45
22:U:39:ASN:HD22	22:U:44:ARG:HD2	1.82	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
1:0:178:U:O2'	1:0:179:C:H5'	2.16	0.45
1:0:193:A:H2'	1:0:414:C:O2	2.16	0.45
1:0:275:G:C2	1:0:376:C:C2	3.05	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:400:C:H2'	1:0:401:C:C6	2.52	0.45
1:0:1119:G:C8	11:J:52:GLN:NE2	2.84	0.45
1:0:1164:U:H4'	1:0:1165:G:H5"	1.99	0.45
1:0:1334:C:H1'	26:Y:204:ARG:HH21	1.81	0.45
1:0:1475:G:N3	1:0:1866:A:H2	2.15	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45
1:0:1917:G:H1'	1:0:1923:G:N2	2.32	0.45
1:0:2295:G:H5'	1:0:2425:A:H4'	1.98	0.45
1:0:2493:C:O2	1:0:2493:C:H2'	2.17	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.45
1:0:2727:A:H2'	1:0:2728:C:H5'	1.98	0.45
1:0:2823:G:O2'	1:0:2824:C:H5'	2.16	0.45
39:0:7140:HOH:O	26:Y:149:GLN:HG3	2.15	0.45
3:B:56:ASP:HB2	3:B:322:ARG:HE	1.82	0.45
11:J:76:ASP:HA	39:J:5907:HOH:O	2.16	0.45
15:N:55:ASP:OD2	31:9:7:G:H4'	2.16	0.45
1:0:63:U:O2'	1:0:64:G:H5'	2.17	0.45
1:0:287:C:H3'	1:0:287:C:H6	1.81	0.45
1:0:343:C:O2'	1:0:344:C:H5'	2.17	0.45
1:0:400:C:H2'	1:0:401:C:H6	1.82	0.45
1:0:693:A:H2'	1:0:694:A:C8	2.52	0.45
1:0:1080:C:O5'	1:0:1080:C:H6	2.00	0.45
1:0:1328:A:C8	26:Y:169:ARG:HD3	2.51	0.45
1:0:1398:G:H2'	1:0:1399:A:O4'	2.17	0.45
1:0:1514:C:O2'	1:0:1515:A:H5'	2.17	0.45
1:0:1766:U:H2'	1:0:1776:A:N6	2.31	0.45
1:0:2513:A:H2'	1:0:2514:U:O4'	2.17	0.45
1:0:2869:G:H5'	39:0:4548:HOH:O	2.16	0.45
3:B:125:GLU:O	3:B:129:ARG:HG3	2.17	0.45
31:9:17:G:O2'	31:9:18:U:H5'	2.16	0.45
1:0:23:G:H2'	1:0:24:G:O4'	2.17	0.45
1:0:123:U:H5'	39:0:6169:HOH:O	2.17	0.45
1:0:151:A:N3	1:0:441:A:H4'	2.32	0.45
1:0:622:G:C5	1:0:623:U:C5	3.04	0.45
1:0:656:G:H2'	1:0:657:G:C8	2.52	0.45
1:0:783:C:O5'	1:0:783:C:H6	2.00	0.45
1:0:957:A:H2'	1:0:958:G:C8	2.52	0.45
1:0:1296:A:O2'	1:0:1297:U:H5'	2.16	0.45
1:0:2043:U:O3'	25:X:23:HIS:HE1	1.99	0.45
1:0:2269:C:C2'	1:0:2270:G:H5'	2.47	0.45
3:B:254:GLN:HG2	3:B:255:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:44:ARG:HG3	15:N:45:ALA:N	2.32	0.45
1:0:80:A:H3'	21:T:43:ASN:OD1	2.16	0.44
1:0:128:A:H3'	1:0:128:A:H8	1.81	0.44
1:0:657:G:H1'	39:0:2960:HOH:O	2.16	0.44
1:0:876:A:N7	1:0:878:G:H1'	2.32	0.44
1:0:1258:G:H8	1:0:1258:G:O5'	2.00	0.44
1:0:1323:G:N2	1:0:1335:C:C2	2.86	0.44
1:0:1387:G:H1'	17:P:28:GLN:HE22	1.80	0.44
1:0:2657:G:H5'	39:0:5938:HOH:O	2.17	0.44
9:H:168:VAL:HG13	39:H:4963:HOH:O	2.16	0.44
1:0:298:C:O5'	1:0:298:C:H6	1.99	0.44
1:0:473:A:O2'	1:0:890:C:H5'	2.17	0.44
1:0:1126:C:O5'	1:0:1126:C:C6	2.66	0.44
1:0:1454:U:H5"	1:0:1455:C:OP2	2.17	0.44
1:0:1526:A:H4'	1:0:1527:A:C5'	2.47	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.34	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.44
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.50	0.44
1:0:2271:G:N3	1:0:2271:G:H2'	2.32	0.44
1:0:2407:G:C2	1:0:2408:A:C4	3.05	0.44
31:9:59:C:H2'	31:9:60:C:H6	1.82	0.44
1:0:32:G:H2'	1:0:33:G:O4'	2.18	0.44
1:0:329:A:H5'	1:0:347:A:H1'	1.99	0.44
1:0:397:A:C4	1:0:418:C:H5'	2.52	0.44
1:0:722:G:C2'	1:0:723:G:H5'	2.48	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
1:0:1730:G:C5'	1:0:1731:C:C6	3.00	0.44
1:0:1827:G:H2'	1:0:1828:G:C8	2.52	0.44
1:0:2087:C:C2	1:0:2658:G:C2	3.06	0.44
1:0:2428:G:H4'	39:0:4707:HOH:O	2.17	0.44
1:0:2638:G:H5'	39:0:3790:HOH:O	2.17	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	1.98	0.44
14:M:99:ARG:NE	14:M:170:ASN:HD22	2.15	0.44
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.82	0.44
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.44
24:W:38:THR:O	24:W:42:ARG:HB2	2.17	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.44
1:0:212:A:O3'	1:0:213:G:H4'	2.17	0.44
1:0:708:A:H2'	1:0:709:G:O4'	2.17	0.44
1:0:1363:G:P	4:C:76:ARG:NH2	2.90	0.44
1:0:1433:G:H2'	1:0:1434:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:C5'	1:0:1868:G:H5"	2.48	0.44
1:0:1909:A:N1	1:0:2128:G:H1'	2.32	0.44
1:0:2002:C:H2'	1:0:2003:U:H5'	1.99	0.44
1:0:2451:G:H5"	39:0:6300:HOH:O	2.16	0.44
1:0:2657:G:N2	1:0:2658:G:H1'	2.33	0.44
1:0:2814:A:O4'	1:0:2816:A:C8	2.70	0.44
1:0:2900:G:O2'	1:0:2901:C:H5'	2.17	0.44
2:A:178:LYS:NZ	39:A:4437:HOH:O	2.50	0.44
12:K:98:VAL:HG13	12:K:102:GLU:HA	2.00	0.44
31:9:1:U:H4'	31:9:3:A:OP1	2.18	0.44
31:9:95:C:O2'	31:9:96:C:H5'	2.17	0.44
1:0:64:G:N2	1:0:70:A:C4	2.85	0.44
1:0:65:C:H2'	1:0:66:G:H8	1.82	0.44
1:0:131:A:OP2	1:0:141:C:H5	2.01	0.44
1:0:256:C:H2'	1:0:257:G:C5'	2.47	0.44
1:0:318:U:H5'	1:0:339:A:N3	2.32	0.44
1:0:962:C:C2'	1:0:963:C:H5'	2.48	0.44
1:0:1209:C:H2'	1:0:1210:G:C8	2.48	0.44
1:0:1544:U:O2'	1:0:1545:C:H5'	2.17	0.44
1:0:1733:A:C2	1:0:1734:C:H1'	2.53	0.44
1:0:1886:A:H61	1:0:2016:U:H3	1.63	0.44
1:0:2103:A:O2'	1:0:2104:C:OP1	2.36	0.44
1:0:2275:G:C6	1:0:2276:U:N3	2.85	0.44
1:0:2679:G:H2'	1:0:2680:A:H3'	1.99	0.44
1:0:2726:U:O4'	1:0:2749:U:C2	2.69	0.44
1:0:2869:G:H8	1:0:2869:G:O5'	2.01	0.44
3:B:244:PRO:HG3	3:B:248:ARG:HH21	1.81	0.44
14:M:157:ASP:HB3	14:M:160:PHE:HD1	1.83	0.44
28:1:28:HIS:O	28:1:32:LYS:N	2.49	0.44
31:9:54:A:H4'	39:9:7345:HOH:O	2.16	0.44
1:0:228:C:C2'	1:0:229:G:H5'	2.48	0.44
1:0:354:A:H2'	1:0:355:C:C6	2.53	0.44
1:0:1501:A:H4'	39:0:4703:HOH:O	2.17	0.44
1:0:1531:U:C2	1:0:1661:A:N1	2.85	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.44
1:0:1632:A:C2'	1:0:1633:C:H5'	2.46	0.44
1:0:1681:G:H5"	1:0:1682:A:H5'	1.99	0.44
1:0:1732:A:C6	1:0:2840:A:H1'	2.52	0.44
1:0:2245:C:H6	1:0:2245:C:O5'	2.01	0.44
1:0:2349:G:H2'	1:0:2350:G:C8	2.52	0.44
1:0:2467:A:H1'	39:0:3524:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2471:G:N3	1:0:2633:A:H2	2.16	0.44
1:0:2892:G:C6	1:0:2893:C:C4	3.06	0.44
5:D:15:GLU:HA	5:D:16:PRO:HD3	1.85	0.44
31:9:3:A:H2'	31:9:26:C:O2	2.18	0.44
1:0:400:C:O2'	1:0:401:C:H5'	2.18	0.44
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.44
1:0:736:A:H8	39:0:6948:HOH:O	2.01	0.44
1:0:1126:C:O2'	1:0:1128:U:H6	2.01	0.44
1:0:1216:G:N2	1:0:1217:G:H1'	2.33	0.44
1:0:1647:G:H2'	1:0:1648:G:O4'	2.17	0.44
1:0:1792:C:C2	1:0:1793:C:H5	2.36	0.44
1:0:2110:G:C2	1:0:2478:U:N3	2.86	0.44
1:0:2254:G:H1'	39:0:4611:HOH:O	2.18	0.44
1:0:2331:C:H1'	1:0:2356:A:C2	2.52	0.44
1:0:2554:U:C6	1:0:2577:A:N6	2.85	0.44
5:D:172:VAL:HG12	5:D:173:GLU:H	1.83	0.44
1:0:577:G:C6	1:0:581:G:O6	2.70	0.44
1:0:690:G:H4'	1:0:741:C:O2	2.18	0.44
1:0:816:G:C5	1:0:817:G:C6	3.06	0.44
1:0:1186:C:N4	1:0:1190:G:H22	2.12	0.44
1:0:1299:G:H5'	39:0:8773:HOH:O	2.17	0.44
1:0:1841:C:OP2	1:0:2022:A:H8	2.00	0.44
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.44
1:0:2001:G:O2'	1:0:2002:C:H5'	2.18	0.44
1:0:2055:A:H5'	19:R:134:SER:HB2	2.00	0.44
1:0:2066:C:H5"	39:0:4041:HOH:O	2.17	0.44
1:0:2076:U:H2'	39:0:6153:HOH:O	2.17	0.44
1:0:2461:U:C2	1:0:2466:G:H1'	2.52	0.44
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.44
1:0:2832:C:H5	39:0:6957:HOH:O	2.01	0.44
3:B:272:ILE:HG22	39:B:7492:HOH:O	2.17	0.44
1:0:81:G:N3	1:0:98:A:C2	2.86	0.44
1:0:119:A:H2'	1:0:120:A:C5'	2.45	0.44
1:0:206:G:H5'	14:M:185:PRO:HD3	1.99	0.44
1:0:533:U:H2'	1:0:2814:A:C6	2.52	0.44
1:0:566:A:H2'	1:0:567:U:C5'	2.48	0.44
1:0:595:U:H2'	1:0:596:C:C6	2.51	0.44
1:0:1200:A:H5'	39:0:7124:HOH:O	2.18	0.44
1:0:1641:A:C8	1:0:1702:U:O4	2.71	0.44
1:0:2120:U:H1'	39:0:3535:HOH:O	2.17	0.44
1:0:2265:U:H2'	1:0:2266:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.53	0.44
1:0:2846:C:H4'	3:B:156:LYS:HB2	1.99	0.44
5:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.44
9:H:23:ILE:HG21	9:H:97:VAL:HG11	2.00	0.44
13:L:136:ALA:HB3	39:L:6166:HOH:O	2.18	0.44
1:0:21:G:C4'	19:R:2:ILE:HG22	2.44	0.43
1:0:506:G:H22	1:0:509:A:H5'	1.76	0.43
1:0:792:G:O2'	1:0:793:A:H5'	2.18	0.43
1:0:927:U:H4'	39:0:3262:HOH:O	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.47	0.43
1:0:1185:U:H2'	1:0:1186:C:C6	2.53	0.43
1:0:1829:A:H2'	1:0:1830:C:C5'	2.46	0.43
1:0:1909:A:H2'	1:0:1910:A:C8	2.53	0.43
1:0:2321:A:H62	1:0:2380:A:H62	1.65	0.43
1:0:2420:G:O2'	1:0:2421:G:H5'	2.17	0.43
1:0:2598:U:O2	1:0:2600:A:H8	2.01	0.43
1:0:2730:G:O2'	1:0:2731:G:H5'	2.17	0.43
1:0:2853:U:C4	1:0:2906:A:N6	2.85	0.43
11:J:75:PRO:HG2	11:J:105:LEU:HD21	2.00	0.43
28:1:2:GLY:O	28:1:6:PRO:HG2	2.18	0.43
31:9:92:G:C6	31:9:93:A:N6	2.86	0.43
1:0:212:A:O4'	1:0:214:U:C6	2.71	0.43
1:0:599:G:H2'	1:0:600:G:C8	2.53	0.43
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.43
1:0:868:G:C5	1:0:887:G:C8	3.06	0.43
1:0:952:G:N3	1:0:2302:A:H2'	2.33	0.43
1:0:1448:A:H4'	39:0:6039:HOH:O	2.18	0.43
1:0:1933:G:O2'	1:0:1934:A:H5'	2.18	0.43
1:0:2507:G:O6	1:0:2511:A:H4'	2.18	0.43
1:0:2739:A:C6	1:0:2740:G:C5	3.06	0.43
19:R:63:ASN:ND2	19:R:75:TRP:HZ2	2.17	0.43
1:0:56:G:H1'	39:0:4338:HOH:O	2.18	0.43
1:0:66:G:C2	1:0:109:U:C4	3.06	0.43
1:0:235:C:O2'	1:0:236:A:H2'	2.18	0.43
1:0:530:C:H2'	1:0:531:G:O4'	2.18	0.43
1:0:596:C:H2'	1:0:597:A:C8	2.53	0.43
1:0:836:G:N3	1:0:836:G:H2'	2.34	0.43
1:0:1188:A:N7	1:0:1189:A:C2	2.87	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.43
1:0:1557:G:H2'	1:0:1558:C:H6	1.83	0.43
1:0:1689:A:H2'	1:0:1689:A:N3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1758:U:C2'	1:0:1759:A:H5'	2.48	0.43
1:0:1788:U:C2	1:0:1805:G:N2	2.87	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
1:0:2364:A:H5"	18:Q:15:LYS:HD3	2.00	0.43
1:0:2552:C:C6	1:0:2577:A:N7	2.86	0.43
5:D:149:ARG:HH12	15:N:15:GLU:HA	1.83	0.43
25:X:74:ALA:HB2	25:X:85:VAL:HG13	2.00	0.43
1:0:67:A:C6	1:0:109:U:H1'	2.53	0.43
1:0:281:U:O2'	1:0:282:C:H5'	2.19	0.43
1:0:549:A:C2	1:0:550:C:C2	3.06	0.43
1:0:658:C:O2'	1:0:662:U:OP1	2.30	0.43
1:0:1127:C:C2'	1:0:1128:U:H5'	2.48	0.43
1:0:1332:C:O2'	1:0:1333:U:H5'	2.19	0.43
1:0:1503:U:C2'	1:0:1504:A:H5'	2.48	0.43
1:0:1821:A:O2'	1:0:1822:A:H5'	2.17	0.43
1:0:387:G:O2'	1:0:388:G:H5'	2.18	0.43
1:0:730:G:H2'	1:0:731:U:C6	2.53	0.43
1:0:869:G:C8	1:0:869:G:OP2	2.72	0.43
1:0:938:G:N2	1:0:1031:G:H1'	2.34	0.43
1:0:1610:G:H2'	1:0:1611:G:O4'	2.18	0.43
1:0:1825:U:O4'	1:0:1999:C:H5"	2.19	0.43
1:0:1861:C:O2'	1:0:1862:C:H5'	2.19	0.43
1:0:1942:A:H2'	39:0:4237:HOH:O	2.18	0.43
1:0:2467:A:H5"	39:0:2924:HOH:O	2.17	0.43
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.43
1:0:815:U:O2'	1:0:816:G:H5'	2.19	0.43
1:0:1074:G:H4'	1:0:1260:G:C6	2.54	0.43
1:0:1076:G:C2	1:0:1084:C:N3	2.86	0.43
1:0:1086:A:N6	24:W:11:VAL:HG11	2.33	0.43
1:0:1135:G:N2	1:0:1228:C:C2	2.87	0.43
1:0:1288:U:H4'	24:W:27:HIS:CD2	2.54	0.43
1:0:1786:C:C5	1:0:1787:C:H5	2.37	0.43
1:0:1853:C:H5'	2:A:228:ILE:O	2.18	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.43
1:0:2097:G:N2	1:0:2098:C:H1'	2.34	0.43
1:0:2103:A:H2'	1:0:2104:C:H5'	2.01	0.43
13:L:3:LYS:NZ	39:L:3752:HOH:O	2.51	0.43
27:Z:78:ILE:HD12	39:Z:3477:HOH:O	2.16	0.43
1:0:944:G:H21	24:W:44:MET:HE2	1.83	0.43
1:0:1102:C:O5'	1:0:1102:C:H6	2.02	0.43
1:0:1162:G:N2	1:0:1185:U:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1397:C:H1'	17:P:28:GLN:OE1	2.18	0.43
1:0:1444:G:H5"	20:S:11:THR:HG22	2.00	0.43
1:0:1742:A:H61	1:0:2037:C:H42	1.66	0.43
1:0:1758:U:H2'	1:0:1759:A:O4'	2.19	0.43
