



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 02:13 AM EST

PDB ID : 1TTT  
Title : Phe-tRNA, elongation factor EF-TU:GDPNP ternary complex  
Authors : Nissen, P.; Kjeldgaard, M.; Thirup, S.; Polekhina, G.; Reshetnikova, L.; Clark, B.F.C.; Nyborg, J.  
Deposited on : 1995-11-16  
Resolution : 2.70 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

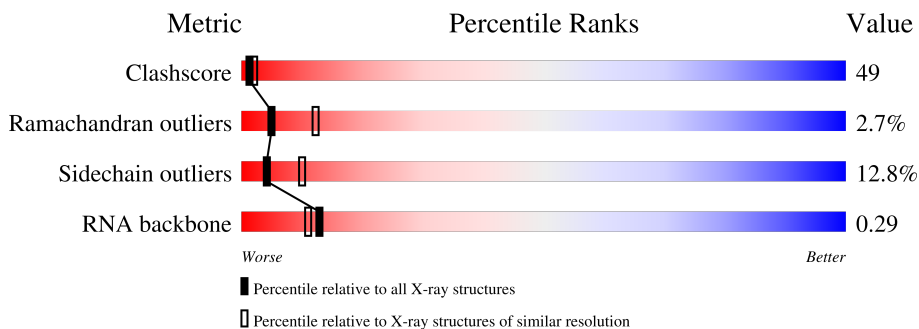
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	76	18% 59% 20%
1	E	76	7% 18% 41% 34%
1	F	76	21% 55% 21%
2	A	405	34% 53% 12%
2	B	405	39% 49% 12%
2	C	405	29% 54% 15%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
1	M2G	D	26	-	-	X	-
1	2MG	E	10	-	-	X	-
1	M2G	E	26	-	-	X	-
1	2MG	F	10	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14573 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 TRANSFER RIBONUCLEIC ACID (YEAST, PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	D	76	1652	746	294	536	76	0	0	0
1	E	76	1652	746	294	536	76	0	0	0
1	F	76	1652	746	294	536	76	0	0	0

- Molecule 2 is a protein called OF ELONGATION FACTOR TU (EF-TU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	405	3144	1986	548	598	12	0	0	0
2	B	405	3144	1986	548	598	12	0	0	0
2	C	405	3144	1986	548	598	12	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 6 is water.

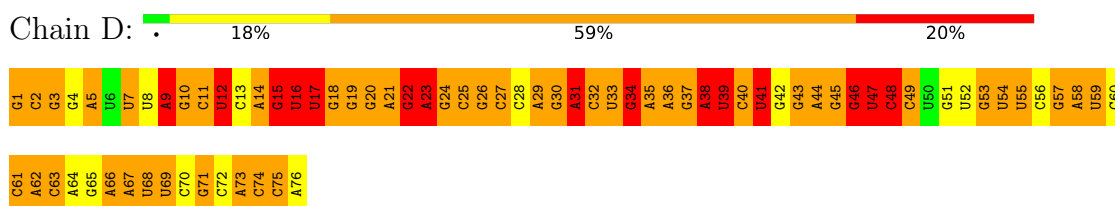
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	6	Total	O	0	0
			6	6		
6	E	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		
6	A	21	Total	O	0	0
			21	21		
6	B	13	Total	O	0	0
			13	13		
6	C	7	Total	O	0	0
			7	7		

### 3 Residue-property plots [i](#)

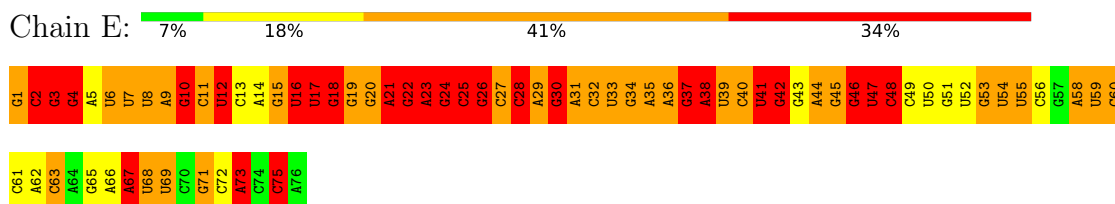
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

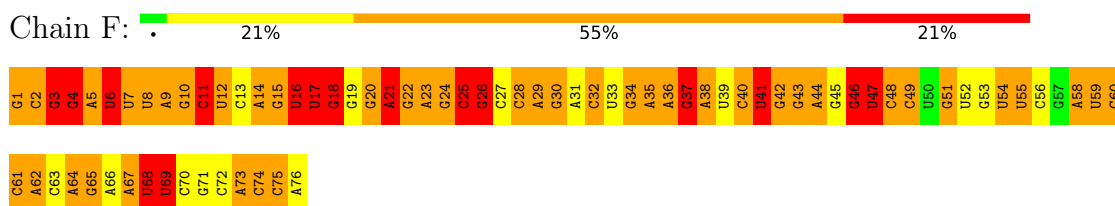
- Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)



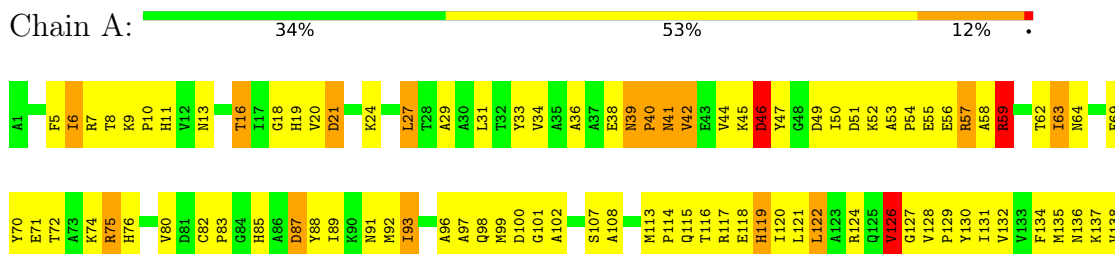
- Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)

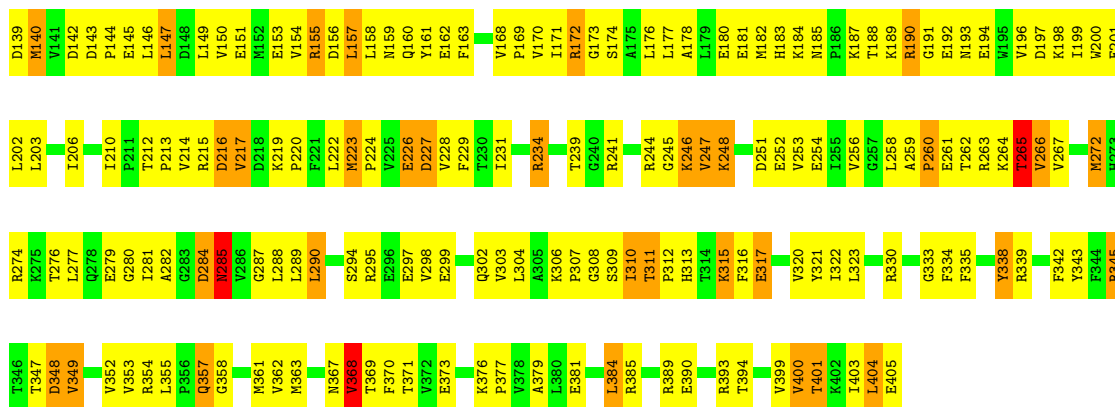


- Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)

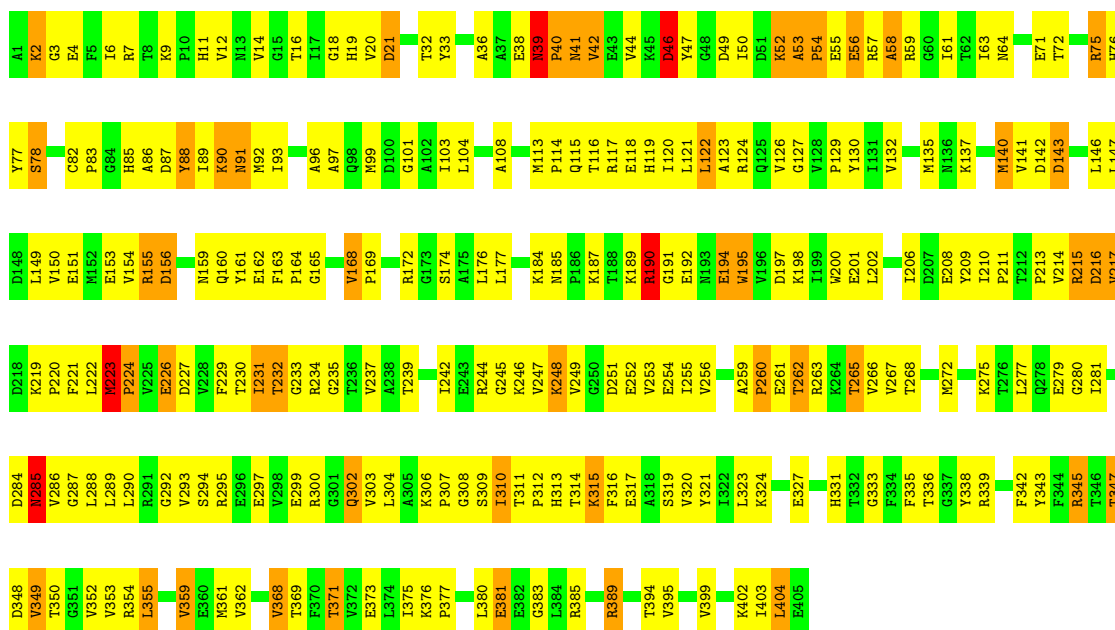


- Molecule 2: OF ELONGATION FACTOR TU (EF-TU)

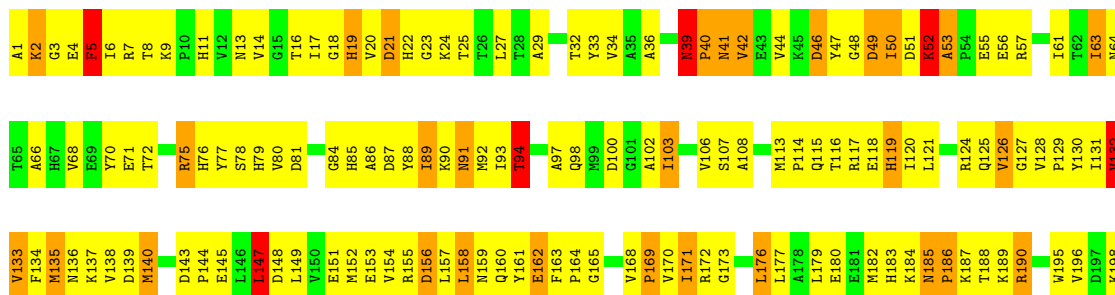
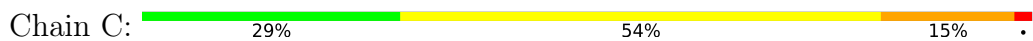




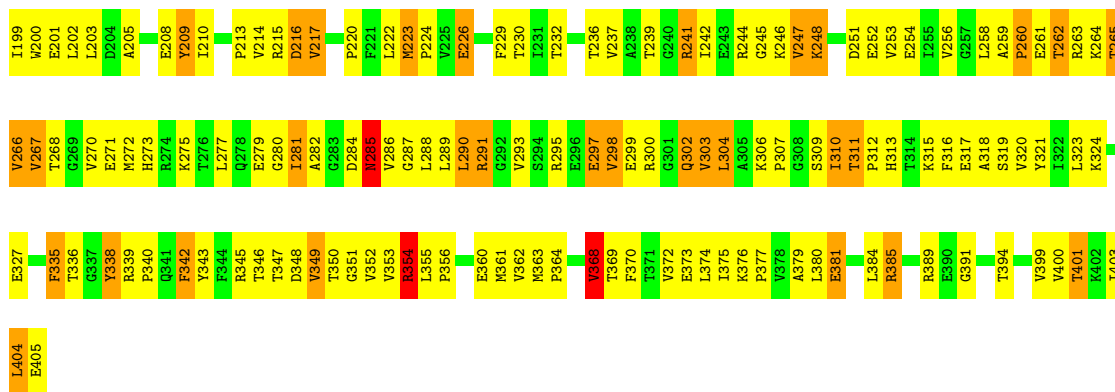
● Molecule 2: OF ELONGATION FACTOR TU (EF-TU)



● Molecule 2: OF ELONGATION FACTOR TU (EF-TU)







## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.84Å 122.35Å 151.55Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	91.1 (25.00-2.70)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.206 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

## 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: OMC, GNP, MG, 5MU, PSU, 2MG, 7MG, M2G, H2U, 5MC, YYG, OMG, 1MA

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	D	0.46	1/1487 (0.1%)	2.28	87/2315 (3.8%)
1	E	0.47	1/1487 (0.1%)	2.25	92/2315 (4.0%)
1	F	0.45	0/1487	2.21	108/2315 (4.7%)
2	A	0.87	1/3204 (0.0%)	1.52	43/4345 (1.0%)
2	B	0.87	0/3204	1.47	27/4345 (0.6%)
2	C	0.86	0/3204	1.52	35/4345 (0.8%)
All	All	0.76	3/14073 (0.0%)	1.80	392/19980 (2.0%)

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	F	2	0
2	A	2	0
All	All	4	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	G	OP3-P	-7.83	1.51	1.61
1	D	1	G	OP3-P	-5.69	1.54	1.61
2	A	400	VAL	CA-CB	-5.18	1.43	1.54