1:0:1812:G:H4'	1:0:1814:G:O4'	2.18	0.43
1:0:1815:A:H8	1:0:1815:A:O5'	2.01	0.43
1:0:1924:A:H8	1:0:1924:A:O5'	2.01	0.43
1:0:2591:C:H2'	1:0:2592:G:H5'	2.01	0.43
1:0:2635:A:C2'	1:0:2636:C:H5'	2.48	0.43
1:0:2686:C:H2'	1:0:2687:G:C8	2.54	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.43
31:9:59:C:H1'	39:9:2772:HOH:O	2.18	0.43
1:0:120:A:C6	28:1:17:THR:HG21	2.53	0.43
1:0:453:A:H4'	1:0:455:A:N7	2.33	0.43
1:0:661:G:C5	1:0:662:U:C4	3.07	0.43
1:0:961:A:H4'	39:0:6342:HOH:O	2.17	0.43
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.43
1:0:1274:A:C6	1:0:1275:C:C4	3.07	0.43
1:0:1399:A:H2'	1:0:1400:C:C6	2.54	0.43
1:0:1594:C:C2	1:0:1601:G:N2	2.86	0.43
1:0:2038:A:C2	1:0:2039:A:C5	3.07	0.43
1:0:2642:G:C6	1:0:2643:G:C5	3.06	0.43
1:0:2738:G:H2'	1:0:2739:A:H8	1.84	0.43
1:0:2835:C:H42	1:0:2845:G:H1	1.65	0.43
1:0:2846:C:H2'	1:0:2847:G:H8	1.82	0.43
1:0:2882:G:H8	1:0:2882:G:O5'	2.01	0.43
39:0:3707:HOH:O	2:A:11:ARG:HD3	2.18	0.43
17:P:55:LYS:HG2	17:P:56:GLY:N	2.34	0.43
1:0:217:C:H2'	1:0:218:C:C6	2.54	0.43
1:0:465:U:C5	1:0:475:G:N2	2.87	0.43
1:0:594:C:C4	1:0:595:U:N3	2.86	0.43
1:0:603:A:H5"	1:0:604:G:OP1	2.19	0.43
1:0:656:G:H1'	39:0:7042:HOH:O	2.18	0.43
1:0:865:G:O2'	1:0:866:U:H5'	2.19	0.43
1:0:1118:A:C8	1:0:1119:G:H5"	2.54	0.43
1:0:1626:A:H2'	1:0:1627:G:C5'	2.49	0.43
1:0:1626:A:O2'	1:0:1627:G:H5'	2.19	0.43
1:0:1730:G:H5'	1:0:1731:C:C5	2.54	0.43
1:0:2297:U:C2	1:0:2298:C:C6	3.07	0.43
1:0:2441:U:H4'	13:L:53:ARG:HD2	2.01	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:99:ARG:HD2	14:M:167:GLY:HA2	2.01	0.43
1:0:24:G:O2'	1:0:25:A:OP2	2.31	0.43
1:0:287:C:H3'	1:0:287:C:C6	2.54	0.43
1:0:458:G:H2'	1:0:459:A:C8	2.54	0.43
1:0:541:C:O2'	1:0:542:A:H5"	2.17	0.43
1:0:759:C:C5	1:0:761:A:C8	3.07	0.43
1:0:940:G:N3	1:0:1032:A:C2	2.86	0.43
1:0:1130:U:O2'	31:9:91:C:H4'	2.18	0.43
1:0:1361:C:H2'	1:0:1362:U:H6	1.83	0.43
1:0:1904:A:H2'	1:0:1905:U:H6	1.84	0.43
1:0:1933:G:C2'	1:0:1934:A:H5'	2.48	0.43
1:0:2329:C:O2'	1:0:2330:U:H5'	2.19	0.43
1:0:2768:A:H5"	39:0:3093:HOH:O	2.19	0.43
39:0:3308:HOH:O	31:9:105:A:H5"	2.19	0.43
3:B:238:ASN:HD22	3:B:240:GLY:H	1.66	0.43
20:S:73:ASP:O	20:S:77:VAL:HG23	2.18	0.43
1:0:48:A:C5	1:0:113:A:C2	3.07	0.42
1:0:295:C:H2'	1:0:296:G:O4'	2.18	0.42
1:0:343:C:H2'	1:0:344:C:C6	2.50	0.42
1:0:664:U:H5	1:0:680:G:C4	2.36	0.42
1:0:812:A:C2	1:0:813:C:C2	3.07	0.42
1:0:1185:U:H5'	39:0:7308:HOH:O	2.18	0.42
1:0:1314:U:H2'	39:0:5081:HOH:O	2.18	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.34	0.42
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:2383:G:C6	1:0:2384:U:C4	3.07	0.42
1:0:2577:A:H5'	39:0:7700:HOH:O	2.19	0.42
1:0:2716:G:O2'	1:0:2717:C:H5'	2.19	0.42
1:0:2795:C:H1'	39:0:8323:HOH:O	2.19	0.42
2:A:70:ALA:HA	2:A:71:PRO:HD3	1.84	0.42
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.89	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
1:0:313:U:H2'	1:0:314:G:H5'	2.00	0.42
1:0:453:A:H5"	39:0:7136:HOH:O	2.20	0.42
1:0:661:G:C5	1:0:686:A:C2	3.07	0.42
1:0:894:A:N1	4:C:87:ARG:NH2	2.67	0.42
1:0:1163:G:H1	1:0:1184:C:N4	2.16	0.42
1:0:1350:U:H4'	39:0:4055:HOH:O	2.19	0.42
1:0:1585:C:N3	1:0:1611:G:C2	2.87	0.42
1:0:1698:U:H5	39:0:7522:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1965:C:H2'	1:0:1966:U:C6	2.54	0.42
1:0:2103:A:HO2'	1:0:2104:C:P	2.41	0.42
1:0:2791:U:O5'	1:0:2791:U:H6	2.02	0.42
24:W:5:VAL:HG11	24:W:153:MET:HE1	2.01	0.42
1:0:256:C:H2'	1:0:257:G:H5'	2.00	0.42
1:0:324:G:C2	1:0:325:U:C6	3.07	0.42
1:0:372:A:H2'	1:0:373:G:H8	1.83	0.42
1:0:840:U:C5	1:0:2648:U:C5	3.07	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.54	0.42
1:0:908:A:O2'	1:0:909:U:H5'	2.19	0.42
1:0:1014:A:C6	1:0:1015:C:H1'	2.54	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.20	0.42
1:0:1307:A:O5'	1:0:1307:A:H8	2.02	0.42
1:0:1379:A:H1'	39:0:5427:HOH:O	2.19	0.42
1:0:1535:G:H2'	1:0:1536:C:C6	2.54	0.42
1:0:1632:A:C3'	1:0:1633:C:H5'	2.49	0.42
1:0:1779:A:H2'	1:0:1780:G:O4'	2.19	0.42
1:0:2328:U:H2'	1:0:2329:C:O4'	2.19	0.42
1:0:2359:G:H3'	39:0:4829:HOH:O	2.19	0.42
37:0:9101:MUL:C10	37:0:9101:MUL:C14	2.97	0.42
14:M:68:ARG:NE	14:M:73:ARG:HH11	2.16	0.42
16:O:32:ARG:HH21	16:O:35:LYS:HZ2	1.67	0.42
31:9:36:C:C5	31:9:37:C:C4	3.07	0.42
1:0:308:U:C2'	21:T:52:ARG:NH2	2.79	0.42
1:0:801:U:O2'	1:0:802:G:H5'	2.19	0.42
1:0:946:C:H2'	1:0:947:U:C6	2.54	0.42
1:0:1338:U:O2'	1:0:1339:G:H5'	2.20	0.42
1:0:1441:G:H2'	1:0:1442:A:H8	1.82	0.42
1:0:1593:C:H2'	1:0:1594:C:C6	2.47	0.42
1:0:1676:G:C6	1:0:1677:U:N3	2.84	0.42
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.42
1:0:1935:C:H2'	1:0:1936:C:C6	2.54	0.42
1:0:2054:A:H5'	39:0:3751:HOH:O	2.18	0.42
19:R:109:MET:HB2	19:R:109:MET:HE3	1.92	0.42
31:9:41:C:H2'	31:9:42:C:C6	2.53	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
1:0:217:C:OP1	1:0:395:A:O2'	2.26	0.42
1:0:338:C:H4'	4:C:174:ILE:HD11	2.01	0.42
1:0:399:C:H1'	14:M:194:GLY:OXT	2.20	0.42
1:0:784:A:H2'	1:0:785:U:O4'	2.19	0.42
1:0:1082:A:H2'	1:0:1083:C:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1168:C:H5'	10:I:83:GLY:HA3	2.00	0.42
1:0:1687:C:H1'	28:1:8:GLN:O	2.20	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:2414:A:H1'	39:0:3480:HOH:O	2.19	0.42
1:0:2600:A:H2'	1:0:2601:A:O4'	2.20	0.42
1:0:2686:C:H2'	1:0:2687:G:H8	1.84	0.42
7:F:32:GLY:N	39:F:3111:HOH:O	2.51	0.42
1:0:314:G:C2	1:0:317:A:C8	3.07	0.42
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.42
1:0:946:C:O2'	1:0:947:U:H5'	2.20	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.19	0.42
1:0:1157:C:O2'	1:0:1158:G:H5'	2.19	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.31	0.42
1:0:1452:G:H1'	35:0:8803:CL:CL	2.57	0.42
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
1:0:1918:U:O2	1:0:1920:C:H3'	2.19	0.42
1:0:1947:G:N2	1:0:1966:U:O2	2.52	0.42
1:0:2397:G:H2'	1:0:2398:A:C8	2.52	0.42
1:0:2485:A:H3'	39:0:5048:HOH:O	2.19	0.42
1:0:2766:A:O2'	1:0:2767:C:H5'	2.19	0.42
1:0:2815:G:N7	11:J:80:LYS:NZ	2.68	0.42
1:0:170:U:H5'	30:3:48:ASN:ND2	2.27	0.42
1:0:561:G:C2	1:0:562:A:N7	2.88	0.42
1:0:595:U:H3'	1:0:595:U:H6	1.85	0.42
1:0:758:A:H2'	1:0:759:C:O4'	2.20	0.42
1:0:933:C:H4'	1:0:1297:U:H4'	2.00	0.42
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.42
1:0:1546:G:H2'	1:0:1547:A:O4'	2.20	0.42
1:0:1692:C:H2'	39:0:6064:HOH:O	2.19	0.42
1:0:1848:G:H4'	39:0:6016:HOH:O	2.20	0.42
1:0:1866:A:N7	1:0:1867:G:H1'	2.35	0.42
1:0:2319:C:H4'	1:0:2322:U:C4	2.55	0.42
1:0:2419:U:H5"	1:0:2420:G:H5'	2.02	0.42
1:0:2583:A:H4'	12:K:43:ARG:O	2.19	0.42
1:0:2715:G:OP1	3:B:16:ARG:NH2	2.53	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
39:0:6217:HOH:O	21:T:38:ARG:NH1	2.51	0.42
15:N:44:ARG:NH1	31:9:4:G:H21	2.17	0.42
1:0:122:C:H5"	39:0:8215:HOH:O	2.19	0.42
1:0:666:A:N7	1:0:667:C:C2	2.88	0.42
1:0:740:G:H2'	1:0:741:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1079:A:H4'	1:0:2078:U:H5'	2.02	0.42
1:0:1384:C:H5'	25:X:30:MET:HG2	2.02	0.42
1:0:1688:G:C6	1:0:1692:C:C5	3.07	0.42
1:0:1739:G:C6	1:0:1740:U:C4	3.07	0.42
1:0:2122:C:O2	14:M:76:ARG:NH2	2.52	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.42
1:0:2300:A:H4'	1:0:2301:A:N3	2.34	0.42
1:0:2555:C:O5'	1:0:2555:C:H6	2.03	0.42
6:E:101:GLU:HB2	6:E:116:THR:O	2.20	0.42
31:9:41:C:H2'	31:9:42:C:H6	1.84	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.19	0.42
1:0:81:G:H5'	21:T:65:VAL:O	2.20	0.42
1:0:187:A:C5'	1:0:188:C:OP2	2.67	0.42
1:0:344:C:H2'	1:0:345:G:O4'	2.19	0.42
1:0:676:C:N4	1:0:677:C:N4	2.68	0.42
1:0:1025:C:H2'	1:0:1026:U:C6	2.55	0.42
1:0:1559:A:C1'	39:0:5067:HOH:O	2.63	0.42
1:0:1847:A:H2'	1:0:1848:G:O4'	2.20	0.42
1:0:2034:U:H4'	39:0:5144:HOH:O	2.20	0.42
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.42
1:0:2289:G:C2'	1:0:2290:U:H5'	2.49	0.42
1:0:2591:C:H2'	1:0:2592:G:C5'	2.49	0.42
1:0:2750:G:H2'	1:0:2751:C:H6	1.84	0.42
2:A:100:PRO:HG2	2:A:103:VAL:HG21	2.01	0.42
9:H:32:ALA:H	9:H:69:ARG:NH1	2.17	0.42
30:3:64:LYS:HB3	30:3:65:THR:H	1.61	0.42
31:9:27:C:O5'	31:9:27:C:H6	2.03	0.42
31:9:112:U:H2'	31:9:113:C:H5'	2.01	0.42
1:0:25:A:H1'	1:0:519:A:C2	2.55	0.42
1:0:74:G:H2'	1:0:75:U:C6	2.55	0.42
1:0:106:A:H1'	39:0:4714:HOH:O	2.19	0.42
1:0:137:U:H3'	1:0:139:C:H41	1.85	0.42
1:0:208:C:C6	1:0:208:C:C3'	3.03	0.42
1:0:749:C:O2'	1:0:750:A:H5'	2.20	0.42
1:0:820:G:N7	2:A:171:LYS:HB2	2.35	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.20	0.42
1:0:1029:U:O2'	1:0:1273:C:OP1	2.37	0.42
1:0:1448:A:N7	1:0:1506:U:C2	2.88	0.42
1:0:1879:U:H1'	39:0:8121:HOH:O	2.20	0.42
1:0:2044:G:H2'	1:0:2045:G:O5'	2.19	0.42
4:C:22:PHE:HD2	4:C:119:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:118:THR:O	4:C:136:VAL:HG13	2.20	0.42
1:0:10:U:C4	1:0:532:A:N7	2.88	0.41
1:0:325:U:H2'	1:0:326:G:H8	1.85	0.41
1:0:640:G:C5	1:0:641:G:N7	2.88	0.41
1:0:657:G:H2'	1:0:658:C:H6	1.85	0.41
1:0:1001:U:O2'	1:0:1002:G:H5'	2.20	0.41
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.41
1:0:1505:U:H6	1:0:1505:U:H2'	1.76	0.41
1:0:1884:G:O6	2:A:190:ARG:HD2	2.20	0.41
1:0:1969:A:N7	1:0:1970:G:C6	2.88	0.41
1:0:2072:G:H3'	1:0:2073:G:H5"	2.01	0.41
1:0:2543:G:O3'	1:0:2590:U:H5'	2.20	0.41
1:0:909:U:H5	39:0:6389:HOH:O	2.03	0.41
1:0:1262:C:H1'	24:W:120:PRO:CG	2.50	0.41
1:0:1391:G:H21	1:0:1434:A:H5"	1.85	0.41
1:0:1396:C:H1'	17:P:1:THR:O	2.19	0.41
1:0:2042:U:H1'	39:0:7090:HOH:O	2.20	0.41
1:0:2291:A:H2'	1:0:2291:A:N3	2.35	0.41
1:0:2549:C:O2'	1:0:2550:U:H5'	2.20	0.41
7:F:1:PRO:HB2	39:F:5897:HOH:O	2.20	0.41
9:H:54:VAL:HG13	9:H:162:PRO:HG3	2.01	0.41
13:L:90:ARG:HA	13:L:119:THR:HB	2.01	0.41
1:0:24:G:C2	1:0:518:G:N3	2.88	0.41
1:0:45:A:N6	1:0:147:G:C4	2.89	0.41
1:0:109:U:O2	1:0:109:U:C2'	2.68	0.41
1:0:317:A:C5'	39:0:8405:HOH:O	2.68	0.41
1:0:422:G:C6	1:0:2446:G:C6	3.08	0.41
1:0:913:A:H8	1:0:913:A:O5'	2.03	0.41
1:0:1528:A:H61	1:0:1663:G:H1'	1.85	0.41
1:0:1758:U:O2'	1:0:1759:A:H5'	2.20	0.41
1:0:1833:U:O2'	1:0:1834:C:H5'	2.19	0.41
1:0:1988:C:H2'	1:0:1989:G:O4'	2.20	0.41
1:0:2067:A:C4	1:0:2068:G:C8	3.08	0.41
1:0:2250:G:H2'	1:0:2251:G:C8	2.54	0.41
1:0:2278:U:H5'	39:0:4608:HOH:O	2.20	0.41
1:0:2307:A:H8	1:0:2307:A:O5'	2.03	0.41
1:0:2379:G:H4'	1:0:2380:A:H3'	2.01	0.41
1:0:2486:A:H2	37:0:9101:MUL:C22	2.32	0.41
1:0:2735:U:H2'	1:0:2736:U:H6	1.83	0.41
37:0:9101:MUL:H131	37:0:9101:MUL:H4	1.78	0.41
2:A:53:ALA:HB1	39:A:1902:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:228:ALA:HA	4:C:229:PRO:HD3	1.90	0.41
9:H:46:TYR:HA	9:H:47:PRO:HD3	1.90	0.41
15:N:108:SER:HA	15:N:109:PRO:HD3	1.81	0.41
19:R:59:PHE:O	19:R:63:ASN:HB3	2.19	0.41
24:W:129:LYS:NZ	31:9:87:U:H2'	2.34	0.41
1:0:182:G:H2'	1:0:183:A:H8	1.86	0.41
1:0:360:A:H2'	1:0:361:C:C6	2.56	0.41
1:0:472:A:N1	1:0:888:U:O2'	2.43	0.41
1:0:559:U:H2'	1:0:560:U:O4'	2.20	0.41
1:0:656:G:H1	1:0:749:C:H42	1.67	0.41
1:0:1061:C:H1'	1:0:2283:G:O6	2.21	0.41
1:0:1150:A:H3'	1:0:1151:G:C5'	2.51	0.41
1:0:1649:G:H5'	39:0:6234:HOH:O	2.20	0.41
1:0:1760:G:P	1:0:1777:G:H22	2.43	0.41