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	G	O4'-C1'-N9	29.42	131.74	108.20
1	D	33	U	O4'-C1'-N1	20.76	124.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	G	O4'-C1'-N9	20.70	124.76	108.20
2	A	39	ASN	C-N-CD	-20.57	75.34	120.60
1	D	21	A	N9-C1'-C2'	-20.07	87.90	114.00
1	E	48	C	O5'-P-OP2	-19.66	87.11	110.70
1	E	15	G	O4'-C1'-N9	-18.97	93.02	108.20
1	D	22	G	N9-C1'-C2'	-18.94	89.38	114.00
2	C	39	ASN	C-N-CD	-18.86	79.10	120.60
1	F	13	C	O4'-C1'-N1	17.62	122.29	108.20
1	D	71	G	O4'-C1'-N9	-17.45	94.24	108.20
2	B	39	ASN	C-N-CD	-17.02	83.16	120.60
1	F	18	G	O4'-C1'-N9	16.54	121.43	108.20
1	D	45	G	O4'-C1'-N9	-16.07	95.34	108.20
1	D	28	C	O4'-C1'-N1	15.57	120.66	108.20
1	D	48	C	O4'-C1'-N1	15.13	120.31	108.20
1	E	21	A	N9-C1'-C2'	-14.93	94.59	114.00
1	F	1	G	O4'-C1'-N9	-14.87	96.30	108.20
1	F	51	G	O4'-C1'-N9	-14.85	96.32	108.20
1	F	21	A	N9-C1'-C2'	-14.69	94.90	114.00
1	E	25	C	O4'-C1'-N1	14.67	119.93	108.20
1	E	38	A	O5'-P-OP1	-14.45	92.69	105.70
1	E	71	G	O4'-C1'-N9	-14.35	96.72	108.20
1	D	18	G	O4'-C1'-N9	14.35	119.68	108.20
1	D	33	U	N1-C1'-C2'	-14.26	95.46	114.00
1	F	11	C	O4'-C1'-N1	14.13	119.50	108.20
1	F	71	G	O4'-C1'-N9	-14.10	96.92	108.20
1	F	68	U	O4'-C1'-N1	13.68	119.15	108.20
1	E	23	A	O4'-C1'-N9	13.38	118.91	108.20
1	F	5	A	O4'-C1'-N9	13.30	118.84	108.20
1	E	3	G	N9-C1'-C2'	-13.22	96.81	114.00
1	E	7	U	O4'-C1'-N1	13.22	118.78	108.20
1	D	47	U	N1-C1'-C2'	13.14	131.08	114.00
1	F	70	C	O4'-C1'-N1	12.76	118.41	108.20
1	D	19	G	O5'-P-OP1	-12.76	94.22	105.70
1	D	47	U	O4'-C1'-N1	12.75	118.40	108.20
1	E	6	U	O4'-C1'-N1	12.54	118.23	108.20
1	D	19	G	N9-C1'-C2'	-12.51	97.74	114.00
1	F	69	U	O4'-C1'-N1	12.37	118.09	108.20
1	E	53	G	O5'-P-OP2	-12.31	94.62	105.70
1	E	59	U	O4'-C1'-N1	12.31	118.05	108.20
1	F	42	G	O4'-C1'-N9	-12.21	98.43	108.20
1	D	38	A	N9-C1'-C2'	-12.15	98.21	114.00
1	E	30	G	O4'-C1'-N9	12.04	117.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	C	O4'-C1'-N1	12.03	117.82	108.20
1	E	36	A	N9-C1'-C2'	-12.00	98.40	114.00
1	D	42	G	O4'-C1'-N9	-11.98	98.62	108.20
1	E	41	U	O4'-C1'-N1	-11.96	98.63	108.20
1	D	41	U	O4'-C1'-N1	-11.70	98.84	108.20
1	E	47	U	N1-C1'-C2'	11.59	129.06	114.00
1	F	48	C	O4'-C1'-N1	11.51	117.41	108.20
1	F	28	C	O4'-C1'-N1	11.45	117.36	108.20
1	F	73	A	N9-C1'-C2'	-11.38	99.21	114.00
1	D	59	U	O4'-C1'-N1	11.35	117.28	108.20
1	F	9	A	O4'-C1'-N9	11.34	117.27	108.20
1	F	24	G	N9-C1'-C2'	-11.26	99.36	114.00
1	D	7	U	N1-C1'-C2'	-11.17	99.48	114.00
1	F	65	G	O4'-C1'-N9	-11.11	99.31	108.20
1	D	61	C	O4'-C1'-N1	11.11	117.08	108.20
1	E	4	G	O5'-P-OP2	-11.07	95.74	105.70
1	F	3	G	N9-C1'-C2'	-10.96	99.75	114.00
1	E	47	U	O5'-P-OP2	-10.90	95.89	105.70
1	D	3	G	N9-C1'-C2'	-10.66	100.14	114.00
1	D	23	A	O4'-C1'-N9	10.44	116.55	108.20
1	E	66	A	O4'-C1'-N9	-10.42	99.86	108.20
1	E	29	A	O4'-C1'-N9	10.41	116.53	108.20
1	F	66	A	O4'-C1'-N9	-10.40	99.88	108.20
1	F	18	G	N9-C1'-C2'	-10.13	100.83	114.00
1	F	48	C	O5'-P-OP2	-10.12	96.59	105.70
1	F	61	C	O4'-C1'-N1	10.11	116.29	108.20
1	F	25	C	O4'-C1'-N1	10.10	116.28	108.20
1	E	3	G	O4'-C1'-N9	10.08	116.26	108.20
1	D	27	C	O4'-C1'-N1	10.05	116.24	108.20
1	E	24	G	O4'-C1'-N9	-9.94	100.25	108.20
1	F	73	A	O4'-C1'-N9	-9.87	100.31	108.20
1	D	31	A	N9-C1'-C2'	-9.80	101.22	112.00
1	E	38	A	N9-C1'-C2'	-9.80	101.22	112.00
1	E	20	G	O4'-C1'-N9	-9.71	100.43	108.20
1	D	30	G	N9-C1'-C2'	-9.67	101.36	112.00
1	D	23	A	N9-C1'-C2'	9.67	126.57	114.00
1	E	44	A	O4'-C1'-N9	9.66	115.93	108.20
1	F	35	A	O4'-C1'-N9	-9.59	100.53	108.20
1	D	73	A	N9-C1'-C2'	-9.36	101.71	112.00
1	F	36	A	O4'-C1'-N9	9.32	115.66	108.20
1	D	25	C	N1-C1'-C2'	-9.29	101.78	112.00
1	D	66	A	O4'-C1'-N9	-9.29	100.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	U	O4'-C1'-N1	-9.27	100.78	108.20
1	E	2	C	OP2-P-O3'	9.24	125.54	105.20
1	F	47	U	N1-C1'-C2'	9.23	126.00	114.00
2	B	184	LYS	CD-CE-NZ	9.22	132.90	111.70
1	E	73	A	O4'-C1'-N9	-9.18	100.86	108.20
1	D	35	A	O4'-C1'-N9	-9.16	100.87	108.20
1	E	56	C	O4'-C1'-N1	-9.15	100.88	108.20
1	D	56	C	O4'-C1'-N1	-9.08	100.93	108.20
1	E	22	G	O5'-P-OP2	-9.08	97.53	105.70
1	E	28	C	N1-C1'-C2'	8.98	125.67	114.00
1	F	15	G	O4'-C1'-N9	-8.94	101.05	108.20
1	E	19	G	O5'-P-OP1	-8.86	97.72	105.70
1	D	18	G	N9-C1'-C2'	-8.82	102.30	112.00
1	F	25	C	N1-C1'-C2'	-8.82	102.30	112.00
1	F	38	A	O4'-C1'-N9	-8.79	101.16	108.20
1	F	43	G	O4'-C1'-N9	-8.77	101.18	108.20
1	F	33	U	O5'-P-OP2	-8.77	97.81	105.70
1	E	67	A	OP2-P-O3'	8.69	124.32	105.20
1	D	37	YYG	OP1-P-O3'	8.63	124.20	105.20
1	D	36	A	O4'-C1'-N9	8.59	115.07	108.20
1	E	6	U	O5'-P-OP1	8.58	120.99	110.70
1	F	24	G	O4'-C1'-N9	8.57	115.06	108.20
1	E	61	C	O4'-C1'-N1	8.42	114.94	108.20
1	E	31	A	O4'-C1'-N9	8.37	114.89	108.20
2	A	59	ARG	NE-CZ-NH1	-8.35	116.12	120.30
1	E	13	C	N1-C1'-C2'	8.34	124.85	114.00
1	D	43	G	O4'-C1'-N9	8.34	114.87	108.20
1	F	51	G	N9-C1'-C2'	8.34	124.84	114.00
1	D	74	C	O4'-C1'-N1	-8.24	101.61	108.20
1	F	47	U	O5'-P-OP2	-8.20	98.32	105.70
1	F	11	C	C2'-C3'-O3'	8.11	127.35	109.50
1	E	28	C	O4'-C1'-N1	8.06	114.65	108.20
1	E	41	U	O5'-P-OP1	8.05	120.36	110.70
1	E	65	G	O5'-P-OP1	-7.95	98.54	105.70
1	F	23	A	O4'-C1'-N9	7.95	114.56	108.20
1	E	60	C	N1-C1'-C2'	-7.94	103.26	112.00
1	D	21	A	C3'-C2'-O2'	-7.90	90.38	113.30
1	F	59	U	O4'-C1'-N1	7.89	114.51	108.20
1	F	44	A	O4'-C1'-N9	-7.87	101.90	108.20
1	F	29	A	O4'-C1'-N9	7.84	114.47	108.20
1	F	7	U	O4'-C1'-N1	-7.83	101.94	108.20
1	D	32	OMC	OP1-P-O3'	-7.80	88.04	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	MET	CG-SD-CE	7.79	112.66	100.20
2	B	223	MET	C-N-CD	-7.77	103.50	120.60
2	A	384	LEU	CB-CG-CD1	-7.77	97.79	111.00
1	E	32	OMC	OP1-P-O3'	-7.77	88.11	105.20
1	E	69	U	C2'-C3'-O3'	7.73	126.52	109.50
2	C	209	TYR	CZ-CE2-CD2	-7.71	112.86	119.80
2	A	163	PHE	N-CA-C	-7.67	90.28	111.00
1	E	52	U	O4'-C1'-N1	7.65	114.32	108.20
1	F	48	C	O5'-P-OP1	7.64	119.87	110.70
1	D	5	A	O4'-C1'-N9	7.64	114.31	108.20
1	D	3	G	O4'-C1'-N9	7.59	114.27	108.20
1	D	1	G	O4'-C1'-N9	-7.52	102.19	108.20
2	A	330	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	E	9	A	O4'-C1'-N9	7.46	114.17	108.20
1	E	18	G	N9-C1'-C2'	-7.45	103.80	112.00
1	F	20	G	O3'-P-O5'	-7.43	89.87	104.00
2	B	349	VAL	CB-CA-C	-7.41	97.32	111.40
1	E	12	U	O4'-C1'-N1	7.40	114.12	108.20
1	F	24	G	O5'-P-OP2	-7.39	99.05	105.70
1	E	21	A	O5'-P-OP2	7.38	119.56	110.70
1	E	68	U	N1-C1'-C2'	-7.37	103.89	112.00
2	C	266	VAL	CB-CA-C	-7.36	97.43	111.40
1	F	6	U	O4'-C1'-N1	7.34	114.07	108.20
2	C	185	ASN	C-N-CD	-7.27	104.60	120.60
1	D	7	U	O4'-C1'-N1	7.26	114.01	108.20
1	E	52	U	O5'-P-OP2	-7.24	99.18	105.70
1	F	11	C	N1-C1'-C2'	7.24	123.42	114.00
1	F	20	G	O5'-P-OP2	-7.24	99.19	105.70
1	E	73	A	N9-C1'-C2'	-7.21	104.07	112.00
1	F	55	PSU	OP2-P-O3'	7.21	121.05	105.20
1	D	53	G	O4'-C1'-N9	-7.17	102.46	108.20
1	F	35	A	O5'-P-OP2	7.15	119.28	110.70
1	E	22	G	O4'-C1'-N9	-7.12	102.50	108.20
1	D	63	C	OP1-P-O3'	-7.09	89.60	105.20
1	D	30	G	O4'-C1'-N9	7.09	113.87	108.20
2	B	42	VAL	N-CA-C	-7.08	91.89	111.00
2	C	132	VAL	N-CA-C	-7.07	91.91	111.00
1	F	22	G	O5'-P-OP2	-7.06	99.34	105.70
2	B	90	LYS	CD-CE-NZ	7.05	127.92	111.70
1	F	3	G	O4'-C1'-N9	7.03	113.83	108.20
1	F	76	A	O4'-C1'-N9	7.03	113.83	108.20
1	F	21	A	P-O5'-C5'	-7.03	109.66	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	A	O4'-C1'-N9	-7.00	102.60	108.20
1	D	9	A	O4'-C1'-N9	7.00	113.80	108.20
2	B	122	LEU	CA-CB-CG	-6.99	99.21	115.30
1	F	53	G	O5'-P-OP1	6.99	119.08	110.70
1	D	64	A	OP1-P-OP2	6.96	130.04	119.60
1	F	31	A	P-O5'-C5'	-6.96	109.77	120.90
1	F	23	A	N9-C1'-C2'	-6.93	104.38	112.00
1	E	47	U	OP2-P-O3'	6.89	120.36	105.20
1	F	43	G	N9-C1'-C2'	-6.87	104.44	112.00
1	D	65	G	O5'-P-OP2	-6.86	99.53	105.70
1	D	36	A	N9-C1'-C2'	-6.84	104.47	112.00
1	D	15	G	O4'-C1'-N9	-6.84	102.73	108.20
1	F	46	7MG	P-O3'-C3'	6.83	127.90	119.70
1	F	20	G	O5'-P-OP1	-6.81	99.57	105.70
1	F	41	U	O4'-C1'-N1	-6.80	102.76	108.20
1	D	22	G	C4'-C3'-O3'	6.80	126.60	113.00
1	E	35	A	O4'-C1'-N9	-6.79	102.77	108.20
1	E	24	G	N9-C1'-C2'	6.78	122.81	114.00
1	F	12	U	N1-C1'-C2'	6.77	122.81	114.00
1	D	68	U	O4'-C1'-N1	6.76	113.61	108.20
1	D	38	A	O5'-P-OP1	-6.75	99.63	105.70
1	D	69	U	C2'-C3'-O3'	6.74	124.48	113.70
2	A	349	VAL	CB-CA-C	-6.73	98.61	111.40
2	B	46	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	E	69	U	O4'-C1'-N1	6.72	113.58	108.20
1	F	53	G	O4'-C1'-N9	-6.71	102.83	108.20
1	F	46	7MG	OP1-P-O3'	6.71	119.95	105.20
1	F	68	U	N1-C1'-C2'	-6.71	104.62	112.00
1	D	3	G	O3'-P-O5'	6.68	116.69	104.00
1	F	31	A	N9-C1'-C2'	-6.68	104.66	112.00
2	A	284	ASP	CB-CG-OD1	-6.64	112.33	118.30
1	D	15	G	N9-C1'-C2'	6.63	122.63	114.00
1	D	21	A	P-O5'-C5'	-6.63	110.28	120.90
2	C	281	ILE	CB-CA-C	-6.61	98.38	111.60
2	C	103	ILE	CB-CA-C	-6.59	98.41	111.60
2	A	367	ASN	N-CA-C	-6.56	93.28	111.00
1	D	62	A	OP2-P-O3'	6.55	119.61	105.20
2	A	59	ARG	NH1-CZ-NH2	6.53	126.59	119.40
2	A	274	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	A	42	VAL	N-CA-C	-6.51	93.43	111.00
1	D	75	C	O5'-P-OP1	6.50	118.49	110.70
1	F	11	C	C3'-C2'-O2'	6.49	132.11	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	C	OP2-P-O3'	6.48	119.46	105.20
1	E	68	U	O4'-C1'-N1	6.48	113.38	108.20
2	B	285	ASN	N-CA-C	-6.47	93.52	111.00
1	E	1	G	OP1-P-O3'	6.43	119.34	105.20
1	F	23	A	OP2-P-O3'	6.42	119.32	105.20
1	E	35	A	C3'-C2'-O2'	-6.39	94.77	113.30
2	C	52	LYS	N-CA-C	6.38	128.23	111.00
2	C	354	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	B	190	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	7	U	O5'-P-OP2	6.33	118.30	110.70
1	E	53	G	O4'-C1'-N9	-6.32	103.15	108.20
2	A	132	VAL	N-CA-C	-6.31	93.96	111.00
2	B	286	VAL	CB-CA-C	-6.31	99.41	111.40
1	D	18	G	OP1-P-O3'	6.29	119.03	105.20
1	F	30	G	O4'-C1'-N9	6.29	113.23	108.20
1	E	20	G	O5'-P-OP1	-6.27	100.06	105.70
1	E	46	7MG	OP2-P-O3'	6.26	118.98	105.20
1	F	8	U	O4'-C1'-N1	-6.26	103.19	108.20
2	A	51	ASP	N-CA-C	-6.25	94.14	111.00
1	D	20	G	N9-C1'-C2'	-6.24	105.14	112.00
1	F	44	A	N9-C1'-C2'	6.21	122.08	114.00
2	C	241	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	121	LEU	CA-CB-CG	-6.20	101.04	115.30
1	D	69	U	O5'-P-OP2	6.20	118.14	110.70
1	E	30	G	C2'-C3'-O3'	6.20	123.62	113.70
2	A	157	LEU	CB-CG-CD1	-6.18	100.50	111.00
2	A	227	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	D	63	C	N1-C1'-C2'	-6.13	105.26	112.00
1	D	64	A	OP2-P-O3'	6.12	118.67	105.20
2	C	127	GLY	N-CA-C	6.10	128.35	113.10
1	D	51	G	N9-C1'-C2'	6.09	121.92	114.00
1	F	20	G	OP2-P-O3'	6.09	118.61	105.20
1	F	21	A	C4'-C3'-O3'	6.09	125.17	113.00
2	A	247	VAL	CB-CA-C	-6.08	99.86	111.40
1	D	3	G	O5'-P-OP2	-6.07	100.24	105.70
2	C	304	LEU	CA-CB-CG	-6.06	101.37	115.30
1	D	24	G	N9-C1'-C2'	-6.04	105.36	112.00
2	A	59	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	C	290	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	E	63	C	OP2-P-O3'	6.03	118.47	105.20
2	B	104	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	E	48	C	O5'-P-OP1	6.02	117.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	C	C2'-C3'-O3'	6.00	123.31	113.70
1	E	75	C	N1-C1'-C2'	-5.98	105.42	112.00
1	E	38	A	O4'-C1'-N9	-5.97	103.42	108.20
2	C	2	LYS	N-CA-C	-5.97	94.88	111.00
1	E	63	C	O5'-P-OP1	5.96	117.86	110.70
1	F	38	A	N9-C1'-C2'	-5.96	105.44	112.00
2	C	203	LEU	CA-CB-CG	-5.95	101.61	115.30
1	F	11	C	O3'-P-O5'	-5.94	92.72	104.00
1	D	61	C	O5'-P-OP1	-5.93	100.36	105.70
1	F	62	A	O5'-P-OP2	-5.93	100.36	105.70
1	E	65	G	OP2-P-O3'	-5.91	92.19	105.20
1	D	29	A	O3'-P-O5'	-5.91	92.77	104.00
2	A	93	ILE	CG1-CB-CG2	-5.89	98.45	111.40
2	B	227	ASP	CB-CG-OD1	-5.87	113.01	118.30
1	E	8	U	N1-C1'-C2'	-5.87	105.55	112.00
1	E	73	A	O5'-P-OP1	5.85	117.72	110.70
1	E	22	G	OP1-P-O3'	5.84	118.05	105.20
1	F	28	C	N1-C1'-C2'	-5.81	105.61	112.00
2	B	355	LEU	CA-CB-CG	-5.81	101.94	115.30
1	E	30	G	N9-C1'-C2'	-5.80	105.62	112.00
1	E	15	G	C4'-C3'-O3'	-5.79	97.24	109.40
2	C	368	VAL	CB-CA-C	-5.79	100.40	111.40
1	E	24	G	OP2-P-O3'	5.77	117.90	105.20
1	D	11	C	N1-C1'-C2'	-5.77	105.66	112.00
1	F	30	G	N9-C1'-C2'	-5.76	105.66	112.00
1	F	67	A	OP2-P-O3'	5.76	117.88	105.20
2	A	310	ILE	N-CA-C	5.75	126.53	111.00
2	A	315	LYS	CD-CE-NZ	5.75	124.93	111.70
1	D	69	U	O3'-P-O5'	-5.75	93.08	104.00
1	E	42	G	C5'-C4'-O4'	-5.75	102.20	109.10
2	C	385	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	A	284	ASP	CB-CG-OD2	5.74	123.47	118.30
2	A	352	VAL	CB-CA-C	-5.74	100.49	111.40
1	F	31	A	O4'-C1'-N9	5.74	112.79	108.20
1	D	57	G	O4'-C1'-N9	-5.73	103.62	108.20
2	A	214	VAL	N-CA-C	-5.72	95.55	111.00
2	C	169	PRO	CA-N-CD	-5.72	103.49	111.50
2	C	323	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	121	LEU	CB-CG-CD1	5.71	120.71	111.00
1	F	32	OMC	OP2-P-O3'	5.69	117.72	105.20
2	B	75	ARG	CB-CA-C	-5.68	99.03	110.40
1	D	22	G	O5'-P-OP2	-5.67	100.59	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	47	U	OP2-P-O3'	5.67	117.67	105.20
2	A	338	TYR	CB-CA-C	-5.66	99.08	110.40
1	F	36	A	O5'-P-OP2	-5.64	100.62	105.70
1	E	35	A	O5'-P-OP2	5.64	117.47	110.70
1	D	23	A	OP2-P-O3'	5.61	117.55	105.20
2	C	75	ARG	N-CA-C	5.60	126.12	111.00
1	F	4	G	O4'-C1'-N9	5.60	112.68	108.20
1	F	69	U	C2'-C3'-O3'	5.59	122.65	113.70
2	A	155	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	3	G	O3'-P-O5'	5.58	114.60	104.00
2	A	285	ASN	N-CA-C	-5.57	95.96	111.00
1	F	14	A	O4'-C1'-N9	5.56	112.65	108.20
1	E	3	G	O3'-P-O5'	5.55	114.56	104.00
2	B	389	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	143	ASP	N-CA-C	-5.55	96.03	111.00
1	E	43	G	N9-C1'-C2'	5.51	121.17	114.00
2	C	147	LEU	CB-CA-C	-5.51	99.73	110.20
1	F	31	A	O5'-P-OP2	5.50	117.30	110.70
1	F	72	C	O4'-C1'-N1	5.50	112.60	108.20
2	B	208	GLU	N-CA-C	5.50	125.84	111.00
1	D	71	G	C2'-C3'-O3'	5.48	122.47	113.70
2	C	5	PHE	N-CA-C	5.48	125.79	111.00
1	D	69	U	P-O3'-C3'	-5.47	113.13	119.70
1	D	52	U	O5'-P-OP2	-5.46	100.78	105.70
2	A	246	LYS	N-CA-C	5.45	125.72	111.00
1	D	70	C	N1-C1'-C2'	-5.45	106.01	112.00
1	E	42	G	O5'-C5'-C4'	-5.45	101.35	111.70
2	C	285	ASN	N-CA-C	-5.44	96.32	111.00
2	C	208	GLU	N-CA-C	5.42	125.65	111.00
1	D	12	U	O4'-C1'-N1	-5.41	103.87	108.20
1	E	69	U	O3'-P-O5'	-5.41	93.71	104.00
2	C	310	ILE	CB-CA-C	-5.40	100.79	111.60
2	A	265	THR	CB-CA-C	-5.40	97.02	111.60
2	A	345	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	E	29	A	O3'-P-O5'	-5.36	93.81	104.00
2	A	87	ASP	CB-CA-C	-5.36	99.67	110.40
1	F	47	U	O4'-C1'-N1	-5.36	103.91	108.20
2	C	298	VAL	CB-CA-C	-5.36	101.21	111.40
1	F	11	C	C4'-C3'-O3'	5.36	123.72	113.00
1	F	62	A	O5'-P-OP1	5.36	117.13	110.70
1	F	74	C	O4'-C1'-N1	-5.35	103.92	108.20
2	C	94	THR	N-CA-CB	5.35	120.46	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	H2U	OP2-P-O3'	5.35	116.97	105.20
1	F	12	U	O5'-P-OP2	5.35	117.12	110.70
2	A	75	ARG	CB-CA-C	-5.34	99.71	110.40
2	A	122	LEU	CB-CG-CD2	-5.34	101.92	111.00
2	A	368	VAL	CB-CA-C	-5.34	101.26	111.40
2	A	310	ILE	CB-CA-C	-5.33	100.94	111.60
2	C	304	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	B	78	SER	N-CA-C	-5.32	96.65	111.00
1	D	23	A	O5'-P-OP2	-5.30	100.93	105.70
1	F	22	G	OP1-P-O3'	5.30	116.87	105.20
1	F	11	C	C1'-C2'-O2'	5.29	126.45	110.60
1	E	35	A	OP2-P-O3'	5.28	116.82	105.20
2	C	338	TYR	C-N-CA	-5.26	108.55	121.70
2	B	345	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	395	VAL	C-N-CA	-5.22	111.33	122.30
1	E	67	A	O4'-C1'-N9	5.22	112.38	108.20
1	F	60	C	N1-C1'-C2'	-5.21	106.27	112.00
1	F	68	U	O5'-P-OP2	-5.21	101.01	105.70
1	D	27	C	O5'-P-OP2	5.21	116.95	110.70
1	E	73	A	O5'-P-OP2	-5.20	101.02	105.70
1	F	11	C	P-O3'-C3'	-5.20	113.47	119.70
1	D	22	G	OP1-P-O3'	5.18	116.61	105.20
2	A	330	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	20	G	O4'-C1'-N9	-5.18	104.06	108.20
2	B	315	LYS	CB-CA-C	-5.17	100.05	110.40
1	F	70	C	N1-C1'-C2'	-5.16	106.33	112.00
2	B	56	GLU	N-CA-C	-5.15	97.09	111.00
1	E	1	G	C2'-C3'-O3'	5.15	121.94	113.70
2	C	42	VAL	N-CA-C	-5.14	97.11	111.00
2	A	272	MET	N-CA-C	-5.14	97.12	111.00
2	A	212	THR	N-CA-C	-5.14	97.12	111.00
2	B	162	GLU	N-CA-C	5.13	124.85	111.00
2	A	323	LEU	CA-CB-CG	5.12	127.08	115.30
2	A	400	VAL	CA-CB-CG1	-5.11	103.24	110.90
1	E	25	C	O5'-P-OP2	-5.10	101.11	105.70
1	F	41	U	O5'-P-OP1	5.10	116.82	110.70
2	C	49	ASP	CB-CG-OD1	-5.10	113.71	118.30
2	A	27	LEU	CA-CB-CG	-5.08	103.61	115.30
2	A	46	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	C	53	ALA	N-CA-C	-5.08	97.27	111.00
1	F	64	A	P-O5'-C5'	-5.08	112.78	120.90
2	A	266	VAL	CB-CA-C	-5.08	101.76	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	C	OP2-P-O3'	5.07	116.36	105.20
1	F	12	U	O3'-P-O5'	5.07	113.62	104.00
2	C	133	VAL	CB-CA-C	-5.05	101.80	111.40
2	C	162	GLU	N-CA-C	5.04	124.61	111.00
2	B	195	TRP	N-CA-CB	-5.04	101.53	110.60
1	E	28	C	O5'-P-OP2	-5.03	101.17	105.70
1	F	56	C	O5'-P-OP1	-5.03	101.17	105.70
1	D	70	C	O5'-P-OP1	5.03	116.73	110.70
1	F	62	A	C1'-C2'-O2'	-5.03	95.52	110.60
1	D	34	OMG	OP1-P-O3'	5.02	116.24	105.20
2	A	126	VAL	CB-CA-C	5.01	120.92	111.40
1	E	31	A	N9-C1'-C2'	-5.01	106.49	112.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	11	C	C2',C3'
2	A	232	THR	CA
2	A	311	THR	CA

There are no planarity outliers.

## 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	D	1652	0	856	116	0
1	E	1652	0	855	131	0
1	F	1652	0	856	108	0
2	A	3144	0	3161	282	0
2	B	3144	0	3160	302	0
2	C	3144	0	3162	362	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
4	D	11	0	8	2	0
4	E	11	0	8	1	0
4	F	11	0	8	1	0
5	A	32	0	13	6	0
5	B	32	0	13	7	0
5	C	32	0	13	7	0
6	A	21	0	0	5	0
6	B	13	0	0	0	0
6	C	7	0	0	1	0
6	D	6	0	0	0	0
6	E	2	0	0	1	0
6	F	1	0	0	0	0
All	All	14573	0	12113	1273	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 49.