1:0:2374:G:H2'	1:0:2375:A:C8	2.55	0.41
1:0:2787:C:H2'	1:0:2788:A:O4'	2.20	0.41
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.57	0.41
1:0:36:C:C2	1:0:447:A:C2	3.09	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
1:0:871:G:C6	1:0:872:U:C4	3.09	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1124:A:H2'	1:0:1124:A:N3	2.34	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.55	0.41
1:0:1486:A:N6	39:0:3379:HOH:O	2.49	0.41
1:0:1748:U:C5	1:0:1749:U:C4	3.08	0.41
1:0:1788:U:O2'	1:0:1789:G:H5'	2.20	0.41
1:0:1929:G:H1'	39:0:4103:HOH:O	2.20	0.41
1:0:2035:C:O5'	1:0:2035:C:H6	2.03	0.41
1:0:2059:U:C2	1:0:2060:A:C8	3.08	0.41
31:9:104:A:H2'	31:9:105:A:H5'	2.03	0.41
1:0:39:G:C2	1:0:444:C:O2	2.74	0.41
1:0:786:G:H1'	1:0:1488:U:O2	2.20	0.41
1:0:822:C:O2	1:0:822:C:C2'	2.68	0.41
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.41
1:0:1015:C:C2	1:0:1016:U:C5	3.09	0.41
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
1:0:1521:C:H2'	1:0:1522:A:O4'	2.21	0.41
1:0:1592:G:C5	1:0:1593:C:C4	3.08	0.41
1:0:1625:U:H5"	39:0:5289:HOH:O	2.20	0.41
1:0:2055:A:H4'	39:0:7274:HOH:O	2.20	0.41
1:0:2361:A:H8	1:0:2361:A:OP2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:43:VAL:HG13	25:X:76:ARG:NH1	2.35	0.41
1:0:210:U:H2'	1:0:211:U:H6	1.86	0.41
1:0:217:C:H2'	1:0:218:C:O4'	2.21	0.41
1:0:317:A:H5'	39:0:8405:HOH:O	2.21	0.41
1:0:372:A:O2'	1:0:373:G:H5'	2.20	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.20	0.41
1:0:686:A:O2'	1:0:747:G:H4'	2.21	0.41
1:0:1189:A:O2'	1:0:1208:C:H2'	2.20	0.41
1:0:1566:C:H2'	1:0:1567:G:H8	1.84	0.41
1:0:1679:C:O2	1:0:1679:C:H2'	2.21	0.41
1:0:1757:U:H6	1:0:1757:U:O5'	2.04	0.41
1:0:2409:C:O2'	1:0:2410:G:H5'	2.21	0.41
2:A:217:ARG:HG2	2:A:229:ALA:HB2	2.03	0.41
24:W:149:LEU:HG	24:W:153:MET:HE2	2.03	0.41
31:9:73:A:H2'	31:9:74:G:O4'	2.20	0.41
1:0:313:U:H2'	1:0:314:G:C5'	2.50	0.41
1:0:395:A:H3'	1:0:397:A:N7	2.36	0.41
1:0:407:A:C2	1:0:408:A:C4	3.08	0.41
1:0:765:G:H4'	4:C:69:HIS:HB2	2.02	0.41
1:0:841:A:C8	1:0:843:A:C8	3.08	0.41
1:0:960:G:H4'	39:0:7253:HOH:O	2.19	0.41
1:0:1013:A:H5"	1:0:2302:A:H61	1.86	0.41
1:0:1202:A:C2'	1:0:1203:G:H5'	2.51	0.41
1:0:1283:G:H2'	1:0:1284:G:O4'	2.20	0.41
1:0:1297:U:P	39:0:3033:HOH:O	2.78	0.41
1:0:1355:A:H2'	1:0:1355:A:N3	2.36	0.41
1:0:1359:U:O5'	1:0:1360:C:H5"	2.21	0.41
1:0:1597:A:O4'	17:P:95:GLU:HG2	2.21	0.41
1:0:1597:A:C4	1:0:1598:A:C8	3.09	0.41
1:0:1902:G:N2	1:0:1936:C:C2	2.89	0.41
1:0:2498:C:C2'	1:0:2499:U:H5'	2.50	0.41
4:C:133:ARG:NH2	39:C:5086:HOH:O	2.53	0.41
7:F:58:GLU:HB3	14:M:8:ILE:HG23	2.03	0.41
12:K:20:CYS:HB2	12:K:29:LEU:HG	2.03	0.41
15:N:151:ASP:HB3	39:N:3251:HOH:O	2.20	0.41
1:0:57:C:H4'	23:V:34:GLN:HE22	1.84	0.41
1:0:61:G:N1	1:0:86:A:N6	2.69	0.41
1:0:130:C:O2'	1:0:131:A:N7	2.48	0.41
1:0:268:U:C4	1:0:269:G:C6	3.09	0.41
1:0:339:A:N6	39:0:6198:HOH:O	2.51	0.41
1:0:644:G:H1'	39:0:5820:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:861:A:H1'	1:0:1488:U:O4	2.20	0.41
1:0:871:G:C5	1:0:872:U:C4	3.09	0.41
1:0:876:A:C6	1:0:878:G:C8	3.08	0.41
1:0:918:G:C2	1:0:926:A:C2	3.09	0.41
1:0:944:G:H21	24:W:44:MET:CE	2.34	0.41
1:0:959:C:O2	1:0:1005:A:N6	2.54	0.41
1:0:1111:U:H2'	1:0:1112:G:C8	2.55	0.41
1:0:1175:G:H1'	1:0:1193:A:C4	2.56	0.41
1:0:1257:C:O2'	1:0:1258:G:H5'	2.21	0.41
1:0:1299:G:N2	39:0:3448:HOH:O	2.54	0.41
1:0:1338:U:H2'	1:0:1339:G:O4'	2.20	0.41
1:0:1506:U:H6	1:0:1506:U:H5'	1.86	0.41
1:0:1531:U:H1'	1:0:1661:A:C2	2.56	0.41
1:0:1608:G:O2'	1:0:1609:C:H5'	2.21	0.41
1:0:1611:G:C2	1:0:1612:A:N7	2.89	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.69	0.41
1:0:1689:A:OP2	1:0:1689:A:H8	2.04	0.41
1:0:1851:G:O2'	1:0:1852:A:H5'	2.21	0.41
1:0:1881:A:OP1	2:A:199:HIS:HE1	2.04	0.41
1:0:1992:U:C2	1:0:1994:A:OP2	2.73	0.41
1:0:2385:G:C4	1:0:2386:U:C5	3.09	0.41
1:0:2455:A:H2'	1:0:2456:A:O4'	2.21	0.41
1:0:2590:U:H2'	1:0:2591:C:H5'	2.01	0.41
1:0:2624:A:O2'	1:0:2625:C:H5'	2.20	0.41
1:0:2629:C:O2'	1:0:2630:G:H5'	2.21	0.41
1:0:2694:A:C6	1:0:2702:A:C8	3.09	0.41
1:0:2904:U:C5	1:0:2905:A:N7	2.89	0.41
2:A:199:HIS:CD2	2:A:201:PHE:H	2.37	0.41
3:B:120:ASP:OD2	3:B:123:ALA:HB3	2.21	0.41
31:9:49:G:H2'	31:9:50:G:O4'	2.21	0.41
31:9:73:A:C6	31:9:74:G:C6	3.09	0.41
1:0:23:G:H8	1:0:23:G:O5'	2.03	0.41
1:0:36:C:N3	1:0:447:A:C2	2.89	0.41
1:0:73:U:O5'	1:0:73:U:H6	2.03	0.41
1:0:204:A:H2'	1:0:205:U:H5'	2.02	0.41
1:0:334:G:H2'	1:0:335:U:O4'	2.21	0.41
1:0:361:C:H2'	1:0:362:G:C8	2.56	0.41
1:0:426:G:H5"	39:0:7523:HOH:O	2.20	0.41
1:0:545:G:N1	1:0:612:U:O2	2.54	0.41
1:0:629:A:H2'	1:0:630:A:H5'	2.03	0.41
1:0:822:C:O2	1:0:823:U:C5	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1156:C:H3'	1:0:1156:C:C6	2.56	0.41
1:0:1274:A:N6	1:0:1275:C:N4	2.69	0.41
1:0:1644:C:C4	1:0:1645:U:C5	3.09	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
1:0:2017:U:H2'	1:0:2018:A:C8	2.55	0.41
1:0:2106:C:O5'	1:0:2106:C:H6	2.04	0.41
1:0:2594:C:O2'	1:0:2595:U:H5'	2.21	0.41
1:0:2732:U:H2'	1:0:2733:U:C6	2.56	0.41
1:0:2791:U:H1'	1:0:2792:A:H5"	2.02	0.41
4:C:118:THR:HG23	4:C:231:ARG:O	2.21	0.41
14:M:180:SER:HB3	39:M:3219:HOH:O	2.21	0.41
1:0:285:A:C2	1:0:368:C:H4'	2.56	0.40
1:0:731:U:H6	1:0:731:U:O5'	2.03	0.40
1:0:958:G:H2'	1:0:959:C:C6	2.56	0.40
1:0:1044:C:H5	39:0:6095:HOH:O	2.02	0.40
1:0:1175:G:H1'	1:0:1193:A:C8	2.56	0.40
1:0:1473:U:H1'	28:1:41:LYS:HE2	2.02	0.40
1:0:1521:C:O2'	1:0:1522:A:H5'	2.21	0.40
1:0:1678:A:C4	1:0:1679:C:C6	3.09	0.40
1:0:1703:G:C2	1:0:1716:A:C4	3.09	0.40
1:0:2057:U:H5	39:0:4741:HOH:O	2.04	0.40
1:0:2622:A:H1'	39:0:8784:HOH:O	2.20	0.40
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.40
39:0:6384:HOH:O	21:T:53:GLY:HA3	2.22	0.40
2:A:121:ALA:O	2:A:124:VAL:HG22	2.21	0.40
4:C:29:ASP:HB2	16:O:3:THR:HG22	2.03	0.40
5:D:67:ASP:HA	5:D:68:PRO:HD3	1.97	0.40
7:F:2:VAL:HG22	7:F:57:GLU:OE1	2.21	0.40
21:T:1:SER:OG	21:T:2:LYS:N	2.54	0.40
22:U:49:LEU:HD13	22:U:51:TRP:HE1	1.86	0.40
1:0:154:C:C2	1:0:155:C:C5	3.09	0.40
1:0:536:A:H3'	39:0:3958:HOH:O	2.21	0.40
1:0:793:A:H2'	1:0:794:U:O4'	2.20	0.40
1:0:1310:U:OP2	4:C:168:ARG:NH1	2.55	0.40
1:0:1310:U:P	4:C:168:ARG:HH11	2.44	0.40
1:0:1572:A:C2	1:0:1573:A:C4	3.10	0.40
1:0:2003:U:H4'	1:0:2004:U:H5	1.86	0.40
1:0:2293:G:H2'	1:0:2294:C:O5'	2.21	0.40
1:0:2321:A:H1'	1:0:2322:U:H2'	2.02	0.40
1:0:2582:G:C2	1:0:2583:A:C8	3.09	0.40
1:0:2597:U:H2'	1:0:2598:U:H5'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2626:C:H2'	1:0:2627:G:H8	1.86	0.40
1:0:2731:G:O2'	1:0:2732:U:H5'	2.21	0.40
1:0:2757:A:C2'	1:0:2758:G:H5'	2.51	0.40
14:M:84:LYS:HA	30:3:46:ILE:O	2.21	0.40
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.51	0.40
27:Z:70:ARG:HD3	27:Z:83:TYR:HB2	2.04	0.40
30:3:11:CYS:HB2	30:3:20:HIS:NE2	2.36	0.40
1:0:12:U:H2'	1:0:13:G:C5'	2.45	0.40
1:0:35:U:H5'	4:C:47:GLY:O	2.21	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.57	0.40
1:0:489:A:H2'	1:0:490:C:O4'	2.21	0.40
1:0:700:A:H2	16:O:69:VAL:HG23	1.87	0.40
1:0:863:G:N3	1:0:1459:A:H2	2.19	0.40
1:0:1059:G:C8	1:0:2491:G:H4'	2.56	0.40
1:0:1421:C:C2	1:0:1422:U:C5	3.09	0.40
1:0:1448:A:C8	1:0:1506:U:C2	3.09	0.40
1:0:1477:C:C5'	1:0:1868:G:C5'	3.00	0.40
1:0:1704:G:O3'	17:P:59:ARG:NH1	2.55	0.40
1:0:1988:C:H5	39:0:3572:HOH:O	2.04	0.40
1:0:2316:G:O2'	1:0:2462:G:O6	2.38	0.40
1:0:2319:C:C3'	1:0:2320:U:H5"	2.52	0.40
1:0:2505:G:H2'	1:0:2506:A:H5'	2.04	0.40
1:0:2722:G:C2	1:0:2761:A:N1	2.89	0.40
1:0:2768:A:H3'	1:0:2768:A:N3	2.35	0.40
1:0:2807:U:OP2	3:B:28:SER:HB2	2.21	0.40
1:0:2838:A:OP1	3:B:307:ARG:NH2	2.54	0.40
39:0:5466:HOH:O	3:B:254:GLN:HG3	2.20	0.40
3:B:215:VAL:O	3:B:219:GLY:HA2	2.22	0.40
4:C:93:LYS:O	4:C:98:ARG:NH2	2.55	0.40
27:Z:49:ARG:O	27:Z:53:ILE:HG13	2.21	0.40
31:9:110:G:C5	31:9:111:U:C5	3.09	0.40
1:0:187:A:N3	1:0:187:A:H2'	2.37	0.40
1:0:814:G:N1	1:0:815:U:C2	2.90	0.40
1:0:1400:C:H2'	1:0:1401:G:H5'	2.03	0.40
1:0:1422:U:H2'	1:0:1423:C:C6	2.57	0.40
1:0:1513:C:H5'	1:0:1574:C:O2'	2.22	0.40
1:0:1587:U:H2'	1:0:1588:G:O4'	2.21	0.40
1:0:1676:G:C5	1:0:1677:U:N3	2.90	0.40
1:0:1747:A:O3'	1:0:2584:G:H5'	2.21	0.40
1:0:1910:A:C2	1:0:2128:G:N3	2.90	0.40
1:0:2055:A:H2'	1:0:2056:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2128:G:H2'	1:0:2129:U:O4'	2.22	0.40
1:0:2294:C:N4	1:0:2314:G:H1	2.19	0.40
1:0:2428:G:C4'	39:0:4707:HOH:O	2.70	0.40
1:0:2439:C:O2'	1:0:2440:C:H5'	2.22	0.40
1:0:2537:G:H5"	1:0:2538:A:C5'	2.51	0.40
1:0:2593:C:O2'	1:0:2594:C:H5'	2.22	0.40
12:K:14:LYS:HB2	12:K:45:PRO:HG2	2.03	0.40
31:9:56:A:C3'	31:9:57:A:H5"	2.52	0.40
1:0:365:G:H2'	1:0:366:U:O4'	2.21	0.40
1:0:387:G:H2'	1:0:388:G:H5'	2.03	0.40
1:0:472:A:H5'	28:1:35:SER:OG	2.22	0.40
1:0:818:A:C6	1:0:819:A:N1	2.90	0.40
1:0:951:A:H2'	1:0:952:G:H5'	2.04	0.40
1:0:1531:U:O2	1:0:1661:A:C2	2.74	0.40
1:0:1574:C:C6	1:0:1575:C:H5	2.40	0.40
1:0:1592:G:O2'	1:0:1593:C:O4'	2.39	0.40
1:0:1679:C:O2	1:0:1685:A:C2	2.75	0.40
1:0:1682:A:H1'	1:0:1685:A:OP2	2.22	0.40
1:0:1695:G:H1'	28:1:9:GLY:HA3	2.02	0.40
1:0:1812:G:H3'	1:0:1812:G:OP1	2.21	0.40
1:0:1893:C:H2'	1:0:1894:C:H5'	2.03	0.40
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.40
1:0:2468:A:N6	30:3:50:GLY:HA2	2.36	0.40
1:0:2867:G:H2'	1:0:2868:C:C6	2.57	0.40
39:0:4064:HOH:O	24:W:9:GLY:HA3	2.21	0.40
6:E:154:ILE:HD11	6:E:157:LYS:HE2	2.04	0.40
12:K:125:ALA:C	12:K:127:ALA:H	2.25	0.40
15:N:113:SER:HB3	39:9:5851:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	235/237 (99%)	210 (89%)	20 (8%)	5 (2%)	7	37
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	17	56
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	13	49
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	6	35
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	25	64
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	24
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	25	64
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	44
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	46
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	19	58
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	22	61
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	5	31
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	6	35
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	61
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	6	35
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	22	61
20	S	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	T	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	U	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
23	V	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	139 (91%)	13 (9%)	0	100	100
25	X	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	47
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	22	61
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	5	29
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	39
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	2	19
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	12	47

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	SER
3	B	306	LYS
7	F	61	MET
11	J	5	GLU
14	M	80	GLY
26	Y	157	ILE
30	3	27	SER
4	C	205	ARG
7	F	91	VAL
7	F	101	ALA
15	N	167	ASP
27	Z	92	SER
30	3	47	GLY
30	3	48	ASN
2	A	34	ASP
2	A	122	SER
4	C	79	ARG
4	C	208	ALA
5	D	137	PRO
6	E	122	THR
11	J	89	HIS
14	M	82	ARG
15	N	70	GLY
15	N	139	TRP
18	Q	48	PRO
28	1	54	ALA
5	D	56	ARG
9	H	171	GLY
10	I	108	HIS
12	K	10	GLN
13	L	37	LYS
14	M	71	SER
15	N	154	LEU
17	P	77	ALA
18	Q	18	PRO
27	Z	70	ARG
30	3	64	LYS
5	D	46	GLY
2	A	37	VAL
7	F	104	ALA
2	A	88	ILE
14	M	110	PRO
19	R	114	VAL

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Mol	Chain	Res	Type
14	M	35	GLY
3	B	2	GLN
25	X	52	PRO
3	B	185	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	179/179 (100%)	169 (94%)	10 (6%)	21	57
3	B	282/282 (100%)	263 (93%)	19 (7%)	16	50
4	C	193/193 (100%)	179 (93%)	14 (7%)	14	46
5	D	117/148 (79%)	109 (93%)	8 (7%)	16	49
6	E	152/152 (100%)	139 (91%)	13 (9%)	10	38
7	F	93/93 (100%)	91 (98%)	2 (2%)	52	79
8	G	27/282 (10%)	23 (85%)	4 (15%)	3	14
9	H	134/145 (92%)	121 (90%)	13 (10%)	8	31
10	I	58/58 (100%)	56 (97%)	2 (3%)	37	70
11	J	118/118 (100%)	112 (95%)	6 (5%)	24	60
12	K	106/106 (100%)	99 (93%)	7 (7%)	16	51
13	L	113/127 (89%)	105 (93%)	8 (7%)	14	47
14	M	158/158 (100%)	146 (92%)	12 (8%)	13	45
15	N	149/149 (100%)	135 (91%)	14 (9%)	8	33
16	O	93/93 (100%)	88 (95%)	5 (5%)	22	58
17	P	113/113 (100%)	110 (97%)	3 (3%)	44	75
18	Q	79/79 (100%)	77 (98%)	2 (2%)	47	77
19	R	117/117 (100%)	111 (95%)	6 (5%)	24	60
20	S	71/71 (100%)	68 (96%)	3 (4%)	30	65
21	T	105/105 (100%)	99 (94%)	6 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/44 (100%)	40 (91%)	4 (9%)	9	34
23	V	51/51 (100%)	47 (92%)	4 (8%)	12	43
24	W	130/130 (100%)	127 (98%)	3 (2%)	50	78
25	X	66/66 (100%)	60 (91%)	6 (9%)	9	34
26	Y	120/120 (100%)	114 (95%)	6 (5%)	24	60
27	Z	60/60 (100%)	57 (95%)	3 (5%)	24	60
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	39 (93%)	3 (7%)	14	47
30	3	79/79 (100%)	73 (92%)	6 (8%)	13	45
All	All	3095/3410 (91%)	2903 (94%)	192 (6%)	18	53