All (1273) 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:E:9:A:H5'	1:E:46:7MG:H1'	1.22	1.15
2:A:217:VAL:HG12	2:A:246:LYS:HD3	1.28	1.11
2:A:54:PRO:HA	2:A:57:ARG:HG3	1.21	1.08
2:A:389:ARG:HG2	2:A:394:THR:HA	1.32	1.05
2:A:101:GLY:HA3	2:A:210:ILE:HD13	1.40	1.02
2:C:158:LEU:HD12	2:C:163:PHE:HB2	1.42	1.00
2:A:85:HIS:HD2	2:A:87:ASP:H	1.05	0.98
1:F:14:A:H2'	1:F:15:G:H5'	1.44	0.98
1:E:23:A:H2'	1:E:24:G:C8	1.98	0.98
2:C:68:VAL:HG22	2:C:79:HIS:HB3	1.47	0.97
2:B:18:GLY:H	2:B:119:HIS:HD2	1.04	0.97
1:F:10:2MG:HM23	1:F:11:C:H1'	1.46	0.97
2:C:18:GLY:H	2:C:119:HIS:HD2	1.06	0.96
1:E:10:2MG:HM23	1:E:11:C:H1'	1.46	0.96
2:C:354:ARG:HG3	2:C:354:ARG:HH11	1.31	0.95
1:E:14:A:H2'	1:E:15:G:H5'	1.49	0.95
2:A:311:THR:HG22	2:A:312:PRO:HD2	1.46	0.95
2:C:56:GLU:HG3	2:C:63:ILE:HG23	1.50	0.93
2:A:55:GLU:HG3	2:A:59:ARG:HG3	1.48	0.93
2:B:217:VAL:HG12	2:B:246:LYS:HD3	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:C:H42	1:E:42:G:H1	0.99	0.92
2:C:389:ARG:HG2	2:C:394:THR:HA	1.51	0.91
1:E:28:C:N4	1:E:42:G:H1	1.66	0.91
1:D:27:C:H42	1:D:43:G:H1	1.16	0.90
2:A:259:ALA:HB1	2:A:260:PRO:HD2	1.53	0.90
2:B:265:THR:HG21	2:B:290:LEU:HB3	1.53	0.90
2:B:19:HIS:HD2	2:B:115:GLN:H	1.14	0.90
2:C:263:ARG:HH21	2:C:297:GLU:HB3	1.37	0.89
2:B:335:PHE:CD1	2:B:361:MET:HB2	2.06	0.89
2:B:53:ALA:HB3	2:B:56:GLU:HB2	1.54	0.89
2:A:97:ALA:HA	2:A:126:VAL:HG13	1.53	0.89
1:D:11:C:H2'	1:D:12:U:H6	1.37	0.89
1:E:25:C:H2'	1:E:26:M2G:C8	2.08	0.88
2:C:169:PRO:HD2	2:C:209:TYR:CE2	2.08	0.88
2:C:316:PHE:HA	2:C:404:LEU:HD22	1.55	0.88
1:D:37:YYG:H31	1:D:37:YYG:H1'	1.55	0.88
2:B:213:PRO:HG2	2:B:215:ARG:CZ	2.03	0.88
1:E:11:C:H2'	1:E:12:U:H6	1.37	0.87
2:B:129:PRO:HB2	2:B:130:TYR:CD1	2.09	0.87
2:B:368:VAL:HG12	2:B:369:THR:H	1.37	0.87
2:A:54:PRO:CA	2:A:57:ARG:HG3	2.05	0.87
1:E:25:C:H2'	1:E:26:M2G:H8	1.37	0.87
1:E:15:G:H2'	1:E:16:H2U:H62	1.55	0.86
2:B:316:PHE:HA	2:B:404:LEU:HD22	1.57	0.86
2:B:354:ARG:HG3	2:B:354:ARG:HH11	1.40	0.86
1:D:11:C:H2'	1:D:12:U:C6	2.11	0.86
2:C:132:VAL:HG23	2:C:209:TYR:HD2	1.41	0.86
2:B:389:ARG:HG2	2:B:394:THR:HA	1.58	0.86
2:B:85:HIS:HD2	2:B:87:ASP:H	1.25	0.85
1:D:30:G:C2'	1:D:31:A:H5'	2.07	0.85
2:B:252:GLU:HA	2:B:266:VAL:HA	1.59	0.84
2:B:335:PHE:CE1	2:B:361:MET:HB2	2.13	0.84
2:B:259:ALA:HB1	2:B:260:PRO:HD2	1.60	0.84
2:C:19:HIS:HD2	2:C:115:GLN:H	1.24	0.84
1:D:15:G:C2'	1:D:16:H2U:H5'	2.08	0.84
2:C:272:MET:HE3	2:C:285:ASN:H	1.43	0.84
1:E:41:U:H2'	1:E:42:G:C8	2.11	0.84
2:B:82:CYS:HB3	2:B:83:PRO:HD2	1.58	0.84
2:C:259:ALA:HB1	2:C:260:PRO:HD2	1.58	0.84
1:F:40:5MC:C2'	1:F:41:U:H5'	2.08	0.84
1:D:23:A:H2'	1:D:24:G:H8	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:A:C2'	1:E:15:G:H5'	2.08	0.83
1:D:13:C:H2'	1:D:14:A:H8	1.43	0.83
1:E:23:A:H2'	1:E:24:G:H8	1.39	0.83
2:B:18:GLY:H	2:B:119:HIS:CD2	1.94	0.83
2:A:217:VAL:CG1	2:A:246:LYS:HD3	2.09	0.83
1:E:36:A:C2'	1:E:37:YYG:H5'	2.08	0.83
2:C:311:THR:HG22	2:C:312:PRO:HD2	1.61	0.82
2:B:129:PRO:HB2	2:B:130:TYR:CE1	2.14	0.82
1:F:16:H2U:H5''	1:F:16:H2U:H62	1.58	0.82
2:A:368:VAL:HG12	2:A:369:THR:H	1.42	0.82
2:B:52:LYS:HB2	2:B:52:LYS:NZ	1.91	0.82
2:B:217:VAL:CG1	2:B:246:LYS:HD3	2.09	0.81
2:B:313:HIS:CD2	2:B:403:ILE:HG21	2.14	0.81
2:C:97:ALA:HA	2:C:126:VAL:HG13	1.62	0.81
1:E:26:M2G:HM12	1:E:44:A:H2	1.45	0.81
1:D:23:A:H2'	1:D:24:G:C8	2.16	0.81
1:E:24:G:C2'	1:E:25:C:H5'	2.10	0.81
2:A:264:LYS:HE2	2:A:307:PRO:HB3	1.62	0.81
2:A:272:MET:HE3	2:A:285:ASN:H	1.45	0.81
1:F:36:A:C2'	1:F:37:YYG:H5'	2.10	0.81
2:B:63:ILE:HG13	2:B:64:ASN:N	1.95	0.81
2:A:63:ILE:HG13	2:A:64:ASN:N	1.95	0.80
1:E:24:G:H2'	1:E:25:C:O4'	1.79	0.80
2:B:19:HIS:CD2	2:B:115:GLN:H	2.00	0.80
1:E:10:2MG:HM23	1:E:11:C:C1'	2.11	0.80
1:E:11:C:H2'	1:E:12:U:C6	2.16	0.80
2:C:158:LEU:HD12	2:C:163:PHE:CB	2.11	0.80
1:D:10:2MG:N2	1:D:26:M2G:H1'	1.97	0.80
1:F:14:A:C2'	1:F:15:G:H5'	2.11	0.80
2:A:224:PRO:HA	2:A:303:VAL:HG22	1.64	0.79
2:A:252:GLU:HA	2:A:266:VAL:HA	1.64	0.79
1:F:9:A:H5'	1:F:46:7MG:H1'	1.63	0.79
1:E:9:A:C5'	1:E:46:7MG:H1'	2.09	0.79
2:A:36:ALA:HA	2:A:42:VAL:HB	1.65	0.79
2:A:55:GLU:HG3	2:A:59:ARG:CG	2.12	0.79
2:C:18:GLY:H	2:C:119:HIS:CD2	1.97	0.79
1:F:64:A:C4'	2:C:391:GLY:HA2	2.12	0.79
1:D:27:C:N4	1:D:43:G:H1	1.81	0.79
1:D:24:G:H2'	1:D:25:C:H6	1.47	0.78
2:B:113:MET:HB3	2:B:114:PRO:HD2	1.64	0.78
1:E:39:PSU:H4'	2:C:360:GLU:CD	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:19:HIS:HD2	2:A:115:GLN:H	1.30	0.78
2:C:335:PHE:CE1	2:C:361:MET:HB2	2.19	0.78
2:B:261:GLU:OE1	2:B:262:THR:HG23	1.84	0.78
2:B:299:GLU:O	2:B:302:GLN:HG3	1.84	0.78
2:A:92:MET:HE3	2:A:119:HIS:HA	1.66	0.77
2:A:313:HIS:CD2	2:A:403:ILE:HG21	2.18	0.77
2:C:19:HIS:CD2	2:C:115:GLN:H	2.02	0.77
2:C:149:LEU:O	2:C:153:GLU:HG3	1.84	0.77
2:C:356:PRO:HD3	2:C:370:PHE:HB3	1.66	0.77
2:B:315:LYS:HB3	2:B:404:LEU:HB2	1.65	0.77
2:B:92:MET:HG3	2:B:119:HIS:CE1	2.20	0.77
2:B:231:ILE:HG22	2:B:234:ARG:HB2	1.66	0.77
2:C:313:HIS:O	2:C:377:PRO:HA	1.86	0.76
1:E:37:YYG:H31	1:E:37:YYG:H1'	1.66	0.76
1:F:37:YYG:H31	1:F:37:YYG:H1'	1.67	0.76
2:C:131:ILE:HD12	2:C:163:PHE:CD1	2.20	0.76
2:B:53:ALA:HB3	2:B:56:GLU:CB	2.15	0.76
2:A:215:ARG:HG2	2:A:282:ALA:O	1.85	0.76
2:B:21:ASP:HA	5:B:406:GNP:HNB3	1.48	0.76
1:D:47:U:O4	1:F:37:YYG:H5''	1.85	0.76
2:A:311:THR:CG2	2:A:312:PRO:HD2	2.16	0.76
2:C:132:VAL:HG22	2:C:169:PRO:HG2	1.65	0.76
2:A:389:ARG:HG2	2:A:394:THR:CA	2.12	0.76
1:F:1:G:C2'	1:F:2:C:H5'	2.16	0.76
1:D:15:G:O2'	1:D:16:H2U:H5'	1.86	0.75
2:C:50:ILE:O	2:C:52:LYS:HG2	1.87	0.75
1:E:36:A:O2'	1:E:37:YYG:H5'	1.85	0.75
1:F:28:C:H2'	1:F:29:A:C8	2.21	0.75
2:C:195:TRP:HA	2:C:195:TRP:CE3	2.21	0.75
2:C:272:MET:CE	2:C:285:ASN:H	2.00	0.75
1:F:1:G:O2'	1:F:2:C:H5'	1.86	0.75
1:F:36:A:O2'	1:F:37:YYG:H5'	1.85	0.74
2:C:68:VAL:CG2	2:C:79:HIS:HB3	2.17	0.74
1:F:40:5MC:H2'	1:F:41:U:H5'	1.68	0.74
2:A:9:LYS:HE3	2:A:71:GLU:OE1	1.88	0.74
2:A:139:ASP:OD1	2:A:140:MET:HG2	1.87	0.74
2:A:261:GLU:OE1	2:A:262:THR:HG23	1.86	0.74
2:B:142:ASP:HA	2:B:147:LEU:HD11	1.70	0.74
1:F:28:C:H42	1:F:42:G:H1	1.36	0.73
2:C:33:TYR:CE1	2:C:44:VAL:HG21	2.23	0.73
2:B:33:TYR:CE2	2:B:44:VAL:HG21	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:HA	2:B:126:VAL:HG13	1.69	0.73
2:C:11:HIS:ND1	2:C:76:HIS:ND1	2.33	0.73
2:B:38:GLU:HG3	2:B:200:TRP:HZ2	1.53	0.73
2:C:256:VAL:HG11	2:C:310:ILE:CG2	2.17	0.73
2:B:315:LYS:CB	2:B:404:LEU:HB2	2.18	0.73
2:C:46:ASP:O	2:C:50:ILE:HG12	1.89	0.73
2:C:287:GLY:C	2:C:288:LEU:HD23	2.09	0.73
2:A:140:MET:HE3	2:A:140:MET:HA	1.71	0.72
1:F:10:2MG:H2'	1:F:11:C:H6	1.54	0.72
2:A:357:GLN:HG2	2:A:358:GLY:N	2.04	0.72
2:B:19:HIS:HD2	2:B:115:GLN:N	1.88	0.72
1:F:37:YYG:H31	1:F:37:YYG:C1'	2.20	0.72
2:C:252:GLU:HA	2:C:266:VAL:HA	1.72	0.72
1:F:64:A:O4'	2:C:391:GLY:HA2	1.89	0.72
1:F:40:5MC:O2'	1:F:41:U:H5'	1.88	0.72
2:C:261:GLU:OE1	2:C:262:THR:HG23	1.90	0.72
1:F:28:C:H2'	1:F:29:A:H8	1.55	0.72
2:B:389:ARG:CG	2:B:394:THR:HA	2.19	0.72
2:A:313:HIS:O	2:A:377:PRO:HA	1.90	0.71
2:C:335:PHE:CD1	2:C:361:MET:HB2	2.25	0.71
1:F:16:H2U:H62	1:F:16:H2U:C5'	2.20	0.71
1:E:30:G:H5''	1:E:31:A:OP2	1.89	0.71
2:A:188:THR:HG23	2:A:192:GLU:HB2	1.72	0.71
2:B:63:ILE:HB	2:B:88:TYR:CE2	2.26	0.71
2:C:338:TYR:O	2:C:353:VAL:HG23	1.90	0.71
2:A:91:ASN:HA	6:A:427:HOH:O	1.91	0.71
2:C:164:PRO:O	2:C:168:VAL:HG23	1.90	0.71
2:B:117:ARG:HD3	2:B:161:TYR:OH	1.91	0.70
2:B:187:LYS:O	2:B:189:LYS:HD3	1.91	0.70
2:A:19:HIS:CG	2:A:113:MET:HB2	2.25	0.70
1:D:26:M2G:N3	1:D:26:M2G:H2'	2.04	0.70
1:E:37:YYG:H31	1:E:37:YYG:C1'	2.21	0.70
2:C:355:LEU:HD22	2:C:362:VAL:HG23	1.72	0.70
2:B:52:LYS:HB2	2:B:52:LYS:HZ2	1.55	0.70
2:A:74:LYS:HG3	6:A:428:HOH:O	1.91	0.70
1:F:8:U:H5'	1:F:49:5MC:OP2	1.92	0.70
2:A:52:LYS:O	2:A:57:ARG:HD2	1.92	0.69
2:B:335:PHE:HD1	2:B:361:MET:HB2	1.57	0.69
2:C:147:LEU:HD13	2:C:172:ARG:HD3	1.72	0.69
2:C:272:MET:HE3	2:C:285:ASN:N	2.06	0.69
2:B:277:LEU:CD2	2:B:280:GLY:HA2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:2MG:CM2	1:E:11:C:H1'	2.22	0.69
2:A:335:PHE:HA	2:A:355:LEU:HD11	1.73	0.69
2:B:272:MET:HE3	2:B:285:ASN:H	1.58	0.69
2:C:117:ARG:HD3	2:C:161:TYR:OH	1.93	0.69
1:E:23:A:O2'	1:E:24:G:H5'	1.93	0.69
2:C:85:HIS:CD2	2:C:87:ASP:H	2.11	0.69
1:E:1:G:C2'	1:E:2:C:H5'	2.23	0.69
2:B:354:ARG:HG3	2:B:354:ARG:NH1	2.07	0.69
2:C:132:VAL:CG2	2:C:209:TYR:HD2	2.05	0.69
1:D:17:H2U:H4'	1:D:18:G:H5''	1.75	0.69
2:B:103:ILE:HD11	2:B:206:ILE:HD11	1.74	0.68
1:D:37:YYG:H31	1:D:37:YYG:C1'	2.23	0.68
1:D:38:A:N3	1:D:38:A:H2'	2.07	0.68
2:C:306:LYS:HB3	2:C:309:SER:HB3	1.74	0.68
1:F:47:U:H5'	1:F:48:C:H5''	1.75	0.68
2:B:223:MET:HB2	2:B:242:ILE:HA	1.75	0.68
2:C:277:LEU:HD23	2:C:280:GLY:HA2	1.74	0.68
1:D:1:G:C2'	1:D:2:C:H5'	2.23	0.68
2:B:215:ARG:HD2	2:B:215:ARG:N	2.08	0.68
2:C:229:PHE:HE1	2:C:239:THR:HG21	1.59	0.68
1:F:10:2MG:HM23	1:F:11:C:C1'	2.23	0.68
2:A:222:LEU:HD11	2:A:303:VAL:HG11	1.74	0.68
2:B:389:ARG:HG2	2:B:394:THR:CA	2.23	0.68
2:A:18:GLY:H	2:A:119:HIS:HD2	1.42	0.68
1:F:19:G:H4'	1:F:20:G:C4	2.29	0.68
1:E:26:M2G:HM12	1:E:44:A:C2	2.27	0.68
2:A:53:ALA:O	2:A:56:GLU:HB2	1.93	0.68
2:B:256:VAL:O	2:B:302:GLN:HB3	1.94	0.68
1:F:1:G:OP3	2:C:300:ARG:NH1	2.27	0.67
2:A:147:LEU:HB3	2:A:172:ARG:NH1	2.09	0.67
2:A:338:TYR:O	2:A:353:VAL:HG23	1.94	0.67
2:C:263:ARG:NH2	2:C:297:GLU:HB3	2.09	0.67
2:B:313:HIS:O	2:B:377:PRO:HA	1.94	0.67
1:D:1:G:O2'	1:D:2:C:H5'	1.94	0.67
1:F:64:A:H4'	2:C:391:GLY:HA2	1.75	0.67
2:A:219:LYS:HB3	2:A:220:PRO:HD2	1.76	0.67
2:B:375:ILE:HG13	2:B:376:LYS:HG3	1.77	0.67
1:D:19:G:H4'	1:D:20:G:C4	2.30	0.67
1:D:24:G:H2'	1:D:25:C:C6	2.29	0.67
1:E:38:A:N3	1:E:38:A:H2'	2.09	0.67
2:C:288:LEU:HD23	2:C:288:LEU:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:YYG:HN20	1:F:37:YYG:C10	2.08	0.66
2:B:40:PRO:CG	2:B:41:ASN:H	2.08	0.66
2:C:56:GLU:CG	2:C:63:ILE:HG23	2.25	0.66
2:A:120:ILE:HD13	2:A:158:LEU:HD23	1.77	0.66
2:B:85:HIS:CD2	2:B:87:ASP:H	2.12	0.66
2:B:198:LYS:HE3	2:B:201:GLU:OE2	1.94	0.66
2:B:89:ILE:HG22	2:B:93:ILE:HD11	1.78	0.66
2:C:85:HIS:HD2	2:C:87:ASP:H	1.42	0.66
2:C:300:ARG:NH2	2:C:348:ASP:OD1	2.29	0.66
2:C:389:ARG:HG2	2:C:394:THR:CA	2.25	0.66
2:C:18:GLY:N	2:C:119:HIS:HD2	1.86	0.66
2:A:46:ASP:O	2:A:50:ILE:HG13	1.96	0.66
2:A:384:LEU:O	2:A:399:VAL:HG23	1.94	0.66
2:B:229:PHE:HE1	2:B:239:THR:HG21	1.60	0.66
2:C:56:GLU:CG	2:C:63:ILE:H	2.09	0.66
1:D:40:5MC:C2'	1:D:41:U:H5'	2.26	0.66
2:A:85:HIS:CD2	2:A:87:ASP:H	1.98	0.66
2:C:19:HIS:HD2	2:C:115:GLN:N	1.92	0.66
1:F:37:YYG:H103	2:A:335:PHE:CE2	2.31	0.65
2:B:248:LYS:HD3	2:B:248:LYS:N	2.11	0.65
1:D:30:G:O2'	1:D:31:A:H5'	1.96	0.65
1:D:39:PSU:O2'	1:D:40:5MC:H5'	1.96	0.65
2:B:18:GLY:N	2:B:119:HIS:HD2	1.87	0.65
1:D:74:C:OP1	2:A:52:LYS:NZ	2.30	0.65
2:C:132:VAL:HG23	2:C:209:TYR:CD2	2.30	0.65
1:D:40:5MC:H2'	1:D:41:U:H5'	1.77	0.65
2:A:33:TYR:CE1	2:A:44:VAL:HG21	2.31	0.65
2:A:306:LYS:HB3	2:A:309:SER:HB3	1.78	0.65
2:C:384:LEU:O	2:C:399:VAL:HG23	1.95	0.65
2:B:53:ALA:HB3	2:B:56:GLU:CG	2.26	0.65
2:B:312:PRO:O	2:B:313:HIS:ND1	2.30	0.65
2:B:354:ARG:HH12	2:B:373:GLU:CD	1.99	0.65
2:B:7:ARG:NH2	2:B:284:ASP:OD1	2.30	0.65
1:F:41:U:H2'	1:F:42:G:O4'	1.95	0.65
2:A:248:LYS:HE3	2:A:251:ASP:OD2	1.97	0.65
2:A:389:ARG:CG	2:A:394:THR:HA	2.19	0.65
2:C:118:GLU:OE2	2:C:389:ARG:NH1	2.30	0.65
2:B:19:HIS:CG	2:B:113:MET:HB2	2.31	0.65
2:C:91:ASN:OD1	2:C:91:ASN:N	2.28	0.65
1:E:24:G:H2'	1:E:25:C:H5'	1.77	0.65
1:E:26:M2G:HM23	1:E:27:C:O4'	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:GLU:OE1	2:C:262:THR:N	2.30	0.65
1:D:58:1MA:H5'	1:F:34:OMG:O6	1.98	0.64
2:B:316:PHE:CA	2:B:404:LEU:HD22	2.26	0.64
2:C:155:ARG:NH2	2:C:170:VAL:HG23	2.12	0.64
2:C:317:GLU:HB3	2:C:401:THR:HG22	1.78	0.64
1:E:36:A:H2'	1:E:37:YYG:H8	1.79	0.64
1:D:16:H2U:H4'	1:D:17:H2U:OP2	1.96	0.64
1:D:47:U:C4	1:F:37:YYG:H5''	2.32	0.64
2:C:253:VAL:N	2:C:265:THR:O	2.30	0.64
2:A:62:THR:HG22	2:A:83:PRO:HB3	1.78	0.64
2:A:155:ARG:NH1	2:A:168:VAL:O	2.30	0.64
1:D:7:U:H4'	1:D:8:U:OP2	1.97	0.64
2:A:55:GLU:OE2	2:A:59:ARG:HD3	1.98	0.64
2:B:4:GLU:O	2:B:275:LYS:HB3	1.97	0.64
2:C:33:TYR:HA	2:C:44:VAL:HG12	1.80	0.64
2:A:150:VAL:O	2:A:154:VAL:HG23	1.97	0.64
2:C:33:TYR:HA	2:C:44:VAL:CG1	2.27	0.64
2:C:56:GLU:HG2	2:C:63:ILE:H	1.62	0.64
2:C:259:ALA:CB	2:C:260:PRO:HD2	2.23	0.64
1:D:38:A:H5''	1:D:39:PSU:OP2	1.98	0.64
1:F:16:H2U:H5''	1:F:16:H2U:C6	2.28	0.63
2:B:9:LYS:NZ	2:B:72:THR:O	2.29	0.63
1:D:35:A:O2'	1:D:36:A:H5'	1.99	0.63
2:A:40:PRO:CG	2:A:41:ASN:H	2.11	0.63
1:E:28:C:H5''	1:E:29:A:OP2	1.98	0.63
1:E:35:A:O2'	1:E:36:A:H5'	1.98	0.63
2:A:317:GLU:HB3	2:A:401:THR:HG22	1.80	0.63
1:F:37:YYG:H103	2:A:335:PHE:CZ	2.33	0.63
1:F:67:A:OP1	2:C:376:LYS:NZ	2.29	0.63
2:A:6:ILE:O	2:A:8:THR:HG23	1.98	0.63
2:C:223:MET:O	2:C:223:MET:HG3	1.98	0.63
2:C:303:VAL:C	2:C:304:LEU:HD23	2.19	0.63
1:E:37:YYG:H141	1:E:37:YYG:H101	1.80	0.63
2:A:97:ALA:HA	2:A:126:VAL:CG1	2.26	0.63
2:A:248:LYS:HD3	2:A:279:GLU:HG3	1.80	0.63
2:A:256:VAL:HG11	2:A:310:ILE:HG22	1.79	0.63
2:A:265:THR:HG21	2:A:290:LEU:HB3	1.81	0.63
2:A:294:SER:OG	2:A:297:GLU:HG3	1.99	0.63
2:B:124:ARG:HG2	2:B:124:ARG:HH11	1.64	0.63
2:C:113:MET:HB3	2:C:114:PRO:HD2	1.81	0.63
2:A:335:PHE:CE1	2:A:361:MET:HB2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLU:HG2	2:B:122:LEU:HD11	1.81	0.63
2:C:40:PRO:CG	2:C:41:ASN:H	2.10	0.63
2:C:6:ILE:O	2:C:8:THR:N	2.30	0.63
2:C:303:VAL:O	2:C:304:LEU:HD23	1.98	0.63
2:A:187:LYS:O	2:A:189:LYS:HD3	1.98	0.63
2:C:36:ALA:HA	2:C:42:VAL:HB	1.80	0.62
2:C:277:LEU:HD23	2:C:280:GLY:CA	2.29	0.62
2:B:209:TYR:O	2:B:211:PRO:HD3	1.99	0.62
2:A:335:PHE:CD1	2:A:361:MET:HB2	2.33	0.62
2:C:342:PHE:O	2:C:348:ASP:HA	1.99	0.62
2:C:217:VAL:O	2:C:245:GLY:HA2	1.99	0.62
2:A:315:LYS:HD3	2:A:405:GLU:OE2	2.00	0.62
2:A:316:PHE:HA	2:A:404:LEU:HD22	1.81	0.62
2:B:97:ALA:HA	2:B:126:VAL:CG1	2.30	0.62
2:B:287:GLY:O	2:B:288:LEU:HD23	2.00	0.62
1:D:67:A:OP1	2:A:376:LYS:NZ	2.28	0.62
2:C:121:LEU:HD13	2:C:161:TYR:CD1	2.35	0.62
1:E:58:1MA:H4'	1:E:59:U:OP1	2.00	0.62
2:C:25:THR:HG23	2:C:50:ILE:HG21	1.81	0.62
1:D:34:OMG:H5''	1:D:35:A:OP2	2.00	0.62
2:A:7:ARG:HH22	2:A:284:ASP:CG	2.03	0.61
2:B:56:GLU:HG3	2:B:63:ILE:HG12	1.80	0.61
2:C:195:TRP:HA	2:C:195:TRP:HE3	1.65	0.61
2:C:229:PHE:HE1	2:C:239:THR:CG2	2.13	0.61
1:D:30:G:H2'	1:D:31:A:H5'	1.81	0.61
2:A:55:GLU:HG3	2:A:59:ARG:CD	2.31	0.61
2:A:261:GLU:OE1	2:A:262:THR:N	2.30	0.61
2:B:96:ALA:HA	2:B:99:MET:HG3	1.83	0.61
2:C:27:LEU:HD21	2:C:202:LEU:CD2	2.31	0.61
2:C:256:VAL:HG11	2:C:310:ILE:HG22	1.79	0.61
2:B:38:GLU:HG3	2:B:200:TRP:CZ2	2.35	0.61
2:C:117:ARG:HH12	2:C:160:GLN:HE22	1.48	0.61
2:C:381:GLU:HG3	2:C:384:LEU:HB2	1.83	0.61
2:B:85:HIS:HD2	2:B:87:ASP:N	1.95	0.61
2:C:16:THR:OG1	2:C:81:ASP:HA	2.00	0.61
2:A:315:LYS:HG2	2:A:373:GLU:HG3	1.83	0.61
2:A:220:PRO:HB3	2:A:306:LYS:HD3	1.83	0.61
1:E:27:C:H5''	6:E:79:HOH:O	2.01	0.60
2:A:55:GLU:O	2:A:59:ARG:HG3	2.01	0.60
2:A:299:GLU:O	2:A:302:GLN:HG3	2.01	0.60
2:A:342:PHE:O	2:A:348:ASP:HA	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:HIS:HE1	2:C:103:ILE:HD12	1.66	0.60
2:C:277:LEU:CD2	2:C:280:GLY:HA2	2.31	0.60
2:A:85:HIS:CD2	2:A:87:ASP:HB2	2.35	0.60
2:C:19:HIS:CG	2:C:113:MET:HB2	2.36	0.60
2:C:336:THR:H	2:C:355:LEU:HD12	1.66	0.60
2:A:143:ASP:OD1	2:A:146:LEU:N	2.32	0.60
1:D:18:G:OP2	1:D:58:1MA:HM11	2.02	0.60
2:A:46:ASP:O	2:A:49:ASP:HB2	2.02	0.60
2:A:129:PRO:HB2	2:A:130:TYR:CD1	2.36	0.60
2:B:354:ARG:NH1	2:B:373:GLU:OE1	2.28	0.60
2:C:147:LEU:HD12	2:C:172:ARG:HH11	1.65	0.60
2:B:108:ALA:HB2	2:B:135:MET:HG2	1.82	0.60
2:B:92:MET:HE3	2:B:119:HIS:HA	1.82	0.60
2:B:189:LYS:HG2	2:B:192:GLU:OE2	2.02	0.60
1:F:8:U:O2	1:F:21:A:H2	1.84	0.60
2:B:55:GLU:HG2	2:B:59:ARG:HD3	1.84	0.60
1:E:9:A:HO2'	1:E:11:C:H5	1.49	0.60
2:A:19:HIS:CD2	2:A:115:GLN:H	2.15	0.60
2:A:113:MET:HB3	2:A:114:PRO:HD2	1.82	0.60
2:C:156:ASP:O	2:C:159:ASN:HB2	2.02	0.60
2:C:354:ARG:HH11	2:C:354:ARG:CG	2.12	0.60
1:D:33:U:H3	1:D:35:A:H3'	1.67	0.59
2:C:126:VAL:HG22	2:C:345:ARG:HA	1.84	0.59
1:D:16:H2U:O2'	1:D:16:H2U:H62	2.02	0.59
2:B:33:TYR:O	2:B:36:ALA:HB3	2.02	0.59
2:B:91:ASN:N	2:B:91:ASN:OD1	2.36	0.59
2:C:9:LYS:HE3	2:C:71:GLU:OE1	2.01	0.59
2:A:222:LEU:HD11	2:A:303:VAL:CG1	2.32	0.59
2:A:277:LEU:HD23	2:A:280:GLY:CA	2.32	0.59
2:A:384:LEU:HD12	2:A:385:ARG:N	2.17	0.59
2:C:13:ASN:ND2	2:C:100:ASP:OD2	2.35	0.59
2:C:180:GLU:O	2:C:183:HIS:HB2	2.03	0.59
2:B:231:ILE:CG2	2:B:234:ARG:HB2	2.31	0.59
2:C:27:LEU:HD13	2:C:134:PHE:CE2	2.38	0.59
2:C:46:ASP:O	2:C:49:ASP:HB2	2.02	0.59
2:A:216:ASP:OD1	2:A:216:ASP:N	2.30	0.59
2:B:202:LEU:HD12	2:B:202:LEU:O	2.02	0.59
2:B:277:LEU:HD23	2:B:280:GLY:HA2	1.84	0.59
2:C:40:PRO:HG2	2:C:41:ASN:H	1.66	0.59
2:C:56:GLU:HG2	2:C:63:ILE:N	2.17	0.59
1:E:41:U:H2'	1:E:42:G:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:VAL:N	2:A:265:THR:O	2.30	0.59
2:C:108:ALA:HB2	2:C:135:MET:CG	2.33	0.59
2:C:315:LYS:HG2	2:C:373:GLU:HG3	1.83	0.59
1:F:28:C:N4	1:F:42:G:H1	1.99	0.59
2:B:355:LEU:HD22	2:B:362:VAL:HG23	1.85	0.59
2:C:5:PHE:CD2	2:C:275:LYS:HD2	2.38	0.59
2:B:311:THR:HG22	2:B:312:PRO:HD2	1.85	0.58
2:A:320:VAL:HG12	2:A:321:TYR:N	2.19	0.58
2:C:117:ARG:HH12	2:C:160:GLN:NE2	2.00	0.58
2:C:281:ILE:N	2:C:284:ASP:OD2	2.29	0.58
2:C:248:LYS:HD3	2:C:248:LYS:N	2.17	0.58
2:B:259:ALA:CB	2:B:260:PRO:HD2	2.21	0.58
2:C:98:GLN:OE1	2:C:226:GLU:HG3	2.03	0.58
2:B:217:VAL:HG12	2:B:246:LYS:CD	2.30	0.58
2:B:336:THR:N	2:B:355:LEU:HD12	2.18	0.58
2:C:29:ALA:O	2:C:33:TYR:HD2	1.85	0.58
2:C:92:MET:HE1	2:C:119:HIS:HA	1.85	0.58
1:D:10:2MG:C2	1:D:26:M2G:H1'	2.38	0.58
2:A:31:LEU:HD13	2:A:70:TYR:OH	2.03	0.58
2:C:138:VAL:HG21	2:C:172:ARG:HB3	1.86	0.58
2:C:311:THR:HG22	2:C:312:PRO:CD	2.33	0.58
2:C:316:PHE:CA	2:C:404:LEU:HD22	2.29	0.58
1:D:2:C:H5''	2:A:88:TYR:CE1	2.39	0.58
1:E:11:C:C2'	1:E:12:U:H6	2.14	0.58
2:A:259:ALA:CB	2:A:260:PRO:HD2	2.20	0.57
2:A:277:LEU:CD2	2:A:280:GLY:HA2	2.33	0.57
2:C:51:ASP:O	2:C:53:ALA:N	2.36	0.57
2:C:248:LYS:N	2:C:251:ASP:OD2	2.29	0.57
2:B:306:LYS:HB3	2:B:309:SER:HB3	1.86	0.57
2:C:266:VAL:HG21	2:C:291:ARG:NH2	2.19	0.57
2:C:375:ILE:O	2:C:376:LYS:HG3	2.03	0.57
1:D:38:A:C2'	1:D:39:PSU:H5''	2.34	0.57
2:B:14:VAL:HA	2:B:101:GLY:O	2.04	0.57
2:B:150:VAL:O	2:B:154:VAL:HG23	2.03	0.57