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	30	ARG
2	A	43	VAL
2	A	51	ARG
2	A	68	ILE
2	A	78	ASP
2	A	131	HIS
2	A	179	MET
2	A	184	THR
2	A	217	ARG
3	B	7	ARG
3	B	20	THR
3	B	27	ASN
3	B	49	THR
3	B	71	VAL
3	B	97	LEU
3	B	98	THR
3	B	103	ASP
3	B	144	THR
3	B	145	HIS
3	B	156	LYS
3	B	162	MET
3	B	171	VAL
3	B	190	MET
3	B	254	GLN

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Mol	Chain	Res	Type
3	B	256	GLN
3	B	277	GLU
3	B	278	PRO
3	B	301	VAL
4	C	17	ASP
4	C	29	ASP
4	C	76	ARG
4	C	78	ARG
4	C	131	PHE
4	C	135	GLU
4	C	136	VAL
4	C	148	VAL
4	C	184	ARG
4	C	187	ARG
4	C	223	LEU
4	C	236	THR
4	C	240	LEU
4	C	243	VAL
5	D	50	VAL
5	D	52	THR
5	D	58	VAL
5	D	73	VAL
5	D	77	ASP
5	D	128	LEU
5	D	136	ARG
5	D	172	VAL
6	E	7	ILE
6	E	10	ASP
6	E	36	PRO
6	E	39	ASP
6	E	40	VAL
6	E	61	THR
6	E	100	ASP
6	E	102	VAL
6	E	115	ARG
6	E	133	VAL
6	E	156	ASP
6	E	159	VAL
6	E	164	ASP
7	F	12	LEU
7	F	55	GLN
8	G	12	ILE

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Mol	Chain	Res	Type
8	G	64	ASN
8	G	65	THR
8	G	73	ASP
9	H	42	ASP
9	H	48	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	91	ARG
9	H	122	LYS
9	H	126	THR
9	H	143	VAL
9	H	154	ARG
9	H	157	TYR
9	H	169	GLU
9	H	173	GLU
10	I	82	THR
10	I	126	THR
11	J	39	VAL
11	J	45	VAL
11	J	47	THR
11	J	52	GLN
11	J	107	ASN
11	J	130	VAL
12	K	10	GLN
12	K	16	SER
12	K	19	THR
12	K	44	HIS
12	K	93	ASN
12	K	109	LEU
12	K	115	ARG
13	L	32	ASP
13	L	35	ARG
13	L	70	ASP
13	L	80	ASP
13	L	102	ASP
13	L	104	ASP
13	L	105	TYR
13	L	145	LEU
14	M	10	ASP
14	M	23	LEU
14	M	68	ARG

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Mol	Chain	Res	Type
14	M	73	ARG
14	M	77	HIS
14	M	81	ARG
14	M	89	THR
14	M	91	ILE
14	M	99	ARG
14	M	123	ASP
14	M	164	THR
14	M	180	SER
15	N	2	THR
15	N	22	GLN
15	N	26	LEU
15	N	43	VAL
15	N	49	THR
15	N	56	ASP
15	N	74	PRO
15	N	134	ASP
15	N	135	VAL
15	N	139	TRP
15	N	162	ASP
15	N	171	HIS
15	N	177	GLU
15	N	180	LEU
16	O	25	VAL
16	O	36	PRO
16	O	43	VAL
16	O	57	THR
16	O	69	VAL
17	P	16	VAL
17	P	91	LYS
17	P	98	ILE
18	Q	18	PRO
18	Q	57	ASP
19	R	13	THR
19	R	52	GLU
19	R	55	GLN
19	R	73	ASP
19	R	110	THR
19	R	125	ARG
20	S	17	ASP
20	S	30	ASP
20	S	44	GLN

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Mol	Chain	Res	Type
21	T	5	ASP
21	T	39	ASN
21	T	71	VAL
21	T	96	VAL
21	T	97	ARG
21	T	115	GLU
22	U	11	THR
22	U	25	ASP
22	U	32	CYS
22	U	53	ASP
23	V	6	GLN
23	V	28	LEU
23	V	49	LEU
23	V	65	ASP
24	W	4	LEU
24	W	38	THR
24	W	146	ILE
25	X	44	ASP
25	X	52	PRO
25	X	72	VAL
25	X	79	GLU
25	X	82	GLU
25	X	88	GLU
26	Y	117	LEU
26	Y	154	ARG
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
26	Y	219	GLU
27	Z	88	PHE
27	Z	92	SER
27	Z	103	VAL
29	2	18	ASN
29	2	46	ASP
29	2	48	ASP
30	3	3	MET
30	3	7	PHE
30	3	21	GLU
30	3	49	ASP
30	3	55	VAL
30	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69)

such sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	221	GLN
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
4	C	73	GLN
4	C	103	ASN
4	C	129	HIS
5	D	103	ASN
5	D	133	ASN
6	E	55	ASN
6	E	143	GLN
6	E	150	GLN
7	F	80	GLN
8	G	64	ASN
9	H	59	GLN
9	H	73	ASN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	23	ASN
12	K	93	ASN
13	L	18	HIS
13	L	41	HIS
13	L	113	GLN
14	M	24	GLN
14	M	29	GLN
14	M	58	GLN
14	M	170	ASN
15	N	40	ASN
15	N	107	ASN
15	N	153	GLN
16	O	100	GLN
17	P	28	GLN
17	P	50	GLN
17	P	88	GLN
17	P	118	GLN
19	R	94	ASN
19	R	98	ASN

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Mol	Chain	Res	Type
19	R	117	HIS
20	S	9	HIS
20	S	44	GLN
20	S	53	ASN
21	T	7	GLN
22	U	39	ASN
22	U	48	ASN
23	V	34	GLN
23	V	60	GLN
24	W	59	GLN
24	W	110	GLN
24	W	141	HIS
25	X	23	HIS
26	Y	129	ASN
26	Y	131	GLN
26	Y	134	HIS
26	Y	149	GLN
26	Y	189	ASN
27	Z	61	HIS
28	1	16	HIS
28	1	28	HIS
29	2	16	ASN
29	2	18	ASN
29	2	45	ASN
30	3	15	ASN
30	3	18	GLN
30	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	263 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	280 (9%)	20 (0%)

All (280) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A

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Mol	Chain	Res	Type
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	204	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	318	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G

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Mol	Chain	Res	Type
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	702	G
1	0	735	C
1	0	736	A
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	836	G
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	882	A
1	0	885	G
1	0	898	G
1	0	905	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1011	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1078	A
1	0	1081	A
1	0	1083	C
1	0	1088	A
1	0	1102	C
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1121	G
1	0	1129	C
1	0	1130	U
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1234	U
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	G

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Mol	Chain	Res	Type
1	0	1342	C
1	0	1353	C
1	0	1354	G
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1427	A
1	0	1460	G
1	0	1474	C
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	1535	G
1	0	1559	A
1	0	1592	G
1	0	1605	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1742	A
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1819	G

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Mol	Chain	Res	Type
1	0	1820	G
1	0	1829	A
1	0	1838	U
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	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	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2104	C
1	0	2110	G
1	0	2134	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	2320	U
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2420	G
1	0	2422	U
1	0	2443	C
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2469	A
1	0	2474	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2607	U
1	0	2608	C
1	0	2609	G
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2792	A

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Mol	Chain	Res	Type
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	41	C
31	9	43	G
31	9	44	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	88	G
31	9	114	G
31	9	122	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	603	A
1	0	604	G
1	0	644	G
1	0	857	A
1	0	871	G
1	0	1080	C
1	0	1352	A
1	0	1377	C
1	0	1667	A
1	0	1730	G
1	0	1979	G
1	0	2011	A

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Mol	Chain	Res	Type
1	0	2103	A
1	0	2467	A
1	0	2536	C
1	0	2718	C
1	0	2761	A
1	0	2791	U
31	9	65	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	UR3	0	2619	1	19,22,23	0.50	0	26,32,35	0.63	1 (3%)
1	1MA	0	628	1,34	16,25,26	1.39	3 (18%)	18,37,40	1.29	3 (16%)
1	PSU	0	2621	1	18,21,22	1.37	2 (11%)	22,30,33	1.25	3 (13%)
1	OMG	0	2588	1	18,26,27	1.13	2 (11%)	19,38,41	0.73	0
1	OMU	0	2587	1	19,22,23	0.36	0	26,31,34	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.29	1.42	1.36
1	0	628	1MA	C2-N3	3.61	1.33	1.29
1	0	2588	OMG	C5-C6	-3.17	1.41	1.47
1	0	628	1MA	C6-N6	2.60	1.34	1.27
1	0	2621	PSU	C6-C5	2.58	1.38	1.35
1	0	2588	OMG	C8-N7	-2.51	1.30	1.35
1	0	628	1MA	C8-N7	-2.14	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.26	120.48	118.20
1	0	628	1MA	CM1-N1-C6	2.88	124.64	120.27
1	0	2621	PSU	C6-N1-C2	-2.81	119.81	122.68
1	0	628	1MA	N1-C2-N3	2.81	129.29	126.02
1	0	2621	PSU	O2-C2-N1	2.67	125.74	122.79
1	0	628	1MA	C5-C6-N1	2.56	117.72	113.90
1	0	2619	UR3	C4-N3-C2	2.29	126.72	124.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	628	1MA	1	0
1	0	2621	PSU	1	0
1	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 304 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	MUL	0	9101	-	36,36,36	1.47	5 (13%)	54,55,55	2.14	17 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	MUL	0	9101	-	-	3/18/79/79	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-5.30	1.39	1.52
37	0	9101	MUL	C5-C14	-2.91	1.53	1.56
37	0	9101	MUL	C12-C11	-2.86	1.53	1.55
37	0	9101	MUL	C10-C11	-2.81	1.53	1.56
37	0	9101	MUL	C9-C10	-2.07	1.53	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	0	9101	MUL	C13-C14-C5	-6.20	109.94	116.31
37	0	9101	MUL	O3-C21-C22	5.49	119.56	110.32
37	0	9101	MUL	C18-C12-C13	5.00	109.33	105.60
37	0	9101	MUL	C14-O3-C21	-3.79	110.79	117.92
37	0	9101	MUL	C8-C9-C4	3.49	111.41	106.56
37	0	9101	MUL	C1-C2-C3	-3.41	101.70	105.52
37	0	9101	MUL	C2-C1-C9	-3.32	101.13	105.61
37	0	9101	MUL	C4-C5-C6	3.30	109.76	106.61
37	0	9101	MUL	C6-C5-C14	-3.17	109.95	112.10
37	0	9101	MUL	C17-C10-C11	-3.00	109.77	112.11
37	0	9101	MUL	C9-C4-C5	-2.72	114.05	118.00
37	0	9101	MUL	C4-C9-C10	-2.69	111.91	116.04
37	0	9101	MUL	C8-C7-C6	-2.49	109.12	112.35
37	0	9101	MUL	O3-C14-C13	2.33	108.76	106.24
37	0	9101	MUL	C23-S1-C22	-2.18	98.06	101.71
37	0	9101	MUL	C12-C19-C20	-2.13	120.96	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	0	9101	MUL	C12-C11-C10	-2.03	112.59	114.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	0	9101	MUL	C13-C12-C19-C20
37	0	9101	MUL	O4-C21-C22-S1
37	0	9101	MUL	O3-C21-C22-S1

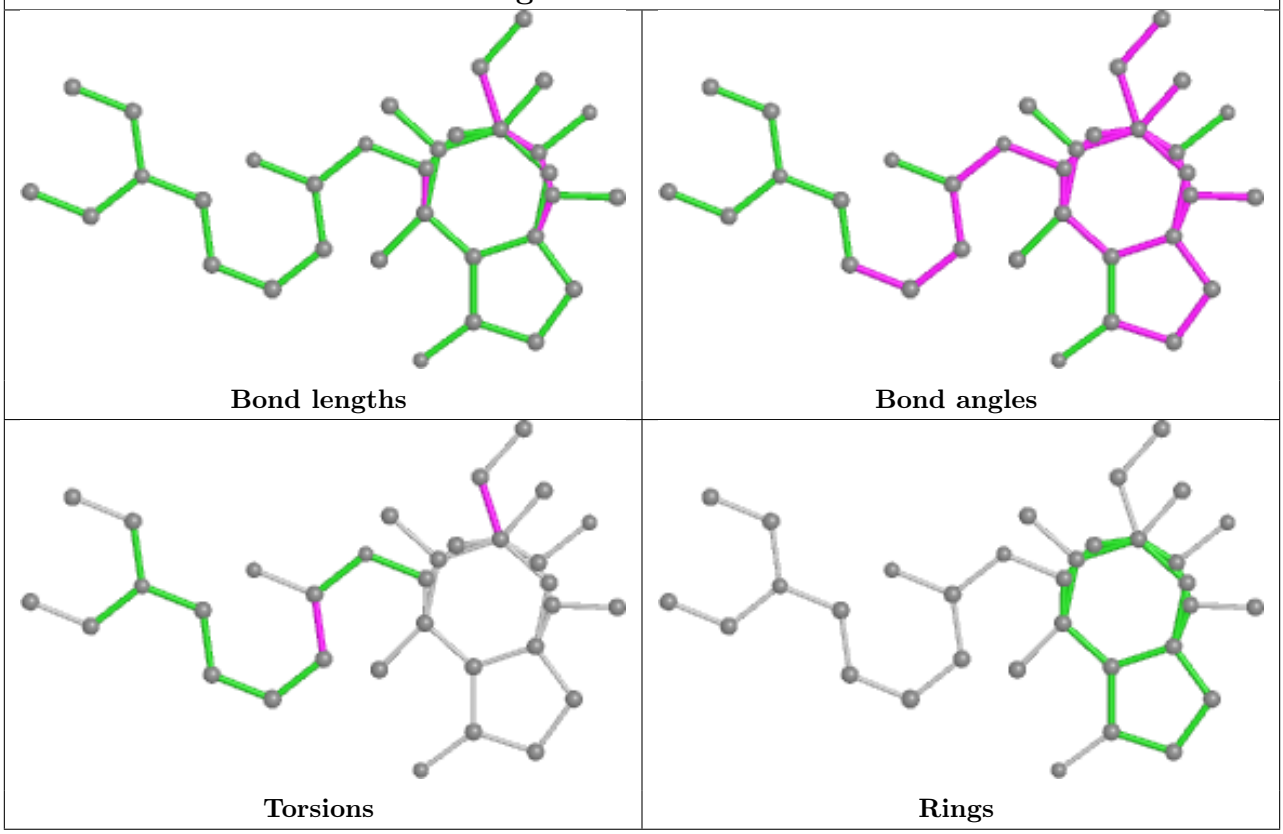
There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	MUL	17	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 then 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.

Ligand MUL 0 9101



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	2749/2923 (94%)	-0.66	3 (0%)	95	95	29, 74, 140, 200	0
2	A	237/237 (100%)	0.04	9 (3%)	40	26	43, 97, 143, 167	0
3	B	337/337 (100%)	-0.40	1 (0%)	94	92	40, 86, 129, 148	0
4	C	246/246 (100%)	-0.39	2 (0%)	86	78	41, 72, 103, 112	0
5	D	140/177 (79%)	1.10	37 (26%)	0	0	118, 160, 184, 191	0
6	E	172/172 (100%)	-0.13	3 (1%)	70	57	76, 104, 134, 146	0
7	F	119/119 (100%)	0.30	8 (6%)	17	10	74, 113, 153, 166	0
8	G	29/348 (8%)	1.00	6 (20%)	1	1	118, 140, 146, 150	0
9	H	160/177 (90%)	0.54	15 (9%)	8	4	77, 104, 146, 162	0
10	I	70/70 (100%)	1.85	32 (45%)	0	0	173, 199, 200, 200	0
11	J	142/142 (100%)	-0.28	0	100	100	55, 80, 104, 123	0
12	K	132/132 (100%)	-0.20	2 (1%)	73	61	54, 79, 112, 118	0
13	L	145/165 (87%)	0.66	26 (17%)	1	1	62, 121, 171, 175	0
14	M	194/194 (100%)	0.09	17 (8%)	10	5	49, 70, 145, 160	0
15	N	186/186 (100%)	0.48	13 (6%)	16	9	82, 118, 178, 187	0
16	O	115/115 (100%)	-0.44	0	100	100	66, 87, 105, 111	0
17	P	143/143 (100%)	-0.22	2 (1%)	75	63	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.02	4 (4%)	36	23	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.48	0	100	100	47, 72, 103, 112	0
20	S	81/81 (100%)	-0.05	2 (2%)	57	43	68, 93, 114, 130	0
21	T	119/119 (100%)	0.23	10 (8%)	11	6	69, 92, 136, 155	0
22	U	53/53 (100%)	0.09	1 (1%)	66	53	94, 114, 136, 145	0
23	V	65/65 (100%)	0.23	3 (4%)	32	20	79, 112, 164, 170	0
24	W	154/154 (100%)	-0.22	2 (1%)	77	65	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	82/82 (100%)	0.11	6 (7%) 15 9	63, 92, 125, 135	0
26	Y	142/142 (100%)	-0.33	2 (1%) 75 63	45, 73, 109, 134	0
27	Z	73/73 (100%)	5.32	53 (72%) 0 0	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.31	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.26	4 (8%) 10 5	48, 95, 145, 146	0
30	3	92/92 (100%)	6.09	79 (85%) 0 0	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.83	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.13	342 (5%) 28 16	29, 85, 168, 200	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	29.8
30	3	82	GLY	26.5
27	Z	35	SER	24.8
30	3	37	ASP	18.0
30	3	41	GLU	16.7
27	Z	46	SER	16.4
27	Z	43	GLY	15.4
30	3	34	LYS	15.1
27	Z	50	VAL	14.5
27	Z	45	VAL	14.2
30	3	32	GLY	14.1
27	Z	58	ASN	13.8
30	3	38	ARG	13.2
30	3	39	GLN	12.9
30	3	83	TRP	12.4
27	Z	44	ARG	12.4
27	Z	51	ALA	12.2
30	3	45	GLY	12.0
30	3	35	TRP	12.0
14	M	70	GLY	11.8
27	Z	59	GLU	11.4
30	3	33	MET	11.2
30	3	30	GLN	11.0
30	3	42	ARG	10.6
27	Z	54	GLU	10.5
30	3	81	GLU	10.4
27	Z	55	SER	10.4
30	3	40	ARG	10.2

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Mol	Chain	Res	Type	RSRZ
30	3	48	ASN	9.8
30	3	9	THR	9.7
30	3	43	ASN	9.6
27	Z	36	GLY	9.2
30	3	36	ILE	9.0
14	M	90	ARG	8.7
27	Z	49	ARG	8.6
30	3	62	THR	8.5
27	Z	47	ARG	8.4
14	M	89	THR	8.2
30	3	31	THR	8.2
30	3	44	SER	8.1
21	T	119	ALA	7.6
30	3	71	CYS	7.5
27	Z	68	GLU	7.5
27	Z	42	TYR	7.3
30	3	56	PRO	7.2
14	M	71	SER	7.2
27	Z	63	CYS	7.2
27	Z	38	PHE	7.1
30	3	27	SER	7.1
30	3	20	HIS	7.1
30	3	58	GLY	7.0
30	3	59	ASP	6.9
30	3	14	CYS	6.7
30	3	47	GLY	6.7
30	3	49	ASP	6.4
30	3	18	GLN	6.3
30	3	5	ARG	6.3
27	Z	37	ARG	6.2
5	D	69	ILE	6.2
30	3	73	GLU	6.2
27	Z	69	ASP	6.2
30	3	57	GLY	6.2
27	Z	53	ILE	6.2
13	L	106	VAL	6.2
30	3	22	VAL	6.1
27	Z	57	MET	6.1
27	Z	82	SER	6.0
30	3	72	GLY	6.0
30	3	23	GLU	5.9
14	M	86	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
27	Z	81	CYS	5.7
5	D	18	ILE	5.7
30	3	15	ASN	5.6
27	Z	48	ARG	5.6
10	I	74	ILE	5.6
30	3	10	TYR	5.5
30	3	8	ASN	5.5
5	D	134	LEU	5.5
27	Z	39	GLY	5.4
30	3	29	ARG	5.4
30	3	66	ASP	5.4
5	D	40	ILE	5.4
5	D	88	LEU	5.4
10	I	70	THR	5.4
27	Z	80	GLN	5.3
10	I	128	THR	5.2
30	3	16	GLU	5.1
30	3	78	HIS	5.1
30	3	80	ARG	5.1
30	3	19	GLU	5.1
30	3	84	ARG	5.1
30	3	21	GLU	4.9
30	3	67	LEU	4.9
7	F	106	ALA	4.9
30	3	28	GLY	4.8
15	N	84	THR	4.8
5	D	66	GLY	4.7
30	3	25	VAL	4.7
30	3	85	ALA	4.7
10	I	97	VAL	4.6
27	Z	65	ASN	4.6
10	I	106	GLN	4.6
30	3	74	CYS	4.5
14	M	77	HIS	4.5
27	Z	56	GLU	4.4
30	3	63	LYS	4.4
5	D	104	PHE	4.4
23	V	1	THR	4.4
30	3	69	TYR	4.4
10	I	117	THR	4.3
5	D	92	GLU	4.3
30	3	13	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
27	Z	67	GLY	4.2
27	Z	77	GLY	4.2
27	Z	88	PHE	4.2
30	3	11	CYS	4.2
30	3	75	GLY	4.2
30	3	55	VAL	4.2
10	I	103	ILE	4.2
15	N	119	GLN	4.1
26	Y	235	GLU	4.1
14	M	79	ALA	4.1
10	I	104	ALA	4.1
30	3	1	MET	4.1
30	3	68	LYS	4.1
30	3	60	LYS	4.0
5	D	93	LEU	4.0
10	I	100	VAL	4.0
2	A	82	VAL	3.9
8	G	73	ASP	3.9
25	X	7	GLU	3.9
30	3	17	HIS	3.9
27	Z	71	VAL	3.8
9	H	133	GLY	3.8
27	Z	52	GLU	3.8
5	D	27	ILE	3.8
30	3	76	LYS	3.8
21	T	117	ASP	3.8
30	3	46	ILE	3.8
9	H	76	LEU	3.8
10	I	94	ASP	3.8
27	Z	70	ARG	3.8
13	L	62	ALA	3.7
14	M	78	LYS	3.7
2	A	24	LYS	3.7
5	D	63	ILE	3.6
20	S	81	ILE	3.6
27	Z	103	VAL	3.6
7	F	75	ILE	3.6
30	3	61	PRO	3.6
27	Z	106	SER	3.6
14	M	80	GLY	3.6
5	D	26	GLY	3.6
30	3	91	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
8	G	66	LEU	3.5
13	L	140	VAL	3.5
14	M	76	ARG	3.5
25	X	10	VAL	3.4
13	L	61	ALA	3.4
5	D	130	VAL	3.4
27	Z	62	ALA	3.3
5	D	44	ILE	3.3
14	M	88	VAL	3.3
5	D	25	MET	3.3
10	I	73	LEU	3.3
29	2	41	HIS	3.3
13	L	76	LEU	3.3
27	Z	93	TYR	3.3
30	3	6	ARG	3.2
5	D	166	ILE	3.2
5	D	128	LEU	3.2
18	Q	95	GLU	3.2
8	G	27	ILE	3.2
13	L	107	LYS	3.2
13	L	49	SER	3.2
14	M	81	ARG	3.2
27	Z	86	TYR	3.2
30	3	65	THR	3.2
27	Z	40	ALA	3.1
30	3	77	ALA	3.1
7	F	49	PHE	3.1
10	I	111	LEU	3.1
5	D	61	PHE	3.1
15	N	172	PHE	3.1
27	Z	60	ASP	3.1
24	W	3	ALA	3.1
5	D	106	PHE	3.1
27	Z	78	ILE	3.1
15	N	179	LEU	3.1
27	Z	85	ASP	3.1
23	V	39	ALA	3.1
30	3	90	PHE	3.0
29	2	36	ASN	3.0
30	3	86	GLY	3.0
27	Z	66	CYS	3.0
21	T	99	THR	3.0