2:C:48:GLY:O	2:C:52:LYS:HB3	2.05	0.57
1:E:26:M2G:CM1	1:E:44:A:H2	2.17	0.57
1:E:75:C:OP1	2:B:52:LYS:HD3	2.03	0.57
2:B:216:ASP:OD1	2:B:216:ASP:N	2.35	0.57
2:A:138:VAL:HG21	2:A:173:GLY:N	2.19	0.57
1:F:44:A:O2'	1:F:45:G:H5'	2.05	0.57
2:B:63:ILE:HB	2:B:88:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:LEU:HB2	5:C:406:GNP:C5	2.35	0.57
2:C:213:PRO:HG2	2:C:215:ARG:CZ	2.35	0.57
2:A:19:HIS:HD2	2:A:115:GLN:N	2.02	0.56
2:A:343:TYR:CE2	2:A:348:ASP:HB2	2.40	0.56
2:A:21:ASP:HA	5:A:406:GNP:HNB3	1.68	0.56
2:B:219:LYS:HB3	2:B:220:PRO:HD2	1.87	0.56
2:C:113:MET:HB3	2:C:114:PRO:CD	2.35	0.56
1:E:32:OMC:H2'	1:E:33:U:H6	1.70	0.56
2:A:75:ARG:NH2	2:A:210:ILE:O	2.30	0.56
2:B:231:ILE:N	2:B:231:ILE:HD13	2.20	0.56
2:C:108:ALA:HB2	2:C:135:MET:HG2	1.86	0.56
2:C:169:PRO:HG2	2:C:209:TYR:CD2	2.41	0.56
2:B:103:ILE:CD1	2:B:206:ILE:HD11	2.35	0.56
2:B:248:LYS:HD2	2:B:279:GLU:OE2	2.06	0.56
2:C:117:ARG:HG3	2:C:161:TYR:HE2	1.68	0.56
2:A:287:GLY:O	2:A:288:LEU:HD23	2.04	0.56
2:B:339:ARG:HD2	2:B:352:VAL:HG22	1.86	0.56
4:D:77:PHE:N	2:A:272:MET:HA	2.21	0.56
2:A:313:HIS:HD2	2:A:403:ILE:CD1	2.18	0.56
2:C:75:ARG:NH2	2:C:210:ILE:O	2.29	0.56
2:C:258:LEU:HD23	2:C:258:LEU:N	2.20	0.56
2:C:281:ILE:HG13	2:C:284:ASP:OD2	2.05	0.56
2:A:343:TYR:HA	2:A:347:THR:O	2.05	0.56
2:B:54:PRO:O	2:B:58:ALA:N	2.36	0.56
2:B:140:MET:CE	2:B:140:MET:HA	2.36	0.56
2:B:247:VAL:C	2:B:248:LYS:HD3	2.26	0.56
1:E:18:G:O6	1:E:55:PSU:H1'	2.06	0.56
2:B:127:GLY:O	2:B:129:PRO:HD3	2.06	0.56
2:C:107:SER:HB2	2:C:137:LYS:HD2	1.88	0.56
2:B:229:PHE:O	2:B:237:VAL:N	2.29	0.56
2:C:368:VAL:HG12	2:C:369:THR:H	1.71	0.56
2:A:118:GLU:OE2	2:A:389:ARG:NH1	2.38	0.56
2:C:79:HIS:HE1	2:C:103:ILE:CD1	2.18	0.56
2:B:40:PRO:HG2	2:B:41:ASN:H	1.70	0.55
1:E:15:G:H2'	1:E:16:H2U:C6	2.32	0.55
1:F:3:G:O2'	1:F:4:G:H5'	2.07	0.55
1:F:34:OMG:H2'	1:F:35:A:O4'	2.06	0.55
2:A:55:GLU:CG	2:A:59:ARG:HG3	2.29	0.55
2:A:143:ASP:O	2:A:147:LEU:HD22	2.07	0.55
2:A:202:LEU:HD12	2:A:202:LEU:O	2.06	0.55
2:B:320:VAL:HG12	2:B:321:TYR:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:H2U:H4'	1:E:18:G:OP2	2.06	0.55
1:F:47:U:H5'	1:F:48:C:C5'	2.36	0.55
2:B:118:GLU:HG2	2:B:122:LEU:CD1	2.35	0.55
2:C:135:MET:CE	2:C:151:GLU:HB2	2.36	0.55
2:C:136:ASN:HA	2:C:173:GLY:O	2.07	0.55
1:D:29:A:H2	1:D:41:U:O2	1.89	0.55
2:C:299:GLU:O	2:C:302:GLN:HG3	2.06	0.55
2:C:336:THR:N	2:C:355:LEU:HD12	2.21	0.55
1:E:1:G:C3'	1:E:2:C:H5'	2.37	0.55
2:A:143:ASP:OD1	2:A:145:GLU:N	2.39	0.55
2:B:63:ILE:HB	2:B:88:TYR:CD2	2.41	0.55
2:B:87:ASP:C	2:B:88:TYR:HD1	2.10	0.55
2:B:177:LEU:N	2:B:177:LEU:HD12	2.21	0.55
2:B:338:TYR:O	2:B:353:VAL:HG23	2.06	0.55
2:C:1:ALA:HB2	2:C:271:GLU:OE2	2.06	0.55
1:E:34:OMG:H8	1:E:34:OMG:O5'	1.90	0.55
2:A:9:LYS:NZ	2:A:72:THR:O	2.29	0.55
2:B:21:ASP:HA	5:B:406:GNP:N3B	2.19	0.55
2:C:177:LEU:HB3	2:C:195:TRP:CD1	2.41	0.55
2:C:315:LYS:HB2	2:C:404:LEU:HB2	1.88	0.55
1:F:36:A:H2'	1:F:37:YYG:H5'	1.89	0.55
2:A:46:ASP:HB2	2:A:49:ASP:OD2	2.07	0.55
1:F:36:A:H2'	1:F:37:YYG:H8	1.89	0.54
2:B:103:ILE:HA	2:B:132:VAL:O	2.07	0.54
2:C:9:LYS:NZ	2:C:72:THR:O	2.31	0.54
2:C:368:VAL:CG1	2:C:369:THR:H	2.20	0.54
2:A:227:ASP:OD1	2:A:228:VAL:N	2.40	0.54
2:B:248:LYS:HE3	2:B:251:ASP:OD2	2.07	0.54
2:C:14:VAL:O	2:C:79:HIS:HA	2.06	0.54
1:F:9:A:C5'	1:F:46:7MG:H1'	2.36	0.54
2:B:256:VAL:HG11	2:B:310:ILE:HG22	1.90	0.54
2:C:19:HIS:NE2	2:C:114:PRO:HD2	2.21	0.54
1:D:2:C:H4'	2:A:88:TYR:HE1	1.72	0.54
2:A:334:PHE:O	2:A:361:MET:HA	2.08	0.54
1:D:45:G:O5'	1:D:45:G:H8	1.91	0.54
2:B:53:ALA:HB1	2:B:54:PRO:CD	2.37	0.54
1:E:16:H2U:H4'	1:E:17:H2U:OP2	1.95	0.54
2:C:63:ILE:HG13	2:C:64:ASN:N	2.22	0.54
2:C:263:ARG:HG3	2:C:264:LYS:H	1.73	0.54
2:A:18:GLY:H	2:A:119:HIS:CD2	2.24	0.54
2:A:315:LYS:HE2	2:A:404:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:SER:OG	2:B:297:GLU:HG3	2.06	0.54
2:C:89:ILE:O	2:C:93:ILE:HD12	2.07	0.54
2:C:140:MET:HA	2:C:140:MET:CE	2.37	0.54
2:C:248:LYS:HE3	2:C:251:ASP:OD2	2.07	0.54
2:A:108:ALA:HB2	2:A:135:MET:HG2	1.88	0.54
1:E:25:C:C2	1:E:26:M2G:C8	2.96	0.54
2:A:27:LEU:HG	2:A:27:LEU:O	2.06	0.54
2:A:38:GLU:OE2	2:A:190:ARG:HG3	2.07	0.54
2:A:38:GLU:HG3	2:A:200:TRP:CZ2	2.43	0.54
2:B:385:ARG:HA	2:B:399:VAL:HA	1.89	0.54
2:C:117:ARG:HG3	2:C:157:LEU:HD11	1.90	0.54
2:C:315:LYS:CB	2:C:404:LEU:HB2	2.38	0.54
1:D:46:7MG:H4'	1:D:47:U:OP2	2.07	0.54
1:E:8:U:O2	1:E:21:A:H2	1.91	0.54
2:C:237:VAL:HG22	2:C:289:LEU:HD13	1.88	0.54
1:F:10:2MG:H2'	1:F:11:C:C6	2.40	0.53
1:F:19:G:OP1	1:F:60:C:N4	2.41	0.53
1:F:26:M2G:N3	1:F:26:M2G:H2'	2.23	0.53
2:B:59:ARG:NH1	2:B:88:TYR:OH	2.41	0.53
2:B:277:LEU:HD23	2:B:280:GLY:CA	2.38	0.53
2:C:169:PRO:CG	2:C:209:TYR:CD2	2.91	0.53
1:F:19:G:H4'	1:F:20:G:N3	2.23	0.53
2:C:216:ASP:N	2:C:216:ASP:OD1	2.41	0.53
2:A:400:VAL:HG12	2:A:401:THR:N	2.24	0.53
2:C:263:ARG:HG3	2:C:264:LYS:N	2.22	0.53
1:F:6:U:H2'	1:F:7:U:C6	2.44	0.53
1:F:25:C:C4	1:F:26:M2G:N7	2.77	0.53
2:B:176:LEU:HB2	5:B:406:GNP:C5	2.39	0.53
1:E:11:C:C2	1:E:12:U:C5	2.97	0.53
2:A:24:LYS:HE3	2:A:82:CYS:O	2.09	0.53
2:B:11:HIS:HE1	2:B:78:SER:OG	1.89	0.53
1:E:3:G:C8	1:E:3:G:H3'	2.43	0.53
1:E:10:2MG:H2'	1:E:11:C:C6	2.43	0.53
2:C:356:PRO:CD	2:C:370:PHE:HB3	2.38	0.53
1:D:2:C:H5''	2:A:88:TYR:HE1	1.74	0.53
2:A:312:PRO:O	2:A:313:HIS:ND1	2.41	0.53
1:F:10:2MG:C4	1:F:11:C:C5	2.97	0.53
2:B:151:GLU:O	2:B:155:ARG:HG3	2.08	0.53
2:B:230:THR:HA	2:B:235:GLY:O	2.09	0.53
2:C:335:PHE:HA	2:C:355:LEU:HD11	1.91	0.53
1:F:3:G:C8	1:F:3:G:H3'	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:GLY:HA3	2:A:210:ILE:CD1	2.26	0.53
1:D:24:G:O2'	1:D:25:C:H5'	2.09	0.53
1:D:34:OMG:HM22	1:D:35:A:H5'	1.91	0.53
1:E:35:A:C2'	1:E:36:A:H5'	2.39	0.53
2:C:399:VAL:HG22	2:C:400:VAL:N	2.23	0.53
2:A:117:ARG:HH12	2:A:160:GLN:HE22	1.57	0.52
2:A:384:LEU:HD12	2:A:385:ARG:H	1.74	0.52
2:B:190:ARG:HG2	2:B:200:TRP:CE2	2.44	0.52
2:C:17:ILE:HD12	2:C:119:HIS:HB3	1.90	0.52
1:D:36:A:O2'	1:D:37:YYG:H5'	2.09	0.52
2:B:313:HIS:HD2	2:B:403:ILE:HD13	1.74	0.52
2:C:106:VAL:HG21	2:C:154:VAL:HG21	1.91	0.52
2:C:169:PRO:HD2	2:C:209:TYR:CD2	2.44	0.52
1:F:26:M2G:C5	1:F:27:C:C5	2.98	0.52
2:A:222:LEU:HD12	2:A:223:MET:N	2.24	0.52
2:A:313:HIS:HD2	2:A:403:ILE:HD13	1.74	0.52
2:B:174:SER:OG	2:B:177:LEU:HD13	2.09	0.52
2:C:161:TYR:O	2:C:162:GLU:HB2	2.10	0.52
1:D:25:C:N3	1:D:26:M2G:C8	2.78	0.52
2:B:88:TYR:HD1	2:B:88:TYR:N	2.07	0.52
2:C:241:ARG:HD2	6:C:412:HOH:O	2.09	0.52
1:D:9:A:H5'	1:D:46:7MG:H1'	1.90	0.52
1:D:11:C:C6	1:D:12:U:H5	2.27	0.52
1:E:36:A:H2'	1:E:37:YYG:H5'	1.89	0.52
1:F:37:YYG:C10	1:F:37:YYG:N20	2.72	0.52
4:F:77:PHE:N	2:C:273:HIS:H	2.07	0.52
2:C:315:LYS:HD3	2:C:405:GLU:HG3	1.90	0.52
1:D:35:A:C2'	1:D:36:A:H5'	2.40	0.52
1:F:11:C:C2	1:F:12:U:C5	2.98	0.52
2:A:62:THR:HB	5:A:406:GNP:O3G	2.10	0.52
2:B:55:GLU:OE2	2:B:59:ARG:NH1	2.40	0.52
2:C:19:HIS:HA	2:C:115:GLN:HB2	1.92	0.52
2:C:222:LEU:HD12	2:C:303:VAL:HG13	1.92	0.52
1:D:10:2MG:HN2	1:D:26:M2G:H1'	1.71	0.52
1:F:10:2MG:CM2	1:F:11:C:H1'	2.32	0.52
2:A:85:HIS:HD2	2:A:87:ASP:N	1.90	0.52
1:D:14:A:C2'	1:D:15:G:H5'	2.40	0.52
2:A:54:PRO:O	2:A:58:ALA:N	2.33	0.52
2:C:102:ALA:O	2:C:131:ILE:HA	2.10	0.52
1:D:11:C:H6	1:D:11:C:O5'	1.93	0.52
1:D:26:M2G:HM12	1:D:44:A:H2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:A:H2'	1:D:30:G:C8	2.45	0.52
2:A:354:ARG:NH1	2:A:373:GLU:OE1	2.30	0.52
2:B:7:ARG:HH22	2:B:284:ASP:CG	2.12	0.52
2:B:61:ILE:O	2:B:61:ILE:HG13	2.10	0.52
2:B:221:PHE:HA	2:B:244:ARG:O	2.10	0.52
2:C:380:LEU:C	2:C:381:GLU:HG2	2.26	0.52
1:E:19:G:H4'	1:E:20:G:C4	2.46	0.51
2:C:318:ALA:HA	2:C:401:THR:HB	1.91	0.51
1:E:24:G:C8	1:E:25:C:C5	2.98	0.51
1:E:34:OMG:H2'	1:E:35:A:O4'	2.10	0.51
2:B:117:ARG:HH12	2:B:160:GLN:HE22	1.59	0.51
2:B:254:GLU:OE1	2:B:308:GLY:N	2.36	0.51
2:C:140:MET:HA	2:C:140:MET:HE3	1.92	0.51
2:A:47:TYR:O	2:A:50:ILE:N	2.40	0.51
2:B:217:VAL:HG12	2:B:246:LYS:NZ	2.25	0.51
2:B:362:VAL:CG2	2:B:368:VAL:HG21	2.41	0.51
1:D:25:C:C2	1:D:26:M2G:C8	2.98	0.51
2:B:368:VAL:HG12	2:B:369:THR:N	2.18	0.51
2:C:237:VAL:HA	2:C:288:LEU:O	2.10	0.51
1:D:13:C:C2	1:D:14:A:C8	2.98	0.51
1:D:14:A:C5	1:D:22:G:C2	2.98	0.51
1:E:1:G:P	2:B:300:ARG:HH11	2.34	0.51
1:E:24:G:C6	1:E:25:C:N3	2.79	0.51
2:C:354:ARG:HG3	2:C:354:ARG:NH1	2.09	0.51
2:A:149:LEU:O	2:A:153:GLU:HG3	2.10	0.51
2:B:190:ARG:HG2	2:B:200:TRP:NE1	2.26	0.51
2:C:70:TYR:O	2:C:77:TYR:HB2	2.10	0.51
1:D:37:YYG:H103	2:B:335:PHE:HE2	1.76	0.51
1:D:66:A:O2'	1:D:67:A:H5'	2.11	0.51
2:A:317:GLU:N	2:A:404:LEU:HD22	2.25	0.51
2:A:333:GLY:HA3	2:A:363:MET:SD	2.50	0.51
1:D:10:2MG:C6	1:D:11:C:C4	2.99	0.51
1:D:15:G:H2'	1:D:16:H2U:H5'	1.92	0.51
1:F:24:G:C6	1:F:25:C:C4	2.99	0.51
2:B:253:VAL:N	2:B:265:THR:O	2.35	0.51
2:C:147:LEU:HB3	2:C:172:ARG:NH1	2.26	0.51
2:C:320:VAL:HG12	2:C:321:TYR:N	2.26	0.51
2:C:355:LEU:CD2	2:C:362:VAL:HG23	2.40	0.51
1:F:64:A:H4'	2:C:391:GLY:CA	2.41	0.51
2:B:55:GLU:HG2	2:B:59:ARG:CD	2.41	0.51
2:B:124:ARG:HB2	2:B:163:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:VAL:HG12	2:B:214:VAL:O	2.11	0.51
2:B:254:GLU:O	2:B:304:LEU:HA	2.11	0.51
2:C:11:HIS:HD1	2:C:76:HIS:CE1	2.24	0.51
1:D:48:C:N4	1:D:59:U:C5	2.79	0.51
1:E:10:2MG:N2	1:E:11:C:C2	2.79	0.51
2:A:188:THR:HG23	2:A:192:GLU:CB	2.41	0.51
1:D:44:A:C6	1:D:45:G:C6	2.99	0.50
1:E:10:2MG:C4	1:E:11:C:C5	2.99	0.50
1:F:27:C:H2'	1:F:28:C:H6	1.75	0.50
2:A:333:GLY:HA2	2:A:362:VAL:O	2.12	0.50
2:B:254:GLU:CD	2:B:308:GLY:H	2.14	0.50
2:C:19:HIS:CD2	2:C:113:MET:HB3	2.46	0.50
1:D:25:C:C4	1:D:26:M2G:N7	2.79	0.50
1:E:24:G:C5	1:E:25:C:C2	3.00	0.50
1:F:24:G:C5	1:F:25:C:C4	2.99	0.50
1:F:24:G:H2'	1:F:25:C:C6	2.46	0.50
1:F:59:U:C5	1:F:60:C:N4	2.79	0.50
2:A:55:GLU:CG	2:A:59:ARG:HD3	2.41	0.50
1:E:24:G:N7	1:E:25:C:C4	2.80	0.50
1:F:26:M2G:C6	1:F:27:C:C4	2.99	0.50
2:A:69:GLU:O	2:A:70:TYR:HB3	2.10	0.50
2:B:113:MET:HB3	2:B:114:PRO:CD	2.40	0.50
2:B:231:ILE:HG22	2:B:234:ARG:HG3	1.92	0.50
2:C:179:LEU:HG	2:C:183:HIS:CE1	2.45	0.50
1:D:14:A:C6	1:D:22:G:C2	2.99	0.50
1:E:1:G:C2	1:E:73:A:N3	2.79	0.50
2:A:151:GLU:HG3	2:A:170:VAL:HG11	1.94	0.50
2:B:88:TYR:N	2:B:88:TYR:CD1	2.79	0.50
1:D:11:C:C2	1:D:12:U:C5	3.00	0.50
1:E:59:U:C5	1:E:60:C:N4	2.78	0.50
1:F:74:C:C4	1:F:75:C:C4	2.98	0.50
5:C:406:GNP:O3G	5:C:406:GNP:O2B	2.29	0.50
1:E:26:M2G:C4	1:E:27:C:C5	2.99	0.50
2:B:190:ARG:HA	2:B:197:ASP:OD1	2.12	0.50
1:D:24:G:C5	1:D:25:C:C5	3.00	0.50
1:F:24:G:C5	1:F:25:C:C5	3.00	0.50
2:B:46:ASP:O	2:B:50:ILE:HG13	2.11	0.50
1:D:48:C:N4	1:D:59:U:C4	2.80	0.50
1:E:25:C:C4	1:E:26:M2G:N7	2.79	0.50
1:F:24:G:N7	1:F:25:C:C5	2.79	0.50
2:A:7:ARG:NH2	2:A:284:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:PRO:HG2	2:A:41:ASN:OD1	2.11	0.50
2:A:140:MET:HA	2:A:140:MET:CE	2.41	0.50
2:B:229:PHE:HE1	2:B:239:THR:CG2	2.25	0.50
2:C:131:ILE:HD12	2:C:163:PHE:CE1	2.47	0.50
1:E:10:2MG:H2'	1:E:11:C:H6	1.76	0.50
1:E:30:G:H8	1:E:30:G:OP2	1.95	0.50
1:F:74:C:C5	1:F:75:C:C4	3.00	0.50
2:A:198:LYS:O	2:A:201:GLU:HB2	2.11	0.50
2:C:21:ASP:HA	5:C:406:GNP:HNB3	1.77	0.50
2:C:34:VAL:CG1	2:C:200:TRP:CE2	2.95	0.50
2:A:139:ASP:OD2	2:A:174:SER:HB2	2.11	0.49
2:A:188:THR:CG2	2:A:192:GLU:HB2	2.40	0.49
2:B:217:VAL:O	2:B:245:GLY:HA2	2.12	0.49
2:C:134:PHE:CD1	2:C:171:ILE:HG22	2.46	0.49
2:C:177:LEU:HD23	2:C:195:TRP:NE1	2.27	0.49
1:F:44:A:O5'	1:F:44:A:H8	1.94	0.49
2:A:98:GLN:OE1	2:A:226:GLU:HG3	2.11	0.49
2:A:315:LYS:HD3	2:A:405:GLU:CD	2.31	0.49
2:B:49:ASP:OD1	2:B:49:ASP:N	2.42	0.49
2:B:217:VAL:CG1	2:B:246:LYS:NZ	2.75	0.49
2:B:231:ILE:HG22	2:B:234:ARG:CB	2.38	0.49
2:C:56:GLU:CD	2:C:63:ILE:H	2.15	0.49
2:C:236:THR:HG21	2:C:293:VAL:HG23	1.93	0.49
2:C:312:PRO:O	2:C:313:HIS:ND1	2.46	0.49
1:F:12:U:C2	1:F:24:G:N2	2.80	0.49
2:C:389:ARG:HA	2:C:394:THR:HA	1.94	0.49
1:D:24:G:C4	1:D:25:C:C6	3.01	0.49
1:D:37:YYG:H103	2:B:335:PHE:CE2	2.46	0.49
1:D:38:A:C3'	1:D:39:PSU:H5''	2.41	0.49
1:F:10:2MG:C6	1:F:26:M2G:C2	3.01	0.49
1:F:68:U:C4	1:F:69:U:C5	3.00	0.49
2:B:33:TYR:CZ	2:B:44:VAL:HG21	2.46	0.49
2:B:143:ASP:HB3	2:B:146:LEU:HB2	1.94	0.49
2:B:404:LEU:N	2:B:404:LEU:HD13	2.27	0.49
1:E:10:2MG:C6	1:E:11:C:C4	3.00	0.49
2:A:213:PRO:HG2	2:A:215:ARG:CZ	2.43	0.49
2:B:85:HIS:CD2	2:B:86:ALA:N	2.80	0.49
2:C:281:ILE:O	2:C:284:ASP:OD2	2.30	0.49
2:C:342:PHE:CD1	2:C:342:PHE:N	2.80	0.49
1:D:14:A:H2'	1:D:15:G:H5'	1.95	0.49
2:B:36:ALA:HA	2:B:42:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LYS:HB3	2:B:91:ASN:OD1	2.12	0.49
2:B:120:ILE:O	2:B:123:ALA:HB3	2.12	0.49
2:C:94:THR:CG2	2:C:346:THR:HG22	2.43	0.49
1:E:29:A:H2'	1:E:30:G:C8	2.48	0.49
2:A:281:ILE:O	2:A:281:ILE:HG13	2.12	0.49
2:B:59:ARG:O	2:B:61:ILE:HG23	2.12	0.49
2:C:33:TYR:CE1	2:C:44:VAL:CG2	2.95	0.49
2:A:121:LEU:HD13	2:A:161:TYR:CD2	2.48	0.49
2:A:322:ILE:HD12	2:A:334:PHE:HE1	1.78	0.49
1:E:7:U:H4'	1:E:8:U:OP2	2.13	0.49
2:A:72:THR:HB	6:A:428:HOH:O	2.12	0.49
2:A:188:THR:HG22	2:A:189:LYS:N	2.28	0.49
2:A:316:PHE:CA	2:A:404:LEU:HD22	2.42	0.49
2:C:145:GLU:HA	2:C:145:GLU:OE1	2.13	0.49
2:C:147:LEU:CD1	2:C:172:ARG:HH11	2.26	0.49
1:D:23:A:C2	1:D:24:G:C5	3.00	0.49
1:E:28:C:N3	1:E:42:G:N2	2.53	0.49
2:C:88:TYR:CD1	2:C:88:TYR:N	2.77	0.49
1:E:2:C:P	2:B:90:LYS:HE3	2.53	0.48
1:E:47:U:O2	1:E:50:U:OP1	2.30	0.48
1:E:54:5MU:OP1	2:B:331:HIS:HE1	1.96	0.48
2:B:156:ASP:O	2:B:159:ASN:N	2.46	0.48
2:B:343:TYR:CD1	2:B:343:TYR:N	2.80	0.48
2:C:217:VAL:HG12	2:C:281:ILE:HG22	1.95	0.48
1:F:74:C:C5	1:F:75:C:N4	2.81	0.48
2:A:38:GLU:HG3	2:A:200:TRP:HZ2	1.78	0.48
2:A:142:ASP:O	2:A:144:PRO:HD3	2.13	0.48
2:C:40:PRO:HG2	2:C:41:ASN:OD1	2.13	0.48
2:C:47:TYR:OH	5:C:406:GNP:O1A	2.28	0.48
2:C:362:VAL:HG21	2:C:368:VAL:HG21	1.95	0.48
2:C:399:VAL:O	2:C:399:VAL:HG13	2.12	0.48
1:F:25:C:H2'	1:F:26:M2G:C8	2.48	0.48
2:A:276:THR:HG22	2:A:277:LEU:N	2.28	0.48
2:B:82:CYS:HB3	2:B:83:PRO:CD	2.37	0.48
2:C:124:ARG:HG2	2:C:125:GLN:OE1	2.13	0.48
1:D:22:G:C6	1:D:23:A:N7	2.81	0.48
1:E:14:A:C3'	1:E:15:G:H5'	2.44	0.48
1:E:24:G:C6	1:E:25:C:C2	3.00	0.48
1:F:59:U:O2'	1:F:60:C:H5'	2.12	0.48
2:A:7:ARG:NH2	2:A:281:ILE:HG12	2.28	0.48
2:B:335:PHE:HE1	2:B:361:MET:HB2	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:VAL:HG12	2:C:277:LEU:HB3	1.94	0.48
1:D:14:A:N6	1:D:22:G:C6	2.82	0.48
1:E:23:A:HO2'	1:E:24:G:H5'	1.79	0.48
2:B:263:ARG:NH1	2:B:297:GLU:HB3	2.28	0.48
2:C:247:VAL:O	2:C:279:GLU:HA	2.12	0.48
2:C:368:VAL:HB	2:C:370:PHE:CD2	2.49	0.48
1:D:14:A:C4	1:D:22:G:N2	2.81	0.48
1:E:1:G:H2'	1:E:2:C:H5'	1.95	0.48
1:E:24:G:C5	1:E:25:C:C4	3.02	0.48
1:F:37:YYG:HN20	1:F:37:YYG:C11	2.27	0.48
2:A:89:ILE:HG22	2:A:93:ILE:HD12	1.95	0.48
2:C:90:LYS:O	2:C:93:ILE:HB	2.13	0.48
2:C:306:LYS:HB3	2:C:309:SER:CB	2.41	0.48
1:E:67:A:OP1	2:B:376:LYS:NZ	2.30	0.48
1:F:17:H2U:O2'	1:F:18:G:OP1	2.30	0.48
1:F:65:G:O2'	2:C:350:THR:OG1	2.29	0.48
2:A:24:LYS:HE2	2:A:24:LYS:HB2	1.50	0.48
2:C:94:THR:HG23	2:C:346:THR:HG22	1.96	0.48
2:C:205:ALA:O	2:C:209:TYR:N	2.38	0.48
2:C:220:PRO:O	2:C:244:ARG:HG3	2.14	0.48
1:D:37:YYG:H8	1:D:37:YYG:O5'	2.14	0.48
1:E:10:2MG:C2	1:E:11:C:C2	3.02	0.48
2:A:13:ASN:HB2	2:A:100:ASP:OD2	2.13	0.48
2:C:56:GLU:HG2	2:C:61:ILE:O	2.13	0.48
2:C:353:VAL:HG13	2:C:370:PHE:CD1	2.49	0.48
2:C:384:LEU:HD12	2:C:385:ARG:N	2.28	0.48
2:C:213:PRO:O	2:C:215:ARG:HD2	2.13	0.48
2:C:362:VAL:HG11	2:C:368:VAL:CG2	2.43	0.48
1:F:24:G:O2'	1:F:25:C:H5'	2.14	0.48
2:A:180:GLU:O	2:A:183:HIS:HB2	2.14	0.48
1:D:14:A:H2'	1:D:14:A:N3	2.28	0.47
1:D:59:U:C5	1:D:60:C:N4	2.82	0.47
2:A:168:VAL:HA	2:A:169:PRO:HD3	1.71	0.47
2:B:113:MET:O	2:B:116:THR:HB	2.14	0.47
2:C:247:VAL:C	2:C:248:LYS:HD3	2.33	0.47
2:A:256:VAL:HG11	2:A:310:ILE:CG2	2.43	0.47
2:A:362:VAL:HG11	2:A:368:VAL:HG21	1.96	0.47
2:B:71:GLU:HB2	2:B:75:ARG:O	2.13	0.47
2:B:130:TYR:CD1	2:B:130:TYR:N	2.81	0.47
2:B:281:ILE:HG12	2:B:284:ASP:OD2	2.14	0.47
2:C:100:ASP:O	2:C:129:PRO:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:MET:HE3	2:C:364:PRO:HD2	1.94	0.47
1:D:26:M2G:C6	1:D:27:C:C5	3.02	0.47
2:A:277:LEU:HD23	2:A:280:GLY:HA2	1.92	0.47
2:B:87:ASP:HB2	2:B:88:TYR:CD1	2.49	0.47
2:B:155:ARG:HD3	2:B:165:GLY:O	2.13	0.47
2:B:219:LYS:HB3	2:B:220:PRO:CD	2.44	0.47
2:B:355:LEU:HB3	2:B:359:VAL:HG12	1.96	0.47
2:C:224:PRO:HA	2:C:303:VAL:HG22	1.97	0.47
1:E:3:G:O2'	1:E:4:G:H5'	2.15	0.47
1:E:10:2MG:OP2	1:E:10:2MG:H3'	2.14	0.47
2:A:171:ILE:HD12	2:A:171:ILE:N	2.29	0.47
2:B:19:HIS:CD2	2:B:113:MET:HB2	2.50	0.47
1:F:47:U:H3'	1:F:47:U:O2	2.15	0.47
2:A:226:GLU:OE2	2:A:227:ASP:HB2	2.15	0.47
2:B:226:GLU:O	2:B:226:GLU:HG2	2.14	0.47
1:E:10:2MG:C6	1:E:11:C:N4	2.83	0.47
1:E:75:C:OP2	2:B:52:LYS:HE2	2.15	0.47
2:A:46:ASP:H	2:A:49:ASP:CG	2.16	0.47
2:C:368:VAL:CG2	2:C:370:PHE:HE2	2.28	0.47
1:D:32:OMC:O5'	1:D:32:OMC:H6	1.97	0.47
1:E:25:C:O2'	1:E:26:M2G:O4'	2.30	0.47
2:A:19:HIS:CE1	2:A:20:VAL:HG12	2.49	0.47
2:A:234:ARG:HB3	2:A:289:LEU:CD2	2.43	0.47
2:B:75:ARG:NH2	2:B:210:ILE:O	2.38	0.47
2:B:231:ILE:HG22	2:B:234:ARG:CG	2.44	0.47
2:C:20:VAL:HA	2:C:84:GLY:HA3	1.97	0.47
2:C:50:ILE:HG12	2:C:50:ILE:H	1.42	0.47
2:C:335:PHE:HA	2:C:355:LEU:CD1	2.44	0.47
1:F:25:C:C4	1:F:26:M2G:C5	3.03	0.47
2:A:277:LEU:HD21	2:A:280:GLY:HA2	1.96	0.47
2:B:40:PRO:HD2	2:B:41:ASN:OD1	2.15	0.47
2:B:141:VAL:O	2:B:141:VAL:HG23	2.15	0.47
2:C:266:VAL:HG21	2:C:291:ARG:HH21	1.80	0.47
2:A:128:VAL:HA	2:A:129:PRO:HD3	1.65	0.47
2:B:38:GLU:OE2	2:B:190:ARG:HG3	2.15	0.47
1:D:39:PSU:O4'	1:D:39:PSU:O4	2.29	0.47
1:E:53:G:H3'	1:E:54:5MU:H71	1.96	0.47
1:F:37:YYG:HN20	1:F:37:YYG:H102	1.79	0.47
2:B:118:GLU:O	2:B:122:LEU:HG	2.15	0.47
2:C:34:VAL:HG12	2:C:200:TRP:CZ2	2.50	0.47
2:C:66:ALA:O	2:C:80:VAL:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:C:H6	1:D:60:C:H2'	1.51	0.46
2:B:90:LYS:HA	2:B:93:ILE:HD12	1.97	0.46
2:B:336:THR:H	2:B:355:LEU:HD12	1.80	0.46
2:B:345:ARG:HH22	2:B:381:GLU:CD	2.18	0.46
2:C:259:ALA:HB1	2:C:260:PRO:CD	2.39	0.46
4:D:77:PHE:N	2:A:285:ASN:O	2.49	0.46
1:E:30:G:C6	1:E:31:A:C5	3.04	0.46
1:F:51:G:H2'	1:F:52:U:O4'	2.15	0.46
2:A:53:ALA:O	2:A:57:ARG:HG2	2.15	0.46
2:A:113:MET:O	2:A:116:THR:HB	2.16	0.46
2:A:229:PHE:HE1	2:A:239:THR:HG21	1.80	0.46
2:B:52:LYS:HA	2:B:57:ARG:HE	1.79	0.46
2:C:214:VAL:HG12	2:C:214:VAL:O	2.14	0.46
2:C:404:LEU:HD13	2:C:404:LEU:N	2.25	0.46
1:E:30:G:C6	1:E:31:A:C6	3.03	0.46