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Mol	Chain	Res	Type	RSRZ
27	Z	79	TRP	3.0
14	M	87	GLY	3.0
6	E	5	LEU	3.0
10	I	92	VAL	3.0
14	M	83	SER	3.0
5	D	89	PRO	3.0
21	T	40	VAL	2.9
27	Z	76	THR	2.9
10	I	68	PRO	2.9
21	T	42	VAL	2.9
10	I	71	ALA	2.9
8	G	69	ARG	2.9
10	I	112	LEU	2.9
7	F	99	THR	2.9
30	3	88	LEU	2.9
17	P	118	GLN	2.9
8	G	23	ILE	2.9
23	V	40	PRO	2.9
15	N	83	LEU	2.9
10	I	102	GLN	2.9
30	3	2	GLN	2.9
10	I	113	SER	2.9
13	L	97	VAL	2.9
9	H	97	VAL	2.8
10	I	109	PRO	2.8
5	D	90	LEU	2.8
10	I	110	ASP	2.8
10	I	93	ALA	2.8
15	N	81	ALA	2.8
15	N	166	ALA	2.8
29	2	48	ASP	2.8
5	D	95	THR	2.8
25	X	8	ARG	2.8
9	H	87	LYS	2.8
13	L	79	ASP	2.8
30	3	3	MET	2.8
13	L	60	GLU	2.8
15	N	175	LEU	2.7
5	D	135	VAL	2.7
5	D	84	LEU	2.7
27	Z	64	PRO	2.7
10	I	98	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
18	Q	64	GLU	2.7
1	0	735	C	2.7
10	I	127	CYS	2.6
10	I	99	GLN	2.6
5	D	57	THR	2.6
1	0	970	U	2.6
15	N	114	LYS	2.6
9	H	86	TYR	2.6
21	T	118	SER	2.5
30	3	24	LYS	2.5
5	D	91	ALA	2.5
10	I	108	HIS	2.5
9	H	66	GLU	2.5
8	G	63	ARG	2.5
2	A	88	ILE	2.5
2	A	36	ASP	2.5
13	L	120	LEU	2.5
9	H	53	ILE	2.5
10	I	72	GLU	2.5
5	D	87	ALA	2.5
10	I	132	VAL	2.5
7	F	15	ASP	2.5
5	D	160	ALA	2.5
5	D	64	ARG	2.5
7	F	17	LEU	2.4
5	D	43	GLU	2.4
5	D	165	PHE	2.4
15	N	145	ALA	2.4
13	L	123	ASP	2.4
30	3	92	GLU	2.4
15	N	101	VAL	2.4
14	M	1	ALA	2.4
7	F	91	VAL	2.4
27	Z	84	CYS	2.4
21	T	101	LEU	2.4
13	L	93	VAL	2.3
5	D	101	THR	2.3
15	N	178	THR	2.3
24	W	96	LEU	2.3
25	X	72	VAL	2.3
21	T	106	GLU	2.3
10	I	101	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
21	T	74	VAL	2.3
30	3	70	ARG	2.3
3	B	128	ILE	2.3
27	Z	89	THR	2.3
9	H	149	VAL	2.3
13	L	78	ALA	2.3
2	A	128	LEU	2.3
13	L	91	VAL	2.3
20	S	28	VAL	2.3
9	H	169	GLU	2.2
13	L	36	ASP	2.2
22	U	25	ASP	2.2
1	0	1169	U	2.2
27	Z	61	HIS	2.2
2	A	58	VAL	2.2
18	Q	75	ILE	2.2
6	E	100	ASP	2.2
9	H	85	ASP	2.2
5	D	24	HIS	2.2
5	D	47	GLN	2.2
7	F	96	ALA	2.2
10	I	119	ALA	2.2
13	L	124	ASP	2.2
5	D	17	ARG	2.2
10	I	105	GLU	2.2
13	L	99	GLU	2.2
12	K	109	LEU	2.2
13	L	130	ARG	2.2
5	D	129	ASP	2.2
12	K	132	VAL	2.2
25	X	85	VAL	2.2
6	E	118	ILE	2.2
9	H	25	GLY	2.2
13	L	108	VAL	2.1
13	L	122	ALA	2.1
2	A	69	LEU	2.1
4	C	63	SER	2.1
25	X	41	PHE	2.1
9	H	141	CYS	2.1
14	M	74	LYS	2.1
2	A	56	ALA	2.1
29	2	45	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
18	Q	85	ILE	2.1
13	L	39	GLU	2.1
15	N	95	ALA	2.1
9	H	50	ILE	2.1
2	A	91	GLY	2.1
13	L	50	GLY	2.0
13	L	66	VAL	2.0
5	D	68	PRO	2.0
10	I	66	GLY	2.0
9	H	146	ALA	2.0
13	L	96	VAL	2.0
17	P	114	LEU	2.0
10	I	118	ASN	2.0
14	M	22	GLU	2.0
21	T	23	VAL	2.0
27	Z	72	ASP	2.0
4	C	246	ARG	2.0
9	H	164	CYS	2.0
26	Y	95	THR	2.0
13	L	81	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	1MA	0	628	23/24	0.97	0.15	49,56,63,64	0
1	OMG	0	2588	24/25	0.97	0.14	50,54,58,60	0
1	PSU	0	2621	20/21	0.97	0.20	59,63,65,66	0
1	UR3	0	2619	21/22	0.98	0.15	61,65,71,72	0
1	OMU	0	2587	21/22	0.98	0.12	60,63,64,64	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
36	SR	0	8997	1/1	-0.10	5.65	200,200,200,200	0
36	SR	0	8971	1/1	0.15	0.12	200,200,200,200	0
34	NA	0	8522	1/1	0.21	0.13	87,87,87,87	0
34	NA	S	8510	1/1	0.40	0.30	69,69,69,69	0
34	NA	0	8506	1/1	0.47	0.60	105,105,105,105	0
34	NA	0	8525	1/1	0.53	0.33	92,92,92,92	0
34	NA	0	8524	1/1	0.54	0.38	47,47,47,47	0
36	SR	B	8987	1/1	0.55	0.82	200,200,200,200	0
32	MG	0	8036	1/1	0.58	0.21	82,82,82,82	0
34	NA	0	8505	1/1	0.59	0.45	56,56,56,56	0
34	NA	0	8553	1/1	0.61	0.20	81,81,81,81	0
34	NA	0	8554	1/1	0.61	0.38	71,71,71,71	0
36	SR	0	8998	1/1	0.62	0.63	169,169,169,169	0
34	NA	9	8572	1/1	0.62	0.32	88,88,88,88	0
32	MG	0	8068	1/1	0.64	0.08	49,49,49,49	0
34	NA	0	8549	1/1	0.64	0.17	83,83,83,83	0
34	NA	0	8556	1/1	0.64	0.80	95,95,95,95	0
32	MG	0	8092	1/1	0.66	0.12	53,53,53,53	0
36	SR	J	8986	1/1	0.66	1.51	200,200,200,200	0
32	MG	0	8090	1/1	0.67	0.93	81,81,81,81	0
36	SR	A	8930	1/1	0.67	0.24	133,133,133,133	0
36	SR	0	8991	1/1	0.68	0.09	190,190,190,190	0
36	SR	0	8958	1/1	0.69	0.07	150,150,150,150	0
36	SR	0	8962	1/1	0.69	0.15	155,155,155,155	0
32	MG	0	8049	1/1	0.69	0.20	61,61,61,61	0
34	NA	0	8564	1/1	0.70	0.57	95,95,95,95	0
34	NA	0	8528	1/1	0.71	0.49	80,80,80,80	0
35	CL	3	8804	1/1	0.73	0.15	96,96,96,96	0
34	NA	0	8501	1/1	0.73	0.22	41,41,41,41	0
36	SR	0	8957	1/1	0.74	0.24	200,200,200,200	0
36	SR	0	8916	1/1	0.74	0.08	129,129,129,129	0
36	SR	0	8994	1/1	0.75	0.72	200,200,200,200	0
34	NA	Q	8540	1/1	0.75	0.29	92,92,92,92	0
32	MG	9	8074	1/1	0.76	0.13	127,127,127,127	0
34	NA	0	8527	1/1	0.76	0.24	60,60,60,60	0
36	SR	0	8922	1/1	0.77	0.47	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8508	1/1	0.77	0.99	70,70,70,70	0
34	NA	9	8543	1/1	0.77	0.17	57,57,57,57	0
32	MG	0	8044	1/1	0.77	0.11	49,49,49,49	0
32	MG	0	8077	1/1	0.77	0.16	47,47,47,47	0
32	MG	0	8081	1/1	0.77	0.45	104,104,104,104	0
36	SR	9	9003	1/1	0.77	0.06	200,200,200,200	0
34	NA	0	8509	1/1	0.78	0.49	66,66,66,66	0
34	NA	0	8568	1/1	0.78	0.57	51,51,51,51	0
34	NA	0	8529	1/1	0.78	0.11	49,49,49,49	0
36	SR	0	8936	1/1	0.78	0.07	109,109,109,109	0
35	CL	N	8807	1/1	0.79	0.38	134,134,134,134	0
36	SR	0	8947	1/1	0.79	0.60	200,200,200,200	0
34	NA	0	8502	1/1	0.80	0.19	51,51,51,51	0
34	NA	0	8566	1/1	0.80	0.89	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.50	96,96,96,96	0
36	SR	0	9006	1/1	0.81	0.49	200,200,200,200	0
32	MG	0	8061	1/1	0.81	0.30	42,42,42,42	0
32	MG	0	8073	1/1	0.81	0.69	110,110,110,110	0
34	NA	0	8550	1/1	0.81	0.19	98,98,98,98	0
36	SR	0	8985	1/1	0.81	0.04	173,173,173,173	0
34	NA	0	8560	1/1	0.82	0.29	64,64,64,64	0
36	SR	0	8979	1/1	0.82	0.10	200,200,200,200	0
34	NA	0	8533	1/1	0.82	0.21	68,68,68,68	0
36	SR	0	8974	1/1	0.83	0.42	191,191,191,191	0
36	SR	0	8977	1/1	0.83	0.14	197,197,197,197	0
36	SR	0	8995	1/1	0.83	0.25	128,128,128,128	0
34	NA	0	8514	1/1	0.83	0.27	61,61,61,61	0
34	NA	0	8545	1/1	0.83	0.31	40,40,40,40	0
32	MG	0	8066	1/1	0.84	0.93	70,70,70,70	0
34	NA	0	8562	1/1	0.84	1.23	85,85,85,85	0
35	CL	0	8805	1/1	0.84	0.39	97,97,97,97	0
34	NA	R	8532	1/1	0.85	0.10	57,57,57,57	0
36	SR	0	9007	1/1	0.85	0.78	180,180,180,180	0
34	NA	0	8552	1/1	0.85	0.31	68,68,68,68	0
36	SR	A	8993	1/1	0.85	0.04	177,177,177,177	0
34	NA	0	8571	1/1	0.85	0.26	89,89,89,89	0
34	NA	0	8531	1/1	0.85	0.27	42,42,42,42	0
36	SR	0	8989	1/1	0.85	0.26	196,196,196,196	0
32	MG	0	8069	1/1	0.86	0.55	68,68,68,68	0
34	NA	0	8511	1/1	0.86	0.21	64,64,64,64	0
36	SR	0	9004	1/1	0.86	0.46	200,200,200,200	0
35	CL	Y	8820	1/1	0.86	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8047	1/1	0.86	0.37	70,70,70,70	0
34	NA	0	8573	1/1	0.87	0.19	92,92,92,92	0
36	SR	0	8992	1/1	0.87	0.10	149,149,149,149	0
36	SR	0	8975	1/1	0.87	0.04	158,158,158,158	0
36	SR	0	8927	1/1	0.87	0.16	172,172,172,172	0
34	NA	0	8565	1/1	0.87	1.16	106,106,106,106	0
32	MG	0	8055	1/1	0.87	0.28	67,67,67,67	0
36	SR	0	8973	1/1	0.87	0.17	134,134,134,134	0
36	SR	0	8960	1/1	0.88	0.11	174,174,174,174	0
36	SR	0	8984	1/1	0.88	0.06	139,139,139,139	0
34	NA	0	8547	1/1	0.88	0.91	81,81,81,81	0
34	NA	M	8539	1/1	0.88	0.12	34,34,34,34	0
34	NA	0	8537	1/1	0.88	0.16	43,43,43,43	0
35	CL	0	8811	1/1	0.88	0.61	99,99,99,99	0
35	CL	0	8822	1/1	0.88	1.36	94,94,94,94	0
36	SR	H	8972	1/1	0.88	0.15	157,157,157,157	0
36	SR	0	8976	1/1	0.88	0.22	185,185,185,185	0
36	SR	9	8980	1/1	0.88	0.05	192,192,192,192	0
36	SR	0	8959	1/1	0.88	0.15	194,194,194,194	0
36	SR	0	8910	1/1	0.89	0.12	113,113,113,113	0
32	MG	0	8039	1/1	0.89	0.27	76,76,76,76	0
34	NA	0	8536	1/1	0.89	0.13	72,72,72,72	0
32	MG	0	8043	1/1	0.89	0.13	55,55,55,55	0
34	NA	0	8558	1/1	0.89	0.60	50,50,50,50	0
36	SR	0	8996	1/1	0.89	0.40	200,200,200,200	0
36	SR	0	8938	1/1	0.89	0.07	200,200,200,200	0
32	MG	0	8072	1/1	0.89	0.08	37,37,37,37	0
36	SR	0	8988	1/1	0.89	0.11	181,181,181,181	0
34	NA	0	8559	1/1	0.90	0.32	94,94,94,94	0
34	NA	0	8518	1/1	0.90	0.40	82,82,82,82	0
36	SR	0	8968	1/1	0.90	0.11	181,181,181,181	0
36	SR	0	8982	1/1	0.90	1.70	200,200,200,200	0
32	MG	0	8033	1/1	0.90	0.26	56,56,56,56	0
36	SR	F	9005	1/1	0.90	0.13	154,154,154,154	0
35	CL	0	8812	1/1	0.90	0.09	58,58,58,58	0
34	NA	0	8544	1/1	0.90	0.17	68,68,68,68	0
36	SR	0	9001	1/1	0.90	0.09	189,189,189,189	0
34	NA	0	8515	1/1	0.90	0.22	45,45,45,45	0
36	SR	0	8970	1/1	0.91	0.06	150,150,150,150	0
34	NA	J	8538	1/1	0.91	0.14	45,45,45,45	0
36	SR	L	8969	1/1	0.91	0.93	198,198,198,198	0
36	SR	0	8914	1/1	0.91	0.32	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	0	8953	1/1	0.91	0.25	185,185,185,185	0
32	MG	0	8087	1/1	0.92	0.18	20,20,20,20	0
36	SR	3	8999	1/1	0.92	0.18	160,160,160,160	0
36	SR	0	8928	1/1	0.92	0.05	164,164,164,164	0
32	MG	0	8004	1/1	0.92	0.15	32,32,32,32	0
32	MG	0	8079	1/1	0.93	0.20	63,63,63,63	0
35	CL	M	8818	1/1	0.93	0.09	73,73,73,73	0
32	MG	0	8058	1/1	0.93	0.06	25,25,25,25	0
34	NA	0	8523	1/1	0.93	0.15	58,58,58,58	0
32	MG	0	8001	1/1	0.93	0.11	28,28,28,28	0
32	MG	0	8053	1/1	0.93	0.05	57,57,57,57	0
36	SR	0	8944	1/1	0.93	0.17	171,171,171,171	0
36	SR	0	8945	1/1	0.93	0.04	111,111,111,111	0
32	MG	0	8010	1/1	0.93	0.18	35,35,35,35	0
36	SR	0	8915	1/1	0.93	0.07	125,125,125,125	0
34	NA	0	8541	1/1	0.94	0.14	46,46,46,46	0
36	SR	0	8946	1/1	0.94	0.26	138,138,138,138	0
34	NA	0	8516	1/1	0.94	0.26	26,26,26,26	0
36	SR	0	8951	1/1	0.94	0.19	177,177,177,177	0
32	MG	2	8060	1/1	0.94	0.09	56,56,56,56	0
36	SR	0	8955	1/1	0.94	0.17	199,199,199,199	0
32	MG	0	8067	1/1	0.94	0.43	42,42,42,42	0
33	K	0	8402	1/1	0.94	0.21	67,67,67,67	0
32	MG	0	8032	1/1	0.94	0.08	64,64,64,64	0
34	NA	0	8574	1/1	0.94	0.80	67,67,67,67	0
36	SR	0	8901	1/1	0.94	0.12	89,89,89,89	0
36	SR	0	8963	1/1	0.94	0.15	135,135,135,135	0
36	SR	0	8967	1/1	0.94	0.07	157,157,157,157	0
34	NA	0	8551	1/1	0.94	0.16	81,81,81,81	0
32	MG	0	8031	1/1	0.94	0.34	71,71,71,71	0
32	MG	0	8082	1/1	0.94	0.41	86,86,86,86	0
32	MG	0	8085	1/1	0.94	0.13	83,83,83,83	0
32	MG	0	8071	1/1	0.94	0.12	50,50,50,50	0
36	SR	0	8924	1/1	0.94	0.17	138,138,138,138	0
32	MG	0	8089	1/1	0.94	0.29	72,72,72,72	0
32	MG	0	8040	1/1	0.94	0.32	100,100,100,100	0
36	SR	3	8932	1/1	0.94	0.29	149,149,149,149	0
32	MG	0	8035	1/1	0.94	0.12	47,47,47,47	0
35	CL	0	8803	1/1	0.94	0.08	66,66,66,66	0
32	MG	T	8057	1/1	0.94	0.03	67,67,67,67	0
37	MUL	0	9101	34/34	0.94	0.26	85,87,104,104	0
35	CL	R	8806	1/1	0.95	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	A	8929	1/1	0.95	0.17	157,157,157,157	0
32	MG	0	8088	1/1	0.95	0.05	39,39,39,39	0
32	MG	0	8038	1/1	0.95	0.12	81,81,81,81	0
36	SR	0	8954	1/1	0.95	0.12	122,122,122,122	0
32	MG	0	8021	1/1	0.95	0.10	28,28,28,28	0
36	SR	0	8908	1/1	0.95	0.06	109,109,109,109	0
35	CL	0	8815	1/1	0.95	0.24	90,90,90,90	0
36	SR	0	8940	1/1	0.95	0.03	117,117,117,117	0
36	SR	1	8913	1/1	0.95	0.17	97,97,97,97	0
34	NA	0	8526	1/1	0.95	0.27	52,52,52,52	0
32	MG	0	8015	1/1	0.95	0.10	25,25,25,25	0
36	SR	0	8981	1/1	0.95	0.10	151,151,151,151	0
32	MG	0	8037	1/1	0.95	0.29	84,84,84,84	0
36	SR	0	8966	1/1	0.95	0.10	110,110,110,110	0
34	NA	0	8542	1/1	0.96	0.52	51,51,51,51	0
32	MG	0	8005	1/1	0.96	0.27	30,30,30,30	0
34	NA	0	8561	1/1	0.96	0.36	73,73,73,73	0
32	MG	0	8003	1/1	0.96	0.16	31,31,31,31	0
32	MG	0	8029	1/1	0.96	0.12	54,54,54,54	0
34	NA	0	8548	1/1	0.96	0.25	52,52,52,52	0
32	MG	B	8042	1/1	0.96	0.08	67,67,67,67	0
34	NA	0	8567	1/1	0.96	0.21	58,58,58,58	0
36	SR	0	8964	1/1	0.96	0.09	149,149,149,149	0
34	NA	0	8530	1/1	0.96	0.31	49,49,49,49	0
35	CL	0	8813	1/1	0.96	0.15	68,68,68,68	0
36	SR	0	8934	1/1	0.96	0.09	114,114,114,114	0
35	CL	0	8814	1/1	0.96	0.41	67,67,67,67	0
34	NA	0	8521	1/1	0.96	0.11	34,34,34,34	0
32	MG	0	8065	1/1	0.96	0.14	41,41,41,41	0
36	SR	B	8950	1/1	0.96	0.28	151,151,151,151	0
36	SR	0	8941	1/1	0.96	0.31	143,143,143,143	0
36	SR	0	8942	1/1	0.96	0.08	129,129,129,129	0
36	SR	0	8943	1/1	0.96	0.17	99,99,99,99	0
35	CL	L	8810	1/1	0.96	0.24	86,86,86,86	0
34	NA	0	8535	1/1	0.96	0.54	45,45,45,45	0
34	NA	C	8503	1/1	0.96	0.32	39,39,39,39	0
36	SR	1	8952	1/1	0.96	0.19	81,81,81,81	0
32	MG	Y	8086	1/1	0.96	0.04	55,55,55,55	0
36	SR	0	8983	1/1	0.96	0.21	185,185,185,185	0
36	SR	0	8949	1/1	0.96	0.10	120,120,120,120	0
32	MG	0	8014	1/1	0.96	0.12	30,30,30,30	0
32	MG	0	8041	1/1	0.96	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
38	CD	O	8705	1/1	0.96	0.03	115,115,115,115	0
32	MG	0	8063	1/1	0.97	0.15	67,67,67,67	0
32	MG	0	8064	1/1	0.97	0.20	48,48,48,48	0
34	NA	0	8563	1/1	0.97	0.18	74,74,74,74	0
32	MG	0	8027	1/1	0.97	0.05	30,30,30,30	0
36	SR	0	8917	1/1	0.97	0.14	121,121,121,121	0
36	SR	0	8919	1/1	0.97	0.17	194,194,194,194	0
36	SR	0	8920	1/1	0.97	0.11	132,132,132,132	0
36	SR	0	9000	1/1	0.97	0.23	200,200,200,200	0
36	SR	0	8921	1/1	0.97	0.09	90,90,90,90	0
34	NA	0	8546	1/1	0.97	1.32	69,69,69,69	0
32	MG	0	8008	1/1	0.97	0.14	15,15,15,15	0
32	MG	0	8009	1/1	0.97	0.21	28,28,28,28	0
32	MG	0	8052	1/1	0.97	0.04	40,40,40,40	0
36	SR	0	8933	1/1	0.97	0.04	122,122,122,122	0
32	MG	0	8007	1/1	0.97	0.17	10,10,10,10	0
32	MG	0	8024	1/1	0.97	0.14	58,58,58,58	0
35	CL	A	8809	1/1	0.97	0.67	96,96,96,96	0
35	CL	B	8819	1/1	0.97	0.76	68,68,68,68	0
35	CL	J	8801	1/1	0.97	0.21	90,90,90,90	0
35	CL	J	8821	1/1	0.97	0.16	70,70,70,70	0
36	SR	0	8978	1/1	0.97	0.04	130,130,130,130	0
32	MG	0	8034	1/1	0.97	0.30	43,43,43,43	0
32	MG	0	8059	1/1	0.97	0.12	40,40,40,40	0
34	NA	0	8534	1/1	0.97	0.22	45,45,45,45	0
34	NA	0	8555	1/1	0.97	0.55	50,50,50,50	0
32	MG	0	8075	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8076	1/1	0.97	0.06	36,36,36,36	0
32	MG	0	8025	1/1	0.97	0.07	44,44,44,44	0
32	MG	0	8078	1/1	0.97	0.23	64,64,64,64	0
38	CD	Z	8703	1/1	0.97	0.14	155,155,155,155	0
38	CD	3	8704	1/1	0.97	0.41	176,176,176,176	0
36	SR	0	8939	1/1	0.98	0.05	145,145,145,145	0
34	NA	0	8517	1/1	0.98	0.20	30,30,30,30	0
35	CL	J	8802	1/1	0.98	0.08	100,100,100,100	0
34	NA	0	8569	1/1	0.98	0.17	72,72,72,72	0
34	NA	0	8570	1/1	0.98	0.11	65,65,65,65	0
36	SR	0	8990	1/1	0.98	0.19	111,111,111,111	0
32	MG	C	8012	1/1	0.98	0.21	19,19,19,19	0
34	NA	0	8520	1/1	0.98	0.19	57,57,57,57	0
35	CL	O	8808	1/1	0.98	0.30	98,98,98,98	0
32	MG	K	8054	1/1	0.98	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8056	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8080	1/1	0.98	0.52	98,98,98,98	0
32	MG	0	8002	1/1	0.98	0.17	26,26,26,26	0
36	SR	0	8902	1/1	0.98	0.13	63,63,63,63	0
36	SR	0	8903	1/1	0.98	0.19	62,62,62,62	0
36	SR	0	9002	1/1	0.98	0.09	188,188,188,188	0
36	SR	0	8956	1/1	0.98	0.23	178,178,178,178	0
32	MG	0	8070	1/1	0.98	0.39	54,54,54,54	0
36	SR	0	8909	1/1	0.98	0.07	89,89,89,89	0
36	SR	0	9008	1/1	0.98	0.16	99,99,99,99	0
32	MG	0	8006	1/1	0.98	0.12	62,62,62,62	0
36	SR	0	8911	1/1	0.98	0.13	109,109,109,109	0
32	MG	0	8046	1/1	0.98	0.21	48,48,48,48	0
32	MG	0	8016	1/1	0.98	0.16	38,38,38,38	0
32	MG	0	8011	1/1	0.98	0.21	18,18,18,18	0
34	NA	0	8557	1/1	0.98	0.07	71,71,71,71	0
32	MG	0	8022	1/1	0.98	0.13	29,29,29,29	0
34	NA	0	8507	1/1	0.98	0.27	39,39,39,39	0
32	MG	0	8091	1/1	0.98	0.18	42,42,42,42	0
32	MG	0	8023	1/1	0.98	0.15	21,21,21,21	0
36	SR	0	8923	1/1	0.98	0.17	120,120,120,120	0
32	MG	0	8093	1/1	0.98	0.10	40,40,40,40	0
34	NA	0	8512	1/1	0.98	0.30	49,49,49,49	0
34	NA	0	8513	1/1	0.98	0.23	63,63,63,63	0
35	CL	0	8816	1/1	0.98	0.71	86,86,86,86	0
32	MG	A	8050	1/1	0.98	0.19	52,52,52,52	0
36	SR	0	8935	1/1	0.98	0.05	106,106,106,106	0
38	CD	U	8701	1/1	0.98	0.04	104,104,104,104	0
32	MG	A	8051	1/1	0.98	0.28	90,90,90,90	0
32	MG	0	8013	1/1	0.98	0.04	21,21,21,21	0
36	SR	0	8948	1/1	0.99	0.08	104,104,104,104	0
36	SR	0	8905	1/1	0.99	0.27	70,70,70,70	0
36	SR	0	8925	1/1	0.99	0.13	105,105,105,105	0
36	SR	0	8926	1/1	0.99	0.16	145,145,145,145	0
36	SR	0	8906	1/1	0.99	0.19	65,65,65,65	0
36	SR	0	8907	1/1	0.99	0.16	63,63,63,63	0
36	SR	0	8931	1/1	0.99	0.10	123,123,123,123	0
32	MG	0	8020	1/1	0.99	0.11	52,52,52,52	0
32	MG	0	8083	1/1	0.99	0.08	59,59,59,59	0
32	MG	0	8084	1/1	0.99	0.16	50,50,50,50	0
32	MG	0	8017	1/1	0.99	0.07	29,29,29,29	0
36	SR	0	8937	1/1	0.99	0.17	108,108,108,108	0