2:A:33:TYR:HB3	2:A:182:MET:HG3	1.98	0.46
2:B:11:HIS:HD1	2:B:76:HIS:CE1	2.33	0.46
2:B:63:ILE:HA	2:B:88:TYR:CD2	2.51	0.46
2:C:120:ILE:HD12	2:C:157:LEU:HG	1.97	0.46
2:C:265:THR:HG23	2:C:291:ARG:O	2.15	0.46
1:D:18:G:O6	1:D:55:PSU:H1'	2.15	0.46
2:A:46:ASP:HB2	2:A:49:ASP:CG	2.36	0.46
2:A:177:LEU:N	2:A:177:LEU:CD1	2.79	0.46
2:B:335:PHE:HE1	2:B:361:MET:SD	2.38	0.46
2:C:90:LYS:O	2:C:93:ILE:N	2.47	0.46
2:C:380:LEU:HB2	2:C:403:ILE:HD13	1.97	0.46
2:C:399:VAL:CG2	2:C:400:VAL:N	2.79	0.46
1:D:11:C:H2'	1:D:12:U:C5	2.50	0.46
1:E:24:G:H3'	1:E:25:C:H6	1.81	0.46
2:A:399:VAL:HG22	2:A:400:VAL:N	2.29	0.46
2:B:36:ALA:CB	2:B:44:VAL:HG12	2.45	0.46
2:B:53:ALA:CB	2:B:56:GLU:HB2	2.36	0.46
2:B:89:ILE:HG22	2:B:93:ILE:CD1	2.45	0.46
2:B:246:LYS:HB2	2:B:280:GLY:O	2.16	0.46
2:B:268:THR:OG1	2:B:289:LEU:HD23	2.15	0.46
2:B:361:MET:O	2:B:361:MET:HG2	2.15	0.46
2:B:362:VAL:HG21	2:B:368:VAL:HG21	1.97	0.46
2:C:324:LYS:O	2:C:327:GLU:N	2.48	0.46
1:D:24:G:C6	1:D:25:C:C4	3.04	0.46
2:A:19:HIS:CD2	2:A:113:MET:HB2	2.50	0.46
2:A:311:THR:HG22	2:A:312:PRO:CD	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:389:ARG:HA	2:A:393:ARG:O	2.16	0.46
2:B:53:ALA:HB1	2:B:54:PRO:HD3	1.96	0.46
2:B:75:ARG:HD3	2:B:77:TYR:OH	2.15	0.46
2:C:85:HIS:CD2	2:C:86:ALA:N	2.84	0.46
2:C:133:VAL:HG12	2:C:134:PHE:N	2.31	0.46
2:C:217:VAL:HG12	2:C:246:LYS:HD3	1.97	0.46
1:D:30:G:C3'	1:D:31:A:H5'	2.42	0.46
1:E:33:U:H4'	1:E:37:YYG:H191	1.97	0.46
2:A:178:ALA:O	2:A:181:GLU:HB3	2.16	0.46
2:B:156:ASP:O	2:B:159:ASN:HB2	2.15	0.46
2:B:177:LEU:N	2:B:177:LEU:CD1	2.79	0.46
2:C:131:ILE:CD1	2:C:163:PHE:CE1	2.99	0.46
2:C:139:ASP:OD1	2:C:139:ASP:N	2.49	0.46
2:C:256:VAL:HG11	2:C:310:ILE:HG21	1.94	0.46
1:D:59:U:O2'	1:D:60:C:H5'	2.16	0.46
1:E:17:H2U:H3'	1:E:18:G:H5''	1.98	0.46
2:A:20:VAL:O	2:A:20:VAL:HG13	2.15	0.46
2:A:368:VAL:CG1	2:A:369:THR:H	2.08	0.46
2:C:199:ILE:N	2:C:199:ILE:HD13	2.30	0.46
1:E:62:A:H2'	1:E:63:C:O4'	2.15	0.46
1:F:18:G:O6	1:F:55:PSU:H1'	2.15	0.46
2:A:102:ALA:O	2:A:131:ILE:HA	2.14	0.46
2:C:134:PHE:CD1	2:C:171:ILE:CG2	2.99	0.46
1:E:24:G:O2'	1:E:25:C:H5'	2.16	0.46
1:E:38:A:H5'	2:C:336:THR:HG22	1.98	0.46
2:A:353:VAL:HG13	2:A:370:PHE:CD1	2.51	0.46
2:B:117:ARG:HH12	2:B:160:GLN:NE2	2.14	0.46
2:C:19:HIS:CD2	2:C:113:MET:CB	2.99	0.46
2:C:131:ILE:O	2:C:209:TYR:HE2	1.99	0.46
4:E:77:PHE:N	2:B:272:MET:HA	2.31	0.45
2:A:193:ASN:HB3	2:A:196:VAL:HB	1.98	0.45
2:A:400:VAL:CG1	2:A:401:THR:N	2.79	0.45
2:B:335:PHE:CE1	2:B:361:MET:CE	2.99	0.45
2:C:11:HIS:CE1	2:C:272:MET:HE2	2.51	0.45
2:C:23:GLY:HA2	5:C:406:GNP:PA	2.56	0.45
2:C:182:MET:SD	2:C:188:THR:HB	2.56	0.45
2:C:310:ILE:HG21	2:C:310:ILE:HD13	1.65	0.45
1:D:25:C:C4	1:D:26:M2G:C8	3.04	0.45
1:F:11:C:HO2'	1:F:12:U:H6	1.63	0.45
2:A:177:LEU:N	2:A:177:LEU:HD12	2.30	0.45
2:A:315:LYS:HD3	2:A:405:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLU:OE2	2:B:389:ARG:NH1	2.49	0.45
2:C:39:ASN:HA	2:C:40:PRO:HD3	1.47	0.45
2:C:265:THR:HG22	2:C:291:ARG:N	2.31	0.45
1:D:22:G:N1	1:D:23:A:N7	2.64	0.45
1:D:26:M2G:CM1	1:D:44:A:H2	2.29	0.45
2:A:36:ALA:CB	2:A:44:VAL:HG12	2.47	0.45
2:B:47:TYR:OH	5:B:406:GNP:O1A	2.30	0.45
2:B:163:PHE:HA	2:B:164:PRO:HD2	1.67	0.45
2:C:33:TYR:HA	2:C:44:VAL:HG11	1.98	0.45
2:A:199:ILE:HG22	2:A:203:LEU:HD12	1.98	0.45
2:A:202:LEU:HD12	2:A:202:LEU:C	2.35	0.45
2:A:334:PHE:CD2	2:A:338:TYR:CD2	3.05	0.45
2:B:55:GLU:CG	2:B:59:ARG:HD2	2.47	0.45
2:B:137:LYS:HB3	2:B:140:MET:HG3	1.97	0.45
2:B:149:LEU:O	2:B:153:GLU:HG3	2.16	0.45
2:C:4:GLU:O	2:C:4:GLU:HG2	2.17	0.45
1:D:58:1MA:HM12	1:D:61:C:H1'	1.97	0.45
2:A:85:HIS:CD2	2:A:87:ASP:CB	3.00	0.45
2:A:276:THR:CG2	2:A:277:LEU:N	2.79	0.45
2:C:63:ILE:CG1	2:C:64:ASN:N	2.80	0.45
2:C:85:HIS:HD2	2:C:86:ALA:N	2.15	0.45
2:C:217:VAL:CG1	2:C:281:ILE:HG22	2.46	0.45
2:C:266:VAL:O	2:C:268:THR:HG23	2.17	0.45
1:D:36:A:C2	1:D:37:YYG:C4	2.99	0.45
2:A:134:PHE:CD1	2:A:171:ILE:CG2	3.00	0.45
2:A:399:VAL:CG2	2:A:400:VAL:N	2.79	0.45
2:B:38:GLU:OE2	2:B:189:LYS:HB3	2.17	0.45
2:B:63:ILE:HA	2:B:88:TYR:HD2	1.81	0.45
2:C:27:LEU:HD21	2:C:202:LEU:HD21	1.98	0.45
2:A:140:MET:SD	5:A:406:GNP:N2	2.89	0.45
2:A:289:LEU:HD12	2:A:289:LEU:HA	1.76	0.45
2:A:320:VAL:CG1	2:A:321:TYR:N	2.80	0.45
2:C:90:LYS:HA	2:C:93:ILE:HD12	1.99	0.45
1:E:44:A:C2'	1:E:45:G:H5'	2.47	0.45
1:F:46:7MG:H81	1:F:46:7MG:H2'	1.65	0.45
2:A:248:LYS:HD2	2:A:279:GLU:OE2	2.17	0.45
2:B:33:TYR:CZ	2:B:44:VAL:CG2	3.00	0.45
2:B:63:ILE:CG2	2:B:88:TYR:HE2	2.30	0.45
2:B:336:THR:N	2:B:355:LEU:CD1	2.80	0.45
2:C:11:HIS:CE1	2:C:272:MET:CE	3.00	0.45
2:C:56:GLU:OE2	2:C:63:ILE:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:VAL:HG12	2:C:267:VAL:O	2.15	0.45
2:C:342:PHE:CE2	2:C:372:VAL:HG21	2.52	0.45
2:A:176:LEU:HB2	5:A:406:GNP:C5	2.47	0.45
2:B:122:LEU:HD23	2:B:122:LEU:HA	1.50	0.45
2:B:124:ARG:HH11	2:B:124:ARG:CG	2.27	0.45
2:B:285:ASN:C	2:B:285:ASN:HD22	2.20	0.45
2:C:33:TYR:CD1	2:C:44:VAL:HG11	2.52	0.45
1:E:37:YYG:C4	1:E:38:A:C8	3.00	0.45
1:E:53:G:C8	1:E:54:5MU:H72	2.51	0.45
2:A:6:ILE:O	2:A:6:ILE:HG22	2.17	0.45
2:A:16:THR:O	2:A:82:CYS:HB2	2.17	0.45
2:B:261:GLU:OE1	2:B:262:THR:N	2.44	0.45
2:C:24:LYS:HB2	2:C:24:LYS:HE2	1.56	0.45
2:C:155:ARG:NH2	2:C:170:VAL:CG2	2.79	0.45
2:C:254:GLU:O	2:C:304:LEU:HA	2.17	0.45
2:A:304:LEU:HD23	2:A:304:LEU:HA	1.67	0.44
2:A:368:VAL:HG12	2:A:369:THR:N	2.22	0.44
2:C:75:ARG:HD2	2:C:77:TYR:OH	2.17	0.44
1:D:32:OMC:HM23	1:D:32:OMC:O3'	2.17	0.44
2:A:313:HIS:CD2	2:A:403:ILE:CD1	2.99	0.44
2:A:322:ILE:HD12	2:A:334:PHE:CE1	2.51	0.44
2:B:19:HIS:CD2	2:B:113:MET:CB	2.99	0.44
2:B:249:VAL:HG13	2:B:268:THR:C	2.37	0.44
2:C:40:PRO:CG	2:C:41:ASN:N	2.79	0.44
2:C:113:MET:O	2:C:116:THR:HB	2.17	0.44
2:C:187:LYS:O	2:C:189:LYS:HD3	2.16	0.44
2:C:336:THR:N	2:C:355:LEU:CD1	2.79	0.44
1:D:14:A:C6	1:D:22:G:N1	2.85	0.44
2:A:171:ILE:N	2:A:171:ILE:CD1	2.79	0.44
2:A:217:VAL:O	2:A:245:GLY:HA2	2.16	0.44
2:A:223:MET:O	2:A:223:MET:HG3	2.12	0.44
1:D:59:U:C2'	1:D:60:C:H5'	2.47	0.44
1:D:62:A:C2'	1:D:63:C:H5'	2.47	0.44
1:F:32:OMC:HM23	1:F:32:OMC:H1'	1.63	0.44
2:A:144:PRO:HA	2:A:147:LEU:HD23	1.99	0.44
2:A:159:ASN:O	2:A:162:GLU:N	2.47	0.44
2:A:258:LEU:HD23	2:A:258:LEU:HA	1.63	0.44
2:B:320:VAL:CG1	2:B:321:TYR:N	2.79	0.44
2:A:115:GLN:O	2:A:119:HIS:HB2	2.18	0.44
2:A:159:ASN:O	2:A:162:GLU:HA	2.17	0.44
2:C:19:HIS:CG	2:C:113:MET:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:GLU:O	2:C:148:ASP:HB2	2.18	0.44
2:C:339:ARG:HD2	2:C:352:VAL:CG2	2.48	0.44
2:C:384:LEU:HD12	2:C:385:ARG:H	1.82	0.44
2:A:19:HIS:CG	2:A:113:MET:CB	3.00	0.44
2:A:53:ALA:HB1	2:A:54:PRO:CD	2.48	0.44
2:A:313:HIS:CD2	2:A:403:ILE:HD13	2.53	0.44
2:A:315:LYS:HE2	2:A:404:LEU:CB	2.48	0.44
1:E:1:G:C4	1:E:73:A:C2	3.05	0.44
1:E:21:A:O2'	1:E:22:G:O4'	2.35	0.44
2:B:342:PHE:O	2:B:348:ASP:HA	2.18	0.44
2:C:33:TYR:CZ	2:C:44:VAL:HB	2.52	0.44
2:C:147:LEU:HD12	2:C:172:ARG:NH1	2.29	0.44
2:C:270:VAL:CG1	2:C:277:LEU:HB3	2.48	0.44
1:D:17:H2U:C4'	1:D:18:G:H5''	2.43	0.44
2:A:202:LEU:O	2:A:206:ILE:HG13	2.18	0.44
2:B:20:VAL:O	2:B:20:VAL:HG13	2.17	0.44
2:B:124:ARG:CG	2:B:124:ARG:NH1	2.79	0.44
2:B:315:LYS:HB2	2:B:404:LEU:HB2	1.94	0.44
2:C:265:THR:CG2	2:C:291:ARG:N	2.80	0.44
2:C:272:MET:O	2:C:275:LYS:HB2	2.18	0.44
2:C:343:TYR:CD1	2:C:343:TYR:N	2.86	0.44
2:C:356:PRO:HG3	2:C:369:THR:O	2.18	0.44
1:D:8:U:O2	1:D:15:G:O6	2.36	0.44
1:D:71:G:C2'	1:D:72:C:H5'	2.47	0.44
2:A:303:VAL:CG1	2:A:304:LEU:N	2.79	0.44
2:B:126:VAL:HG13	2:B:126:VAL:O	2.18	0.44
2:C:89:ILE:HD13	2:C:89:ILE:HG23	1.84	0.44
2:C:177:LEU:N	2:C:177:LEU:HD12	2.33	0.44
2:C:223:MET:HB2	2:C:242:ILE:HA	1.99	0.44
2:B:2:LYS:HB3	2:B:3:GLY:H	1.58	0.43
2:B:304:LEU:HA	2:B:304:LEU:HD23	1.59	0.43
2:C:155:ARG:NH1	2:C:165:GLY:O	2.46	0.43
1:E:26:M2G:CM1	1:E:44:A:C2	2.96	0.43
2:A:181:GLU:OE1	2:A:181:GLU:HA	2.18	0.43
2:A:303:VAL:HG13	2:A:304:LEU:N	2.33	0.43
2:B:213:PRO:HG2	2:B:215:ARG:NH2	2.31	0.43
2:C:52:LYS:HA	2:C:57:ARG:CZ	2.48	0.43
2:C:171:ILE:CG2	2:C:172:ARG:N	2.80	0.43
1:E:32:OMC:HM22	1:E:32:OMC:O2	2.18	0.43
2:A:36:ALA:HB2	2:A:44:VAL:HG12	1.99	0.43
2:A:52:LYS:HG3	2:A:53:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:345:ARG:HB2	6:A:414:HOH:O	2.18	0.43
2:A:354:ARG:HH11	2:A:354:ARG:HG3	1.83	0.43
5:A:406:GNP:H2'	5:A:406:GNP:H8	1.24	0.43
2:B:32:THR:OG1	2:B:33:TYR:N	2.51	0.43
2:B:83:PRO:O	2:B:83:PRO:HG2	2.18	0.43
2:B:222:LEU:HB3	2:B:244:ARG:HG2	2.00	0.43
2:C:144:PRO:O	2:C:147:LEU:HB2	2.19	0.43
2:C:363:MET:HE2	2:C:363:MET:HB3	1.85	0.43
2:A:40:PRO:HD2	2:A:41:ASN:OD1	2.18	0.43
2:A:96:ALA:HA	2:A:99:MET:HG3	2.00	0.43
2:A:335:PHE:CD1	2:A:361:MET:CB	3.00	0.43
2:C:126:VAL:HG13	2:C:126:VAL:O	2.18	0.43
2:C:135:MET:HE3	2:C:151:GLU:HB2	2.01	0.43
1:D:13:C:C2	1:D:14:A:N7	2.86	0.43
1:D:62:A:H2'	1:D:63:C:O4'	2.18	0.43
1:E:23:A:C6	1:E:24:G:C6	3.05	0.43
2:C:248:LYS:HE3	2:C:251:ASP:CG	2.39	0.43
2:C:315:LYS:HB3	2:C:315:LYS:HE2	1.79	0.43
2:C:324:LYS:H	2:C:327:GLU:HB2	1.83	0.43
1:D:19:G:H8	1:D:19:G:H2'	1.37	0.43
1:F:3:G:C8	1:F:3:G:C3'	3.01	0.43
1:F:21:A:C5	1:F:46:7MG:C6	3.06	0.43
2:A:146:LEU:HD12	2:A:146:LEU:O	2.18	0.43
2:C:289:LEU:HD12	2:C:289:LEU:HA	1.68	0.43
1:E:24:G:H3'	1:E:25:C:C6	2.53	0.43
1:F:37:YYG:H31	1:F:37:YYG:C2'	2.49	0.43
2:A:191:GLY:H	2:A:197:ASP:CG	2.21	0.43
2:A:368:VAL:CG1	2:A:369:THR:N	2.79	0.43
2:B:347:THR:HG22	2:B:348:ASP:N	2.34	0.43
2:A:29:ALA:HB1	2:A:45:LYS:O	2.18	0.43
2:A:72:THR:CG2	2:A:203:LEU:HD22	2.49	0.43
2:A:118:GLU:O	2:A:122:LEU:HG	2.19	0.43
2:A:124:ARG:HG2	2:A:124:ARG:HH11	1.83	0.43
2:B:11:HIS:O	2:B:12:VAL:HG23	2.18	0.43
2:B:316:PHE:HB2	2:B:402:LYS:O	2.18	0.43
2:C:53:ALA:HB3	2:C:56:GLU:OE1	2.17	0.43
2:C:316:PHE:CZ	2:C:372:VAL:HB	2.54	0.43
2:B:63:ILE:CB	2:B:88:TYR:CE2	2.99	0.43
2:B:132:VAL:HG22	2:B:169:PRO:HG2	2.01	0.43
2:C:117:ARG:HG3	2:C:161:TYR:CE2	2.50	0.43
2:C:215:ARG:HG2	2:C:282:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:OMG:C2'	1:F:35:A:H5'	2.49	0.43
2:A:113:MET:HB3	2:A:114:PRO:CD	2.46	0.43
2:B:117:ARG:NH1	2:B:160:GLN:HE22	2.17	0.43
2:B:124:ARG:NH2	2:B:385:ARG:NH2	2.67	0.43
2:B:342:PHE:CD1	2:B:342:PHE:N	2.87	0.43
2:B:350:THR:O	2:B:375:ILE:HG23	2.19	0.43
2:C:21:ASP:O	2:C:23:GLY:N	2.52	0.43
2:C:248:LYS:N	2:C:248:LYS:CD	2.80	0.43
1:E:3:G:C8	1:E:3:G:C3'	3.00	0.42
1:E:21:A:O5'	1:E:21:A:H8	2.01	0.42
1:F:37:YYG:N20	1:F:37:YYG:C11	2.82	0.42
2:A:34:VAL:HG13	6:A:426:HOH:O	2.18	0.42
2:A:140:MET:CG	5:A:406:GNP:N2	2.82	0.42
2:A:254:GLU:OE1	2:A:308:GLY:N	2.46	0.42
2:B:21:ASP:CA	5:B:406:GNP:HNB3	2.24	0.42
2:B:103:ILE:HD11	2:B:206:ILE:CD1	2.46	0.42
2:B:140:MET:HA	2:B:140:MET:HE2	2.00	0.42
1:F:62:A:H2'	1:F:63:C:O4'	2.20	0.42
2:A:122:LEU:HA	2:A:122:LEU:HD23	1.81	0.42
2:A:160:GLN:HE21	2:A:160:GLN:HB3	1.50	0.42
2:A:184:LYS:O	2:A:185:ASN:HB3	2.19	0.42
2:A:306:LYS:HB3	2:A:309:SER:CB	2.47	0.42
2:B:232:THR:O	2:B:234:ARG:N	2.53	0.42
2:B:247:VAL:O	2:B:279:GLU:HA	2.18	0.42
2:B:333:GLY:HA2	2:B:362:VAL:O	2.19	0.42
2:B:339:ARG:HB3	2:B:352:VAL:HG22	2.01	0.42
1:D:36:A:C2	1:D:37:YYG:N9	2.87	0.42
2:A:263:ARG:HH21	2:A:297:GLU:HB3	1.85	0.42
2:B:176:LEU:O	2:B:176:LEU:HD12	2.19	0.42
2:C:177:LEU:N	2:C:177:LEU:CD1	2.82	0.42
2:C:315:LYS:HA	2:C:372:VAL:O	2.20	0.42
1:D:8:U:H5'	1:D:49:5MC:OP2	2.20	0.42
1:E:39:PSU:H4'	2:C:360:GLU:OE2	2.19	0.42
1:E:44:A:O2'	1:E:45:G:H5'	2.20	0.42
1:F:48:C:OP2	1:F:48:C:H6	2.02	0.42
2:A:71:GLU:HB3	2:A:76:HIS:HA	2.01	0.42
2:C:21:ASP:O	5:C:406:GNP:H5'2	2.19	0.42
1:D:29:A:O2'	1:D:30:G:H5'	2.19	0.42
2:A:5:PHE:N	2:A:276:THR:O	2.41	0.42
2:B:39:ASN:HA	2:B:40:PRO:HD3	1.44	0.42
2:B:143:ASP:O	2:B:146:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:MET:HA	2:B:224:PRO:HD2	1.61	0.42
1:E:9:A:O2'	1:E:11:C:H5	2.03	0.42
1:E:51:G:H4'	2:B:339:ARG:HG2	2.01	0.42
1:F:10:2MG:C5	1:F:11:C:C5	3.07	0.42
1:F:11:C:H2'	1:F:12:U:C6	2.55	0.42
2:B:404:LEU:HD12	2:B:404:LEU:HA	1.73	0.42
2:C:128:VAL:HA	2:C:129:PRO:HD3	1.95	0.42
2:C:184:LYS:O	2:C:185:ASN:HB3	2.19	0.42
2:C:198:LYS:O	2:C:201:GLU:N	2.53	0.42
2:C:311:THR:HA	2:C:312:PRO:HD3	1.88	0.42
1:E:14:A:C3'	1:E:15:G:C5'	2.98	0.42
1:E:34:OMG:H1'	1:E:34:OMG:HM23	1.06	0.42
1:F:10:2MG:N3	1:F:11:C:C6	2.87	0.42
1:F:54:5MU:H2'	1:F:55:PSU:O4'	2.20	0.42
2:B:19:HIS:CD2	2:B:115:GLN:NE2	2.87	0.42
2:B:194:GLU:O	2:B:197:ASP:N	2.52	0.42
2:B:226:GLU:O	2:B:300:ARG:HG3	2.20	0.42
2:C:185:ASN:HA	2:C:186:PRO:HD3	1.11	0.42
2:C:335:PHE:CD1	2:C:361:MET:CB	2.99	0.42
1:D:2:C:H4'	2:A:88:TYR:CE1	2.52	0.42
1:E:10:2MG:N1	1:E:11:C:C4	2.88	0.42
1:E:37:YYG:O6	1:E:37:YYG:H132	2.20	0.42
2:A:136:ASN:CG	2:A:137:LYS:H	2.23	0.42
2:B:248:LYS:N	2:B:248:LYS:CD	2.79	0.42
2:B:293:VAL:O	2:B:293:VAL:HG23	2.18	0.42
2:C:6:ILE:HA	2:C:6:ILE:HD13	1.81	0.42
2:C:154:VAL:O	2:C:158:LEU:HB2	2.20	0.42
2:C:338:TYR:C	2:C:340:PRO:HD3	2.40	0.42
2:A:234:ARG:HB3	2:A:289:LEU:HD22	2.02	0.42
2:B:140:MET:HA	2:B:140:MET:HE3	2.01	0.42
2:B:215:ARG:N	2:B:215:ARG:CD	2.80	0.42
2:C:21:ASP:CG	5:C:406:GNP:H5'2	2.40	0.42
2:C:143:ASP:HA	2:C:144:PRO:HD2	1.53	0.42
2:B:222:LEU:HD11	2:B:303:VAL:HG11	2.01	0.42
2:B:262:THR:HG23	2:B:262:THR:H	1.47	0.42
2:B:380:LEU:HD23	2:B:380:LEU:HA	1.80	0.42
2:C:169:PRO:CD	2:C:209:TYR:CD2	3.03	0.42
2:C:248:LYS:O	2:C:251:ASP:OD2	2.38	0.42
1:E:24:G:C5	1:E:25:C:N3	2.88	0.41
1:F:55:PSU:C6	1:F:55:PSU:C3'	3.02	0.41
2:C:13:ASN:N	2:C:100:ASP:OD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:A:H2'	1:E:37:YYG:C8	2.49	0.41
1:E:71:G:C2'	1:E:72:C:H5'	2.50	0.41
2:A:310:ILE:HG23	2:A:311:THR:N	2.34	0.41
2:C:32:THR:HB	2:C:44:VAL:HA	2.01	0.41
2:C:115:GLN:O	2:C:119:HIS:N	2.42	0.41
2:C:304:LEU:HD23	2:C:304:LEU:N	2.12	0.41
1:E:71:G:H8	1:E:71:G:H5''	1.85	0.41
2:A:313:HIS:CD2	2:A:403:ILE:CG2	2.99	0.41
2:A:322:ILE:HG13	2:A:362:VAL:HG11	2.02	0.41
2:B:124:ARG:HG2	2:B:124:ARG:NH1	2.33	0.41
2:C:389:ARG:CG	2:C:394:THR:HA	2.36	0.41
1:E:27:C:O2'	1:E:28:C:OP1	2.29	0.41
2:A:127:GLY:O	2:A:129:PRO:HD3	2.20	0.41
2:A:147:LEU:HD13	2:A:147:LEU:HA	1.69	0.41
2:A:316:PHE:C	2:A:404:LEU:HD22	2.39	0.41
2:B:146:LEU:HD12	2:B:146:LEU:HA	1.72	0.41
2:B:191:GLY:H	2:B:197:ASP:CG	2.23	0.41
2:C:213:PRO:HG2	2:C:215:ARG:NE	2.35	0.41
1:E:1:G:C2	1:E:73:A:C2	3.09	0.41
1:E:37:YYG:H101	1:E:37:YYG:C14	2.48	0.41
1:F:15:G:H2'	1:F:16:H2U:H62	2.02	0.41
2:A:229:PHE:CD1	2:A:229:PHE:N	2.89	0.41
2:C:21:ASP:C	2:C:23:GLY:H	2.23	0.41
2:C:252:GLU:HA	2:C:265:THR:O	2.20	0.41
2:C:350:THR:HG22	2:C:351:GLY:N	2.34	0.41
1:F:37:YYG:H141	1:F:37:YYG:O22	2.20	0.41
2:B:176:LEU:HD12	2:B:176:LEU:C	2.40	0.41
2:B:176:LEU:CB	5:B:406:GNP:C6	2.99	0.41
2:B:230:THR:C	2:B:231:ILE:HD13	2.41	0.41
2:B:310:ILE:HG21	2:B:310:ILE:HD12	1.61	0.41
2:C:316:PHE:CE1	2:C:372:VAL:HB	2.55	0.41
2:C:355:LEU:CD2	2:C:362:VAL:CG2	2.98	0.41
1:E:48:C:H6	1:E:48:C:OP2	2.04	0.41
1:F:27:C:H2'	1:F:28:C:C6	2.55	0.41
2:A:6:ILE:HG21	2:A:6:ILE:HD12	1.80	0.41
2:A:157:LEU:HD12	2:A:157:LEU:HA	1.32	0.41
2:A:370:PHE:HB2	2:A:371:THR:H	1.69	0.41
2:B:255:ILE:HD13	2:B:255:ILE:HG21	1.83	0.41
2:C:190:ARG:H	2:C:190:ARG:HG3	1.72	0.41
2:C:376:LYS:HA	2:C:377:PRO:HD3	1.77	0.41
2:B:176:LEU:HB3	5:B:406:GNP:C6	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:VAL:H	2:B:217:VAL:HG23	1.50	0.41
2:B:299:GLU:N	2:B:302:GLN:OE1	2.51	0.41
2:C:248:LYS:HE3	2:C:251:ASP:OD1	2.21	0.41
2:C:312:PRO:HB2	2:C:377:PRO:HB2	2.02	0.41
1:D:14:A:C5	1:D:22:G:N2	2.89	0.41
1:D:31:A:C2	1:D:40:5MC:C2	3.09	0.41
1:D:53:G:H2'	1:D:54:5MU:O4'	2.20	0.41
1:E:16:H2U:H61	1:E:16:H2U:H2'	0.80	0.41
1:F:67:A:C5	1:F:68:U:C5	3.08	0.41
1:F:74:C:N4	1:F:75:C:N4	2.69	0.41
2:A:11:HIS:O	2:A:215:ARG:NH1	2.42	0.41
2:A:219:LYS:HB2	2:A:244:ARG:HD3	2.03	0.41
2:A:254:GLU:CD	2:A:307:PRO:HA	2.41	0.41
2:A:362:VAL:HG13	2:A:368:VAL:HG22	2.03	0.41
2:B:54:PRO:O	2:B:58:ALA:HB2	2.21	0.41
2:B:155:ARG:HB3	2:B:165:GLY:O	2.20	0.41
2:B:324:LYS:O	2:B:327:GLU:N	2.53	0.41
2:B:362:VAL:CG1	2:B:368:VAL:HG21	2.51	0.41
2:C:33:TYR:HE1	2:C:44:VAL:HG21	1.83	0.41
2:C:128:VAL:HG12	2:C:130:TYR:H	1.85	0.41
2:C:136:ASN:CG	2:C:137:LYS:H	2.23	0.41
2:C:199:ILE:O	2:C:199:ILE:HG22	2.21	0.41
2:C:284:ASP:HB3	2:C:286:VAL:HG12	2.03	0.41
2:C:321:TYR:OH	2:C:327:GLU:OE1	2.28	0.41
1:D:12:U:O2	1:D:13:C:N1	2.54	0.41
1:E:59:U:C4	1:E:60:C:N3	2.89	0.41
1:F:9:A:HO2'	1:F:11:C:H5	1.65	0.41
1:F:34:OMG:H1'	1:F:34:OMG:HM23	1.18	0.41
2:A:9:LYS:CB	2:A:10:PRO:CD	2.99	0.41
2:A:390:GLU:O	2:A:393:ARG:HG2	2.21	0.41
2:C:134:PHE:CE1	2:C:171:ILE:HG22	2.56	0.41
2:C:136:ASN:OD1	2:C:137:LYS:N	2.49	0.41
2:C:265:THR:HG21	2:C:290:LEU:HB3	2.02	0.41
2:C:284:ASP:CB	2:C:286:VAL:CG1	2.99	0.41
2:C:349:VAL:CG2	2:C:374:LEU:HD22	2.51	0.41
2:A:160:GLN:C	2:A:162:GLU:H	2.25	0.40
2:A:254:GLU:O	2:A:304:LEU:HA	2.21	0.40
2:B:36:ALA:HB2	2:B:44:VAL:HG12	2.03	0.40
2:B:168:VAL:HA	2:B:169:PRO:HD2	1.65	0.40
2:B:220:PRO:O	2:B:244:ARG:HG3	2.21	0.40
2:B:222:LEU:CD1	2:B:303:VAL:CG1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:LYS:HB2	2:C:3:GLY:H	1.50	0.40
2:C:182:MET:SD	2:C:196:VAL:CG2	3.09	0.40
2:C:217:VAL:CG1	2:C:281:ILE:CG2	3.00	0.40
2:C:222:LEU:CD1	2:C:303:VAL:CG1	2.99	0.40
2:A:310:ILE:HG21	2:A:310:ILE:HD13	1.87	0.40
2:B:299:GLU:HG2	2:B:302:GLN:OE1	2.21	0.40
2:C:106:VAL:HG21	2:C:154:VAL:CG2	2.51	0.40
2:C:172:ARG:O	2:C:198:LYS:HE2	2.21	0.40
2:A:40:PRO:HG2	2:A:41:ASN:H	1.82	0.40
2:A:223:MET:HA	2:A:224:PRO:HD2	1.65	0.40
2:B:87:ASP:HB2	2:B:88:TYR:CE1	2.56	0.40
2:B:172:ARG:O	2:B:198:LYS:HE2	2.21	0.40
2:B:194:GLU:HB3	2:B:195:TRP:H	1.66	0.40
2:C:259:ALA:CB	2:C:260:PRO:CD	2.98	0.40
1:E:28:C:O2	1:E:28:C:H2'	2.21	0.40
1:E:32:OMC:H1'	1:E:32:OMC:HM23	1.27	0.40
1:F:16:H2U:H2'	1:F:16:H2U:H61	1.53	0.40
1:F:61:C:H2'	1:F:62:A:C8	2.57	0.40
2:B:371:THR:O	2:B:371:THR:HG22	2.17	0.40
2:A:310:ILE:CG2	2:A:311:THR:N	2.79	0.40
2:B:383:GLY:HA2	2:B:399:VAL:CG2	2.52	0.40
2:C:66:ALA:O	2:C:80:VAL:HG13	2.22	0.40
2:C:133:VAL:HG23	2:C:168:VAL:CG1	2.51	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	403/405 (100%)	362 (90%)	35 (9%)	6 (2%)	10 26
2	B	403/405 (100%)	359 (89%)	31 (8%)	13 (3%)	4 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	403/405 (100%)	353 (88%)	36 (9%)	14 (4%)	3 8
All	All	1209/1215 (100%)	1074 (89%)	102 (8%)	33 (3%)	5 12

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	40	PRO
2	B	2	LYS
2	B	53	ALA
2	B	54	PRO
2	C	5	PHE
2	C	50	ILE
2	C	52	LYS
2	A	41	ASN
2	A	194	GLU
2	B	58	ALA
2	C	19	HIS
2	C	40	PRO
2	A	260	PRO
2	B	40	PRO
2	B	41	ASN
2	B	194	GLU
2	C	7	ARG
2	C	41	ASN
2	C	260	PRO
2	A	379	ALA
2	C	22	HIS
2	C	291	ARG
2	C	55	GLU
2	C	379	ALA
2	B	292	GLY
2	B	224	PRO
2	B	260	PRO
2	B	368	VAL
2	C	368	VAL
2	C	186	PRO
2	B	233	GLY
2	A	368	VAL
2	B	359	VAL

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	338/338 (100%)	297 (88%)	41 (12%)	<b>5</b> <b>11</b>
2	B	338/338 (100%)	299 (88%)	39 (12%)	<b>5</b> <b>13</b>
2	C	338/338 (100%)	288 (85%)	50 (15%)	<b>3</b> <b>7</b>
All	All	1014/1014 (100%)	884 (87%)	130 (13%)	<b>4</b> <b>10</b>

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	ILE
2	A	16	THR
2	A	21	ASP
2	A	39	ASN
2	A	46	ASP
2	A	57	ARG
2	A	59	ARG
2	A	63	ILE
2	A	80	VAL
2	A	107	SER
2	A	119	HIS
2	A	126	VAL
2	A	140	MET
2	A	147	LEU
2	A	156	ASP
2	A	172	ARG
2	A	190	ARG
2	A	216	ASP
2	A	217	VAL
2	A	223	MET
2	A	226	GLU
2	A	231	ILE
2	A	234	ARG
2	A	241	ARG
2	A	247	VAL
2	A	248	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	265	THR
2	A	267	VAL
2	A	285	ASN
2	A	290	LEU
2	A	295	ARG
2	A	298	VAL
2	A	311	THR
2	A	317	GLU
2	A	339	ARG
2	A	348	ASP
2	A	349	VAL
2	A	357	GLN
2	A	381	GLU
2	A	401	THR
2	A	404	LEU
2	B	6	ILE
2	B	16	THR
2	B	21	ASP
2	B	39	ASN
2	B	46	ASP
2	B	52	LYS
2	B	88	TYR
2	B	91	ASN
2	B	140	MET
2	B	155	ARG
2	B	156	ASP
2	B	168	VAL
2	B	185	ASN
2	B	190	ARG
2	B	215	ARG
2	B	216	ASP
2	B	217	VAL
2	B	223	MET
2	B	226	GLU
2	B	231	ILE
2	B	232	THR
2	B	248	LYS
2	B	262	THR
2	B	265	THR
2	B	267	VAL
2	B	285	ASN
2	B	295	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	302	GLN
2	B	307	PRO
2	B	310	ILE
2	B	314	THR
2	B	317	GLU
2	B	319	SER
2	B	323	LEU
2	B	347	THR
2	B	349	VAL
2	B	371	THR
2	B	381	GLU
2	B	404	LEU
2	C	5	PHE
2	C	21	ASP
2	C	39	ASN
2	C	46	ASP
2	C	52	LYS
2	C	63	ILE
2	C	78	SER
2	C	89	ILE
2	C	91	ASN
2	C	94	THR
2	C	119	HIS
2	C	126	VAL
2	C	132	VAL
2	C	140	MET
2	C	147	LEU
2	C	152	MET
2	C	156	ASP
2	C	158	LEU
2	C	171	ILE
2	C	176	LEU
2	C	190	ARG
2	C	216	ASP
2	C	217	VAL
2	C	223	MET
2	C	226	GLU
2	C	230	THR
2	C	232	THR
2	C	247	VAL
2	C	248	LYS
2	C	262	THR