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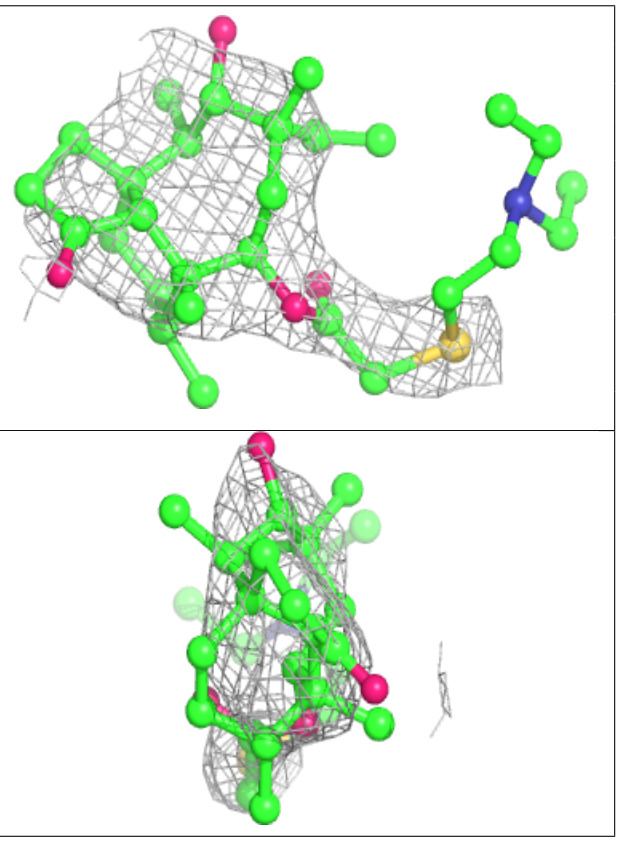
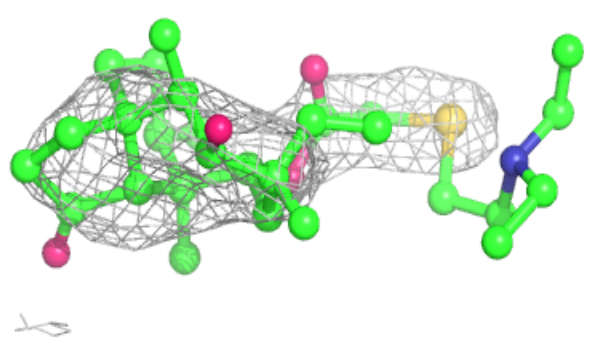
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	R	8912	1/1	0.99	0.23	106,106,106,106	0
36	SR	S	8961	1/1	0.99	0.10	127,127,127,127	0
32	MG	0	8026	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8048	1/1	0.99	0.31	38,38,38,38	0
36	SR	0	8965	1/1	0.99	0.17	135,135,135,135	0
34	NA	0	8519	1/1	0.99	0.18	44,44,44,44	0
35	CL	0	8817	1/1	0.99	0.11	63,63,63,63	0
36	SR	0	8918	1/1	0.99	0.13	84,84,84,84	0
32	MG	0	8018	1/1	0.99	0.18	42,42,42,42	0
32	MG	0	8062	1/1	0.99	0.28	47,47,47,47	0
32	MG	0	8028	1/1	0.99	0.13	14,14,14,14	0
32	MG	0	8019	1/1	0.99	0.16	10,10,10,10	0
38	CD	1	8702	1/1	0.99	0.13	68,68,68,68	0
36	SR	0	8904	1/1	0.99	0.16	64,64,64,64	0
32	MG	0	8030	1/1	1.00	0.48	60,60,60,60	0
34	NA	0	8504	1/1	1.00	0.09	22,22,22,22	0
32	MG	0	8045	1/1	1.00	0.12	44,44,44,44	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 MUL 0 9101:

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 (i)

There are no such residues in this entry.