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Mol	Chain	Res	Type
2	C	265	THR
2	C	267	VAL
2	C	285	ASN
2	C	295	ARG
2	C	297	GLU
2	C	298	VAL
2	C	302	GLN
2	C	303	VAL
2	C	307	PRO
2	C	311	THR
2	C	319	SER
2	C	335	PHE
2	C	342	PHE
2	C	347	THR
2	C	349	VAL
2	C	354	ARG
2	C	368	VAL
2	C	381	GLU
2	C	401	THR
2	C	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	19	HIS
2	A	64	ASN
2	A	67	HIS
2	A	85	HIS
2	A	98	GLN
2	A	115	GLN
2	A	119	HIS
2	A	160	GLN
2	A	183	HIS
2	A	285	ASN
2	A	313	HIS
2	A	341	GLN
2	B	19	HIS
2	B	64	ASN
2	B	85	HIS
2	B	115	GLN
2	B	119	HIS
2	B	160	GLN

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Mol	Chain	Res	Type
2	B	185	ASN
2	B	331	HIS
2	B	341	GLN
2	B	367	ASN
2	C	19	HIS
2	C	67	HIS
2	C	85	HIS
2	C	119	HIS
2	C	160	GLN
2	C	183	HIS
2	C	285	ASN
2	C	341	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	75/76 (98%)	27 (36%)	5 (6%)
1	E	75/76 (98%)	32 (42%)	11 (14%)
1	F	75/76 (98%)	24 (32%)	6 (8%)
All	All	225/228 (98%)	83 (36%)	22 (9%)

All (83) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	4	G
1	D	5	A
1	D	9	A
1	D	12	U
1	D	14	A
1	D	15	G
1	D	16	H2U
1	D	17	H2U
1	D	21	A
1	D	22	G
1	D	23	A
1	D	31	A
1	D	34	OMG
1	D	38	A
1	D	39	PSU
1	D	41	U
1	D	44	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	46	7MG
1	D	47	U
1	D	48	C
1	D	57	G
1	D	67	A
1	D	68	U
1	D	69	U
1	D	73	A
1	D	75	C
1	D	76	A
1	E	2	C
1	E	3	G
1	E	4	G
1	E	5	A
1	E	6	U
1	E	10	2MG
1	E	11	C
1	E	12	U
1	E	16	H2U
1	E	17	H2U
1	E	18	G
1	E	22	G
1	E	23	A
1	E	24	G
1	E	25	C
1	E	26	M2G
1	E	28	C
1	E	30	G
1	E	33	U
1	E	37	YYG
1	E	38	A
1	E	40	5MC
1	E	41	U
1	E	42	G
1	E	45	G
1	E	47	U
1	E	48	C
1	E	67	A
1	E	68	U
1	E	69	U
1	E	73	A
1	E	75	C

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Mol	Chain	Res	Type
1	F	3	G
1	F	4	G
1	F	5	A
1	F	6	U
1	F	11	C
1	F	17	H2U
1	F	18	G
1	F	21	A
1	F	22	G
1	F	23	A
1	F	25	C
1	F	26	M2G
1	F	30	G
1	F	37	YYG
1	F	38	A
1	F	41	U
1	F	43	G
1	F	46	7MG
1	F	47	U
1	F	58	1MA
1	F	68	U
1	F	69	U
1	F	73	A
1	F	75	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	3	G
1	D	16	H2U
1	D	21	A
1	D	22	G
1	D	46	7MG
1	E	3	G
1	E	16	H2U
1	E	17	H2U
1	E	21	A
1	E	22	G
1	E	25	C
1	E	27	C
1	E	30	G
1	E	46	7MG

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Mol	Chain	Res	Type
1	E	47	U
1	E	69	U
1	F	3	G
1	F	11	C
1	F	16	H2U
1	F	21	A
1	F	22	G
1	F	46	7MG

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

42 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	OMG	E	34	1	18,26,27	1.07	2 (11%)	19,38,41	1.61	3 (15%)
1	H2U	D	17	1	18,21,22	0.71	1 (5%)	21,30,33	2.03	5 (23%)
1	5MC	E	49	1	18,22,23	0.39	0	26,32,35	0.86	2 (7%)
1	2MG	D	10	1	18,26,27	1.02	2 (11%)	16,38,41	1.13	2 (12%)
1	5MC	F	49	1	18,22,23	0.98	1 (5%)	26,32,35	0.99	2 (7%)
1	5MC	E	40	1	18,22,23	2.58	1 (5%)	26,32,35	1.16	2 (7%)
1	5MU	D	54	1	19,22,23	4.44	1 (5%)	28,32,35	3.48	5 (17%)
1	PSU	E	39	1	18,21,22	0.88	1 (5%)	22,30,33	1.06	1 (4%)
1	7MG	F	46	1	22,26,27	3.20	2 (9%)	29,39,42	2.01	5 (17%)
1	2MG	E	10	1	18,26,27	1.01	2 (11%)	16,38,41	1.25	2 (12%)
1	OMC	F	32	1	19,22,23	0.42	0	26,31,34	0.85	1 (3%)
1	1MA	D	58	1	16,25,26	1.43	3 (18%)	18,37,40	1.10	2 (11%)
1	PSU	E	55	1	18,21,22	0.65	0	22,30,33	1.11	2 (9%)
1	5MC	F	40	1	18,22,23	2.94	1 (5%)	26,32,35	2.97	3 (11%)
1	YYG	E	37	1	31,42,43	1.63	7 (22%)	33,62,65	2.33	13 (39%)
1	OMG	D	34	1	18,26,27	1.05	2 (11%)	19,38,41	1.19	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	1MA	E	58	1	16,25,26	1.39	2 (12%)	18,37,40	1.34	4 (22%)
1	H2U	F	17	1	18,21,22	1.10	1 (5%)	21,30,33	1.47	5 (23%)
1	5MC	D	40	1	18,22,23	1.93	1 (5%)	26,32,35	1.34	4 (15%)
1	M2G	F	26	1	20,27,28	1.07	2 (10%)	22,40,43	0.97	2 (9%)
1	5MU	F	54	1	19,22,23	1.49	1 (5%)	28,32,35	0.70	1 (3%)
1	7MG	E	46	1	22,26,27	3.17	2 (9%)	29,39,42	2.01	5 (17%)
1	PSU	D	39	1	18,21,22	0.64	0	22,30,33	1.00	2 (9%)
1	PSU	F	55	1	18,21,22	0.78	0	22,30,33	0.94	1 (4%)
1	2MG	F	10	1	18,26,27	1.02	2 (11%)	16,38,41	1.14	2 (12%)
1	OMC	E	32	1	19,22,23	0.35	0	26,31,34	1.18	2 (7%)
1	M2G	E	26	1	20,27,28	1.07	2 (10%)	22,40,43	2.91	6 (27%)
1	5MU	E	54	1	19,22,23	1.90	1 (5%)	28,32,35	0.89	2 (7%)
1	PSU	D	55	1	18,21,22	0.75	0	22,30,33	0.98	1 (4%)
1	H2U	E	16	1	18,21,22	0.62	0	21,30,33	3.20	9 (42%)
1	OMG	F	34	1	18,26,27	1.08	2 (11%)	19,38,41	1.54	3 (15%)
1	H2U	E	17	1	18,21,22	1.12	2 (11%)	21,30,33	2.84	6 (28%)
1	YYG	F	37	1	31,42,43	1.55	4 (12%)	33,62,65	2.56	12 (36%)
1	1MA	F	58	1	16,25,26	1.45	2 (12%)	18,37,40	1.02	2 (11%)
1	7MG	D	46	1	22,26,27	3.53	3 (13%)	29,39,42	1.95	6 (20%)
1	5MC	D	49	1	18,22,23	0.55	1 (5%)	26,32,35	1.70	4 (15%)
1	PSU	F	39	1	18,21,22	0.82	0	22,30,33	1.57	2 (9%)
1	YYG	D	37	1	31,42,43	1.75	6 (19%)	33,62,65	2.90	14 (42%)
1	OMC	D	32	1	19,22,23	0.37	0	26,31,34	0.98	2 (7%)
1	H2U	F	16	1	18,21,22	1.07	1 (5%)	21,30,33	3.05	11 (52%)
1	M2G	D	26	1	20,27,28	1.03	2 (10%)	22,40,43	1.29	4 (18%)
1	H2U	D	16	1	18,21,22	0.72	0	21,30,33	2.07	4 (19%)

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	OMG	E	34	1	-	3/5/27/28	0/3/3/3
1	H2U	D	17	1	-	6/7/38/39	0/2/2/2
1	5MC	E	49	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	D	10	1	-	2/5/27/28	0/3/3/3
1	5MC	F	49	1	-	0/7/25/26	0/2/2/2
1	5MC	E	40	1	-	2/7/25/26	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	7MG	F	46	1	-	0/7/37/38	0/3/3/3
1	2MG	E	10	1	-	1/5/27/28	0/3/3/3
1	OMC	F	32	1	-	0/9/27/28	0/2/2/2
1	1MA	D	58	1	-	2/3/25/26	0/3/3/3
1	PSU	E	55	1	-	2/7/25/26	0/2/2/2
1	5MC	F	40	1	-	0/7/25/26	0/2/2/2
1	YYG	E	37	1	-	14/20/42/43	0/3/4/4
1	OMG	D	34	1	-	2/5/27/28	0/3/3/3
1	1MA	E	58	1	-	0/3/25/26	0/3/3/3
1	H2U	F	17	1	-	4/7/38/39	0/2/2/2
1	5MC	D	40	1	-	0/7/25/26	0/2/2/2
1	M2G	F	26	1	-	1/7/29/30	0/3/3/3
1	5MU	F	54	1	-	0/7/25/26	0/2/2/2
1	7MG	E	46	1	-	1/7/37/38	0/3/3/3
1	PSU	D	39	1	-	4/7/25/26	0/2/2/2
1	PSU	F	55	1	-	1/7/25/26	0/2/2/2
1	2MG	F	10	1	-	0/5/27/28	0/3/3/3
1	OMC	E	32	1	-	2/9/27/28	0/2/2/2
1	M2G	E	26	1	-	3/7/29/30	0/3/3/3
1	5MU	E	54	1	-	0/7/25/26	0/2/2/2
1	PSU	D	55	1	-	1/7/25/26	0/2/2/2
1	H2U	E	16	1	-	4/7/38/39	0/2/2/2
1	OMG	F	34	1	-	1/5/27/28	0/3/3/3
1	H2U	E	17	1	-	2/7/38/39	0/2/2/2
1	YYG	F	37	1	-	4/20/42/43	0/3/4/4
1	1MA	F	58	1	-	2/3/25/26	0/3/3/3
1	7MG	D	46	1	-	2/7/37/38	0/3/3/3
1	5MC	D	49	1	-	0/7/25/26	0/2/2/2
1	PSU	F	39	1	-	0/7/25/26	0/2/2/2
1	YYG	D	37	1	-	9/20/42/43	0/3/4/4
1	OMC	D	32	1	-	1/9/27/28	0/2/2/2
1	H2U	F	16	1	-	0/7/38/39	0/2/2/2
1	M2G	D	26	1	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	H2U	D	16	1	-	6/7/38/39	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	5MU	C5M-C5	-19.29	1.02	1.50
1	D	46	7MG	C8-N9	-15.67	1.37	1.46
1	F	46	7MG	C8-N9	-14.52	1.37	1.46
1	E	46	7MG	C8-N9	-14.49	1.37	1.46
1	F	40	5MC	CM5-C5	-12.42	1.19	1.50
1	E	40	5MC	CM5-C5	-10.83	1.23	1.50
1	D	40	5MC	CM5-C5	-8.09	1.30	1.50
1	E	54	5MU	C5M-C5	-8.05	1.30	1.50
1	F	54	5MU	C5M-C5	-6.26	1.35	1.50
1	D	37	YYG	O23-C21	-4.95	1.25	1.34
1	F	37	YYG	O23-C21	-4.72	1.26	1.34
1	E	37	YYG	O23-C21	-4.37	1.26	1.34
1	F	58	1MA	C2-N3	4.10	1.34	1.29
1	F	49	5MC	CM5-C5	3.94	1.60	1.50
1	E	58	1MA	C2-N3	3.90	1.33	1.29
1	D	37	YYG	O17-C16	3.77	1.30	1.21
1	F	16	H2U	C2-N1	3.72	1.40	1.35
1	D	58	1MA	C2-N3	3.71	1.33	1.29
1	F	37	YYG	O18-C16	-3.71	1.24	1.33
1	E	37	YYG	O18-C16	-3.67	1.24	1.33
1	D	46	7MG	CM7-N7	3.58	1.58	1.45
1	F	17	H2U	C2-N1	3.51	1.40	1.35
1	E	17	H2U	C2-N1	3.50	1.40	1.35
1	D	37	YYG	O22-C21	3.45	1.28	1.21
1	D	46	7MG	C5-N7	3.29	1.39	1.35
1	F	46	7MG	C5-N7	3.23	1.39	1.35
1	E	46	7MG	C5-N7	3.07	1.39	1.35
1	E	37	YYG	C15-N20	3.01	1.52	1.45
1	F	37	YYG	C4-N3	-2.78	1.35	1.40
1	E	34	OMG	C5-C6	-2.73	1.41	1.47
1	E	37	YYG	O22-C21	2.73	1.26	1.21
1	D	58	1MA	C6-N6	2.72	1.34	1.27
1	D	37	YYG	C4-N3	-2.72	1.35	1.40
1	F	34	OMG	C5-C6	-2.69	1.41	1.47
1	E	37	YYG	C4-N3	-2.66	1.35	1.40
1	D	37	YYG	C15-N20	2.65	1.51	1.45
1	E	58	1MA	C6-N6	2.54	1.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	1MA	C6-N6	2.52	1.33	1.27
1	D	26	M2G	C5-C6	-2.51	1.42	1.47
1	E	37	YYG	C8-N7	-2.51	1.30	1.35
1	D	37	YYG	C8-N7	-2.46	1.30	1.35
1	F	26	M2G	C8-N7	-2.46	1.30	1.35
1	E	26	M2G	C5-C6	-2.45	1.42	1.47
1	F	10	2MG	C5-C6	-2.45	1.42	1.47
1	F	34	OMG	C8-N7	-2.43	1.30	1.35
1	F	10	2MG	C8-N7	-2.42	1.30	1.35
1	D	10	2MG	C8-N7	-2.42	1.30	1.35
1	D	26	M2G	C8-N7	-2.41	1.30	1.35
1	E	34	OMG	C8-N7	-2.41	1.30	1.35
1	F	26	M2G	C5-C6	-2.40	1.42	1.47
1	D	10	2MG	C5-C6	-2.37	1.42	1.47
1	D	34	OMG	C8-N7	-2.36	1.31	1.35
1	E	26	M2G	C8-N7	-2.36	1.31	1.35
1	E	10	2MG	C8-N7	-2.35	1.31	1.35
1	F	37	YYG	C8-N7	-2.30	1.31	1.35
1	D	17	H2U	C2-N1	2.25	1.38	1.35
1	D	34	OMG	C5-C6	-2.25	1.42	1.47
1	E	10	2MG	C5-C6	-2.23	1.42	1.47
1	E	39	PSU	O4'-C1'	-2.21	1.40	1.43
1	E	17	H2U	O2-C2	2.17	1.27	1.23
1	E	37	YYG	C21-N20	2.14	1.40	1.34
1	D	49	5MC	CM5-C5	-2.01	1.45	1.50
1	D	58	1MA	C8-N7	-2.00	1.31	1.35

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	40	5MC	CM5-C5-C6	-14.42	103.59	122.85
1	D	54	5MU	C5M-C5-C4	12.48	132.50	118.77
1	D	54	5MU	C5M-C5-C6	-11.33	107.72	122.85
1	E	17	H2U	O4'-C1'-N1	9.30	121.96	109.30
1	E	26	M2G	CM1-N2-C2	9.19	139.72	120.55
1	E	16	H2U	O2-C2-N1	-7.56	113.62	123.11
1	D	37	YYG	C3-N3-C4	7.46	129.95	116.71
1	E	16	H2U	C4-N3-C2	-7.27	119.76	125.79
1	D	49	5MC	CM5-C5-C6	7.12	132.35	122.85
1	D	17	H2U	C4-N3-C2	-6.88	120.08	125.79
1	F	46	7MG	N9-C8-N7	6.79	113.09	103.38
1	D	46	7MG	N9-C8-N7	6.76	113.05	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	7MG	N9-C8-N7	6.74	113.01	103.38
1	F	16	H2U	C4-N3-C2	-6.63	120.29	125.79
1	F	37	YYG	C14-C15-C16	-6.48	91.39	110.30
1	E	16	H2U	O4'-C1'-N1	6.43	118.06	109.30
1	E	37	YYG	C3-N3-C4	6.40	128.07	116.71
1	D	37	YYG	C14-C15-C16	-6.00	92.79	110.30
1	F	16	H2U	N3-C2-N1	5.98	122.98	116.65
1	D	37	YYG	C16-C15-N20	5.98	124.52	110.72
1	F	37	YYG	C3-N3-C4	5.78	126.97	116.71
1	D	54	5MU	O2'-C2'-C3'	-5.69	93.43	111.82
1	E	17	H2U	O3'-C3'-C2'	-5.69	93.43	111.82
1	F	37	YYG	C16-C15-N20	5.60	123.65	110.72
1	F	16	H2U	O2-C2-N3	-5.37	111.49	121.50
1	F	39	PSU	O2'-C2'-C3'	-5.29	94.70	111.82
1	D	37	YYG	C19-O18-C16	5.27	127.85	115.94
1	E	37	YYG	O18-C16-O17	-5.19	113.69	123.84
1	F	16	H2U	O2-C2-N1	-5.08	116.73	123.11
1	E	26	M2G	O3'-C3'-C4'	5.04	125.63	111.05
1	E	26	M2G	CM2-N2-C2	-5.03	110.06	120.55
1	D	16	H2U	O4'-C1'-N1	5.01	116.13	109.30
1	E	40	5MC	CM5-C5-C6	-4.97	116.21	122.85
1	F	34	OMG	CM2-O2'-C2'	-4.85	101.80	114.52
1	D	37	YYG	C13-C14-C15	4.73	122.53	113.21
1	D	37	YYG	C15-N20-C21	4.66	132.27	120.90
1	E	46	7MG	O3'-C3'-C4'	-4.60	97.75	111.05
1	D	16	H2U	O2-C2-N1	-4.58	117.36	123.11
1	D	40	5MC	O4'-C1'-N1	4.55	118.77	108.36
1	D	16	H2U	C4-N3-C2	-4.46	122.09	125.79
1	E	34	OMG	O2'-C2'-C1'	-4.43	100.32	109.09
1	F	46	7MG	O4'-C1'-N9	4.42	115.32	109.30
1	D	46	7MG	O4'-C1'-N9	4.28	115.13	109.30
1	E	17	H2U	C5-C4-N3	4.24	121.41	116.65
1	E	34	OMG	CM2-O2'-C2'	-4.06	103.88	114.52
1	F	37	YYG	C14-C13-C12	-3.96	103.70	112.66
1	E	16	H2U	O4-C4-C5	-3.94	113.76	122.17
1	F	37	YYG	O23-C21-N20	3.92	117.69	110.80
1	E	26	M2G	O2'-C2'-C3'	3.83	124.20	111.82
1	F	37	YYG	C14-C15-N20	-3.81	103.18	110.88
1	E	32	OMC	CM2-O2'-C2'	-3.81	104.54	114.52
1	D	37	YYG	O23-C21-O22	-3.78	119.03	124.58
1	E	37	YYG	O18-C16-C15	3.76	121.14	111.52
1	E	46	7MG	C4-C5-N7	3.76	110.75	105.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	7MG	C4-C5-N7	3.70	110.67	105.53
1	E	32	OMC	C2'-C1'-N1	-3.66	107.12	114.22
1	D	46	7MG	C4-C5-N7	3.62	110.55	105.53
1	E	26	M2G	O2'-C2'-C1'	3.57	124.03	110.85
1	F	46	7MG	O3'-C3'-C2'	3.54	123.28	111.82
1	E	17	H2U	C4-N3-C2	-3.53	122.86	125.79
1	D	37	YYG	C14-C13-C12	3.46	120.47	112.66
1	F	37	YYG	C4-N3-C2	-3.42	111.76	122.15
1	E	37	YYG	C15-N20-C21	3.40	129.21	120.90
1	D	17	H2U	N3-C2-N1	3.40	120.25	116.65
1	F	49	5MC	O3'-C3'-C4'	3.37	120.80	111.05
1	E	37	YYG	C4-N3-C2	-3.35	111.97	122.15
1	D	37	YYG	C4-N3-C2	-3.31	112.09	122.15
1	F	32	OMC	O2'-C2'-C1'	-3.29	102.66	109.08
1	E	37	YYG	C13-C14-C15	3.26	119.62	113.21
1	D	32	OMC	C2'-C1'-N1	-3.25	107.92	114.22
1	D	40	5MC	O2'-C2'-C3'	-3.20	101.48	111.82
1	E	55	PSU	O2'-C2'-C1'	-3.17	103.68	111.23
1	F	17	H2U	N3-C2-N1	3.17	120.00	116.65
1	F	17	H2U	C4-N3-C2	-3.16	123.17	125.79
1	E	37	YYG	C14-C15-C16	-3.10	101.26	110.30
1	F	16	H2U	O3'-C3'-C4'	3.06	119.90	111.05
1	D	54	5MU	O4'-C1'-N1	-3.03	101.44	108.36
1	F	16	H2U	O4'-C1'-N1	-3.03	105.17	109.30
1	D	17	H2U	O2-C2-N1	-3.01	119.33	123.11
1	E	16	H2U	O3'-C3'-C2'	-2.97	102.23	111.82
1	E	10	2MG	O3'-C3'-C4'	2.96	119.62	111.05
1	E	46	7MG	O4'-C1'-N9	-2.93	105.30	109.30
1	D	26	M2G	CM2-N2-CM1	2.91	124.79	115.77
1	E	16	H2U	N3-C2-N1	2.91	119.73	116.65
1	E	58	1MA	N1-C2-N3	2.90	129.41	126.02
1	F	16	H2U	O3'-C3'-C2'	2.84	121.02	111.82
1	D	34	OMG	CM2-O2'-C2'	-2.81	107.16	114.52
1	F	34	OMG	O2'-C2'-C1'	-2.74	103.66	109.09
1	E	37	YYG	C16-C15-N20	2.74	117.04	110.72
1	D	46	7MG	O3'-C3'-C4'	2.72	118.92	111.05
1	E	49	5MC	O2'-C2'-C3'	2.72	120.63	111.82
1	D	37	YYG	O23-C21-N20	2.72	115.58	110.80
1	F	37	YYG	O3'-C3'-C2'	2.70	120.55	111.82
1	D	58	1MA	N1-C2-N3	2.69	129.16	126.02
1	F	16	H2U	O2'-C2'-C3'	2.69	120.53	111.82
1	E	37	YYG	C24-O23-C21	2.69	118.84	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	1MA	C5-C6-N1	2.67	117.88	113.90
1	F	55	PSU	C6-C5-C4	2.67	120.06	118.20
1	F	58	1MA	N1-C2-N3	2.64	129.10	126.02
1	E	37	YYG	C11-C12-N1	-2.63	105.05	106.53
1	E	37	YYG	O6-C6-C5	2.61	128.80	124.17
1	E	46	7MG	O5'-C5'-C4'	2.61	117.86	108.99
1	E	54	5MU	O3'-C3'-C4'	-2.60	103.53	111.05
1	E	16	H2U	O3'-C3'-C4'	-2.59	103.55	111.05
1	D	17	H2U	O3'-C3'-C4'	-2.59	103.56	111.05
1	D	16	H2U	O4-C4-C5	-2.59	116.64	122.17
1	F	17	H2U	O2-C2-N3	-2.58	116.70	121.50
1	F	39	PSU	C6-C5-C4	2.57	120.00	118.20
1	F	37	YYG	O22-C21-N20	-2.56	120.66	124.85
1	E	58	1MA	C5-C6-N1	2.54	117.68	113.90
1	F	26	M2G	N1-C2-N2	-2.51	115.90	118.04
1	F	16	H2U	O4-C4-N3	-2.50	116.31	120.28
1	D	58	1MA	C5-C6-N1	2.49	117.61	113.90
1	D	26	M2G	CM2-N2-C2	-2.48	115.37	120.55
1	D	46	7MG	O3'-C3'-C2'	-2.47	103.83	111.82
1	E	17	H2U	N3-C2-N1	-2.47	114.05	116.65
1	F	37	YYG	O6-C6-C5	2.46	128.53	124.17
1	F	37	YYG	O2'-C2'-C1'	-2.45	101.82	110.85
1	D	10	2MG	CM2-N2-C2	-2.44	118.46	123.86
1	D	49	5MC	C5-C6-N1	-2.43	120.84	123.34
1	F	16	H2U	O4-C4-C5	-2.43	116.98	122.17
1	D	37	YYG	O6-C6-C5	2.43	128.47	124.17
1	F	17	H2U	O2-C2-N1	-2.43	120.06	123.11
1	D	46	7MG	O2'-C2'-C1'	2.42	118.12	110.02
1	E	17	H2U	O2-C2-N3	-2.42	116.99	121.50
1	D	37	YYG	C3-N3-C2	-2.41	117.88	120.13
1	E	16	H2U	O2-C2-N3	-2.39	117.05	121.50
1	D	39	PSU	O2'-C2'-C3'	-2.34	104.25	111.82
1	E	10	2MG	O6-C6-C5	2.33	128.93	124.37
1	D	55	PSU	C6-C5-C4	2.31	119.81	118.20
1	D	34	OMG	O3'-C3'-C2'	2.30	117.70	111.17
1	F	40	5MC	C5-C6-N1	-2.30	120.98	123.34
1	D	34	OMG	O6-C6-C5	2.29	128.85	124.37
1	F	10	2MG	O2'-C2'-C3'	2.29	119.24	111.82
1	D	40	5MC	C5-C6-N1	-2.27	121.00	123.34
1	D	40	5MC	C2'-C1'-N1	-2.27	106.79	113.22
1	F	16	H2U	C5-C4-N3	2.26	119.19	116.65
1	E	37	YYG	O23-C21-N20	2.25	114.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	PSU	C6-C5-C4	2.24	119.77	118.20
1	E	58	1MA	O2'-C2'-C1'	2.24	119.11	110.85
1	D	10	2MG	O6-C6-C5	2.23	128.74	124.37
1	F	17	H2U	C5-C4-N3	2.23	119.15	116.65
1	E	40	5MC	C5-C6-N1	-2.22	121.06	123.34
1	E	39	PSU	C6-C5-C4	2.22	119.75	118.20
1	F	37	YYG	C19-O18-C16	2.21	120.94	115.94
1	E	49	5MC	C5-C6-N1	-2.20	121.08	123.34
1	F	26	M2G	O6-C6-C5	2.19	128.66	124.37
1	D	26	M2G	O6-C6-C5	2.19	128.65	124.37
1	F	49	5MC	C5-C6-N1	-2.16	121.11	123.34
1	D	32	OMC	O3'-C3'-C2'	-2.16	105.03	111.17
1	F	46	7MG	O3'-C3'-C4'	2.15	117.28	111.05
1	D	26	M2G	O2'-C2'-C1'	2.15	118.81	110.85
1	F	54	5MU	C6-C5-C4	2.15	119.83	118.03
1	F	40	5MC	O3'-C3'-C4'	2.14	117.25	111.05
1	E	37	YYG	O23-C21-O22	-2.14	121.44	124.58
1	F	10	2MG	O6-C6-C5	2.14	128.55	124.37
1	D	49	5MC	O3'-C3'-C4'	2.14	117.23	111.05
1	D	39	PSU	C6-C5-C4	2.14	119.69	118.20
1	E	34	OMG	O6-C6-C5	2.13	128.53	124.37
1	D	17	H2U	O4-C4-C5	-2.11	117.67	122.17
1	F	34	OMG	O6-C6-C5	2.10	128.48	124.37
1	D	54	5MU	C6-C5-C4	2.09	119.78	118.03
1	D	37	YYG	C24-O23-C21	-2.08	113.21	115.66
1	E	54	5MU	C6-C5-C4	2.07	119.77	118.03
1	E	58	1MA	O2'-C2'-C3'	-2.05	105.18	111.82
1	E	26	M2G	O6-C6-C5	2.04	128.36	124.37
1	D	49	5MC	O2'-C2'-C3'	2.04	118.42	111.82
1	D	37	YYG	O3'-C3'-C4'	-2.02	105.20	111.05
1	E	16	H2U	C5-C6-N1	2.00	118.21	111.61

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	16	H2U	O4'-C1'-N1-C6
1	D	16	H2U	C2'-C1'-N1-C2
1	D	17	H2U	O4'-C4'-C5'-O5'
1	D	17	H2U	C3'-C4'-C5'-O5'
1	D	32	OMC	C3'-C2'-O2'-CM2
1	D	37	YYG	O23-C21-N20-C15

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Mol	Chain	Res	Type	Atoms
1	D	39	PSU	O4'-C1'-C5-C4
1	D	39	PSU	O4'-C1'-C5-C6
1	D	46	7MG	O4'-C4'-C5'-O5'
1	D	46	7MG	C3'-C4'-C5'-O5'
1	E	16	H2U	O4'-C1'-N1-C6
1	E	16	H2U	C2'-C1'-N1-C6
1	E	17	H2U	C2'-C1'-N1-C2
1	E	26	M2G	O4'-C4'-C5'-O5'
1	E	26	M2G	C3'-C4'-C5'-O5'
1	E	32	OMC	C1'-C2'-O2'-CM2
1	E	34	OMG	C1'-C2'-O2'-CM2
1	E	37	YYG	C11-C12-C13-C14
1	E	37	YYG	C13-C14-C15-N20
1	E	37	YYG	C14-C15-N20-C21
1	E	40	5MC	O4'-C4'-C5'-O5'
1	F	17	H2U	C2'-C1'-N1-C2
1	F	34	OMG	C1'-C2'-O2'-CM2
1	F	37	YYG	C12-C13-C14-C15
1	F	37	YYG	C16-C15-N20-C21
1	D	37	YYG	O22-C21-N20-C15
1	E	37	YYG	O23-C21-N20-C15
1	D	34	OMG	O4'-C4'-C5'-O5'
1	E	40	5MC	C3'-C4'-C5'-O5'
1	F	58	1MA	O4'-C4'-C5'-O5'
1	E	37	YYG	O22-C21-N20-C15
1	F	17	H2U	C2'-C1'-N1-C6
1	E	37	YYG	C13-C14-C15-C16
1	D	16	H2U	O4'-C4'-C5'-O5'
1	D	16	H2U	C3'-C4'-C5'-O5'
1	D	39	PSU	C3'-C4'-C5'-O5'
1	D	58	1MA	O4'-C4'-C5'-O5'
1	D	58	1MA	C3'-C4'-C5'-O5'
1	E	16	H2U	C3'-C4'-C5'-O5'
1	E	37	YYG	C3'-C4'-C5'-O5'
1	F	37	YYG	C3'-C4'-C5'-O5'
1	F	58	1MA	C3'-C4'-C5'-O5'
1	D	37	YYG	C16-C15-N20-C21
1	D	17	H2U	C2'-C1'-N1-C6
1	E	17	H2U	C2'-C1'-N1-C6
1	D	34	OMG	C3'-C4'-C5'-O5'
1	D	39	PSU	O4'-C4'-C5'-O5'
1	E	37	YYG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	E	37	YYG	C12-C13-C14-C15
1	D	37	YYG	N20-C15-C16-O18
1	E	46	7MG	C3'-C4'-C5'-O5'
1	F	37	YYG	O4'-C4'-C5'-O5'
1	E	37	YYG	N20-C15-C16-O18
1	D	37	YYG	C13-C14-C15-C16
1	E	37	YYG	C14-C15-C16-O17
1	E	37	YYG	C14-C15-C16-O18
1	E	37	YYG	N20-C15-C16-O17
1	D	37	YYG	C14-C15-C16-O18
1	D	37	YYG	N20-C15-C16-O17
1	F	17	H2U	O4'-C4'-C5'-O5'
1	F	26	M2G	C4'-C5'-O5'-P
1	D	37	YYG	C14-C15-C16-O17
1	D	10	2MG	C3'-C4'-C5'-O5'
1	E	37	YYG	N1-C12-C13-C14
1	D	16	H2U	C2'-C1'-N1-C6
1	E	16	H2U	C4'-C5'-O5'-P
1	D	10	2MG	O4'-C4'-C5'-O5'
1	F	17	H2U	C3'-C4'-C5'-O5'
1	D	17	H2U	O4'-C1'-N1-C2
1	D	17	H2U	C4'-C5'-O5'-P
1	E	10	2MG	C4'-C5'-O5'-P
1	E	26	M2G	C4'-C5'-O5'-P
1	E	34	OMG	O4'-C4'-C5'-O5'
1	D	17	H2U	C2'-C1'-N1-C2
1	E	34	OMG	C3'-C4'-C5'-O5'
1	D	55	PSU	O4'-C1'-C5-C4
1	E	55	PSU	O4'-C1'-C5-C4
1	E	32	OMC	C3'-C2'-O2'-CM2
1	E	55	PSU	O4'-C1'-C5-C6
1	F	55	PSU	O4'-C1'-C5-C6
1	D	16	H2U	O4'-C1'-N1-C2
1	D	37	YYG	C13-C14-C15-N20

There are no ring outliers.

38 monomers are involved in 156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	34	OMG	3	0
1	D	17	H2U	3	0
1	D	10	2MG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	49	5MC	1	0
1	D	54	5MU	1	0
1	E	39	PSU	2	0
1	F	46	7MG	4	0
1	E	10	2MG	12	0
1	F	32	OMC	1	0
1	D	58	1MA	3	0
1	E	55	PSU	1	0
1	F	40	5MC	3	0
1	E	37	YYG	12	0
1	D	34	OMG	2	0
1	E	58	1MA	1	0
1	F	17	H2U	1	0
1	D	40	5MC	4	0
1	F	26	M2G	7	0
1	F	54	5MU	1	0
1	E	46	7MG	2	0
1	D	39	PSU	5	0
1	F	55	PSU	3	0
1	F	10	2MG	9	0
1	E	32	OMC	3	0
1	E	26	M2G	11	0
1	E	54	5MU	3	0
1	D	55	PSU	1	0
1	E	16	H2U	4	0
1	F	34	OMG	4	0
1	E	17	H2U	3	0
1	F	37	YYG	17	0
1	D	46	7MG	2	0
1	D	49	5MC	1	0
1	D	37	YYG	8	0
1	D	32	OMC	2	0
1	F	16	H2U	5	0
1	D	26	M2G	11	0
1	D	16	H2U	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
5	GNP	B	406	3	29,34,34	1.65	3 (10%)	33,54,54	2.54	8 (24%)
5	GNP	C	406	3	29,34,34	2.17	5 (17%)	33,54,54	4.12	14 (42%)
4	PHE	E	77	1	10,11,12	0.99	1 (10%)	10,13,15	1.96	2 (20%)
4	PHE	F	77	1	10,11,12	1.25	2 (20%)	10,13,15	2.14	2 (20%)
4	PHE	D	77	1	10,11,12	1.11	1 (10%)	10,13,15	2.49	2 (20%)
5	GNP	A	406	3	29,34,34	1.82	7 (24%)	33,54,54	4.29	19 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GNP	B	406	3	-	9/14/38/38	0/3/3/3
5	GNP	C	406	3	-	5/14/38/38	0/3/3/3
4	PHE	E	77	1	-	1/5/6/8	0/1/1/1
4	PHE	F	77	1	-	1/5/6/8	0/1/1/1
4	PHE	D	77	1	-	0/5/6/8	0/1/1/1
5	GNP	A	406	3	-	9/14/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	406	GNP	PB-O3A	-7.91	1.49	1.59
5	B	406	GNP	PB-O3A	-6.18	1.51	1.59
5	C	406	GNP	PG-O1G	5.04	1.54	1.46
5	A	406	GNP	PB-O3A	-4.73	1.53	1.59
5	A	406	GNP	C6-N1	3.70	1.39	1.33
5	A	406	GNP	PB-O2B	-3.64	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	406	GNP	PG-O2G	-3.48	1.47	1.56
5	B	406	GNP	C6-N1	3.46	1.39	1.33
5	C	406	GNP	C6-N1	3.11	1.38	1.33
5	B	406	GNP	PG-O2G	-3.08	1.48	1.56
4	D	77	PHE	CA-N	-3.02	1.39	1.48
5	A	406	GNP	PG-O2G	-2.94	1.48	1.56
4	F	77	PHE	CA-N	-2.86	1.39	1.48
4	E	77	PHE	CA-N	-2.51	1.40	1.48
5	A	406	GNP	PG-O1G	2.27	1.49	1.46
5	A	406	GNP	PB-N3B	-2.18	1.57	1.63
4	F	77	PHE	O-C	2.13	1.28	1.19
5	A	406	GNP	PG-O3G	-2.13	1.51	1.56
5	C	406	GNP	C2-N1	2.07	1.39	1.35

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	GNP	C1'-N9-C4	15.91	154.59	126.64
5	C	406	GNP	C1'-N9-C4	-14.63	100.94	126.64
5	C	406	GNP	O2B-PB-O1B	11.12	133.22	109.92
5	A	406	GNP	C5-C6-N1	-9.26	110.76	123.43
5	B	406	GNP	C5-C6-N1	-9.10	110.99	123.43
5	C	406	GNP	C5-C6-N1	-7.53	113.13	123.43
5	A	406	GNP	C2-N1-C6	6.52	126.29	115.93
4	F	77	PHE	CG-CB-CA	-6.35	101.24	114.10
5	A	406	GNP	O2B-PB-O1B	6.13	122.77	109.92
4	D	77	PHE	CG-CB-CA	-5.54	102.88	114.10
5	A	406	GNP	O4'-C1'-C2'	-5.52	98.86	106.93
4	D	77	PHE	CB-CA-C	-5.51	101.13	111.47
5	B	406	GNP	C2-N1-C6	5.35	124.43	115.93
5	A	406	GNP	C2-N3-C4	-5.34	109.25	115.36
4	E	77	PHE	CB-CA-C	-5.33	101.48	111.47
5	C	406	GNP	O3A-PB-N3B	5.18	120.97	106.59
5	C	406	GNP	C2-N3-C4	-5.15	109.47	115.36
5	A	406	GNP	O2G-PG-O3G	4.86	120.58	107.64
5	B	406	GNP	O1G-PG-N3B	-4.48	105.17	111.77
5	C	406	GNP	O1B-PB-N3B	-4.38	105.31	111.77
5	B	406	GNP	C2-N3-C4	-4.21	110.55	115.36
5	C	406	GNP	C2-N1-C6	4.09	122.42	115.93
5	B	406	GNP	C1'-N9-C4	-3.99	119.64	126.64
5	A	406	GNP	C4-C5-N7	3.42	112.97	109.40
5	A	406	GNP	O5'-C5'-C4'	-3.29	97.68	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	GNP	O3'-C3'-C4'	-3.29	101.55	111.05
5	B	406	GNP	O1B-PB-N3B	-3.26	106.97	111.77
5	A	406	GNP	C3'-C2'-C1'	-3.20	96.16	100.98
5	C	406	GNP	O5'-C5'-C4'	2.95	119.14	108.99
5	A	406	GNP	O2A-PA-O5'	-2.80	94.72	107.75
5	C	406	GNP	O2'-C2'-C3'	2.80	120.88	111.82
5	A	406	GNP	PB-O3A-PA	2.76	142.34	132.62
5	C	406	GNP	O5'-PA-O1A	2.76	119.86	109.07
4	E	77	PHE	CG-CB-CA	-2.73	108.57	114.10
5	A	406	GNP	O3G-PG-O1G	-2.71	106.64	113.45
5	A	406	GNP	N3-C2-N1	-2.57	123.80	127.22
5	C	406	GNP	C3'-C2'-C1'	2.55	104.81	100.98
5	C	406	GNP	O2A-PA-O1A	2.51	124.62	112.24
5	B	406	GNP	O2B-PB-O3A	2.45	112.82	104.64
5	A	406	GNP	O4'-C4'-C5'	2.32	117.01	109.37
5	A	406	GNP	O2A-PA-O1A	2.30	123.59	112.24
4	F	77	PHE	CB-CA-C	-2.23	107.29	111.47
5	C	406	GNP	C4-C5-C6	-2.22	118.67	120.80
5	A	406	GNP	C4-C5-C6	-2.20	118.69	120.80
5	C	406	GNP	C4-C5-N7	2.16	111.66	109.40
5	A	406	GNP	O3'-C3'-C2'	-2.10	105.02	111.82
5	B	406	GNP	PA-O5'-C5'	-2.00	109.94	121.68

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	77	PHE	O-C-CA-CB
4	F	77	PHE	O-C-CA-CB
5	A	406	GNP	PB-N3B-PG-O1G
5	A	406	GNP	PG-N3B-PB-O1B
5	A	406	GNP	PA-O3A-PB-O1B
5	A	406	GNP	PA-O3A-PB-O2B
5	A	406	GNP	C5'-O5'-PA-O3A
5	A	406	GNP	C5'-O5'-PA-O1A
5	B	406	GNP	PB-N3B-PG-O1G
5	B	406	GNP	PG-N3B-PB-O1B
5	B	406	GNP	PA-O3A-PB-O1B
5	B	406	GNP	PA-O3A-PB-O2B
5	B	406	GNP	C5'-O5'-PA-O3A
5	C	406	GNP	PB-N3B-PG-O1G
5	C	406	GNP	PG-N3B-PB-O1B

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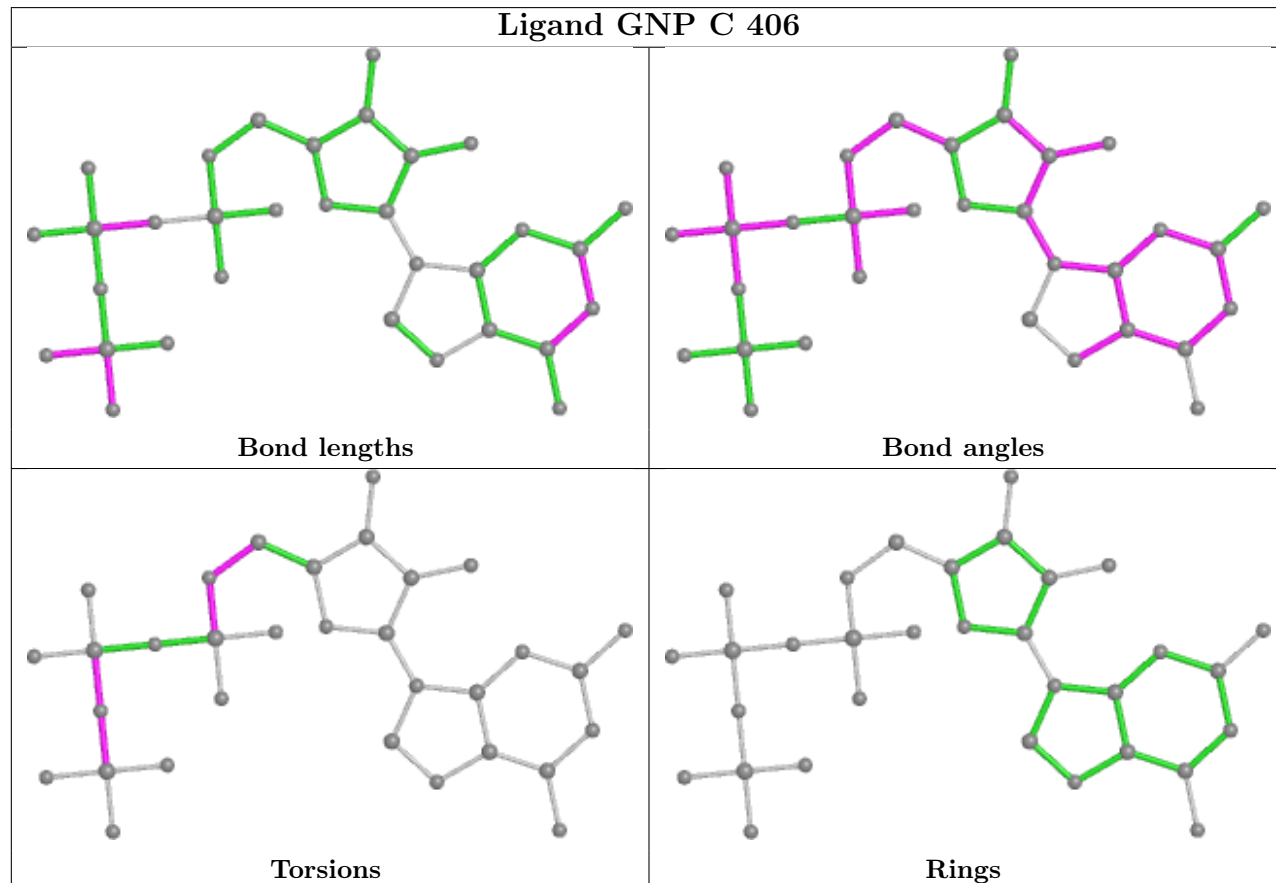
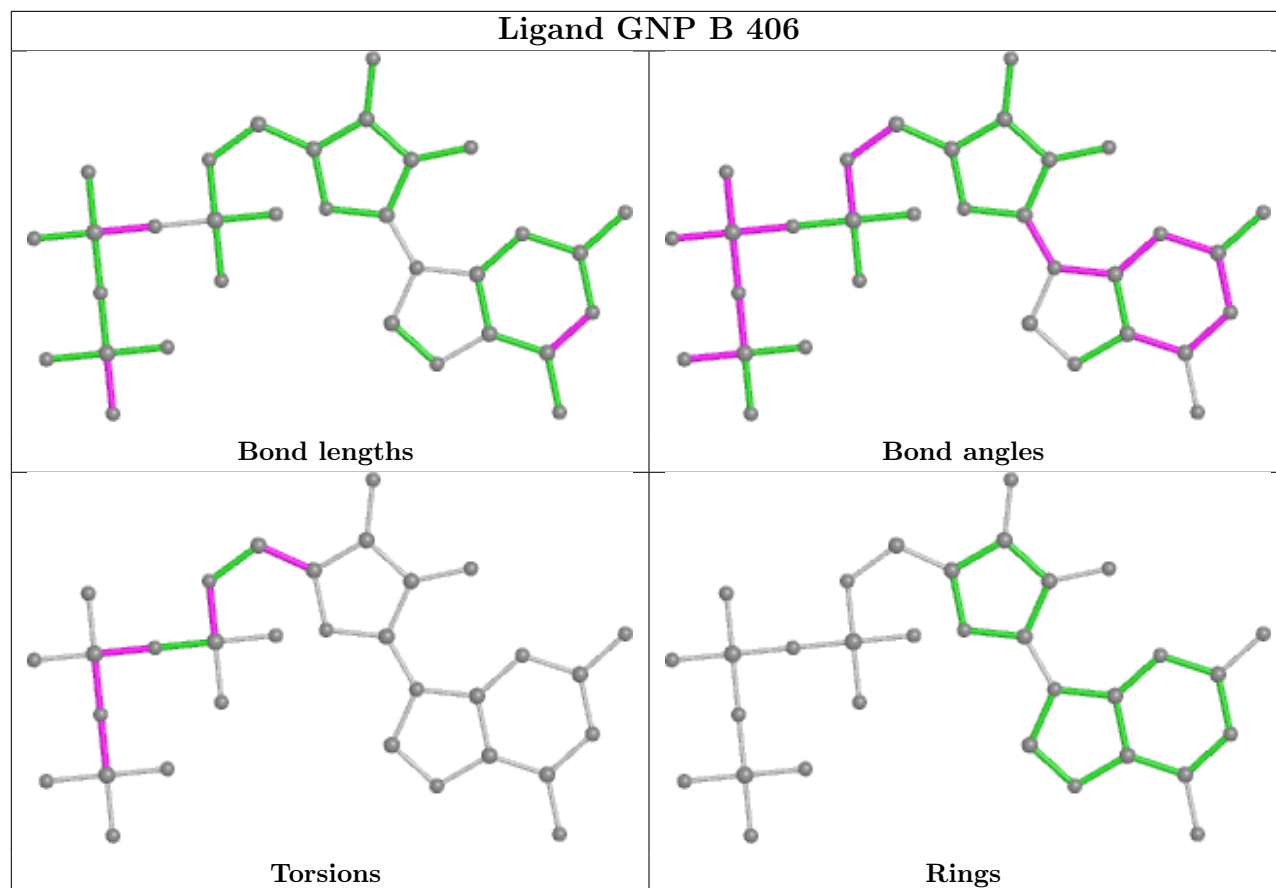
Mol	Chain	Res	Type	Atoms
5	B	406	GNP	C3'-C4'-C5'-O5'
5	B	406	GNP	O4'-C4'-C5'-O5'
5	A	406	GNP	O4'-C4'-C5'-O5'
5	A	406	GNP	C5'-O5'-PA-O2A
5	B	406	GNP	C5'-O5'-PA-O1A
5	B	406	GNP	C5'-O5'-PA-O2A
5	C	406	GNP	C5'-O5'-PA-O2A
5	A	406	GNP	C3'-C4'-C5'-O5'
5	C	406	GNP	C4'-C5'-O5'-PA
5	C	406	GNP	C5'-O5'-PA-O3A

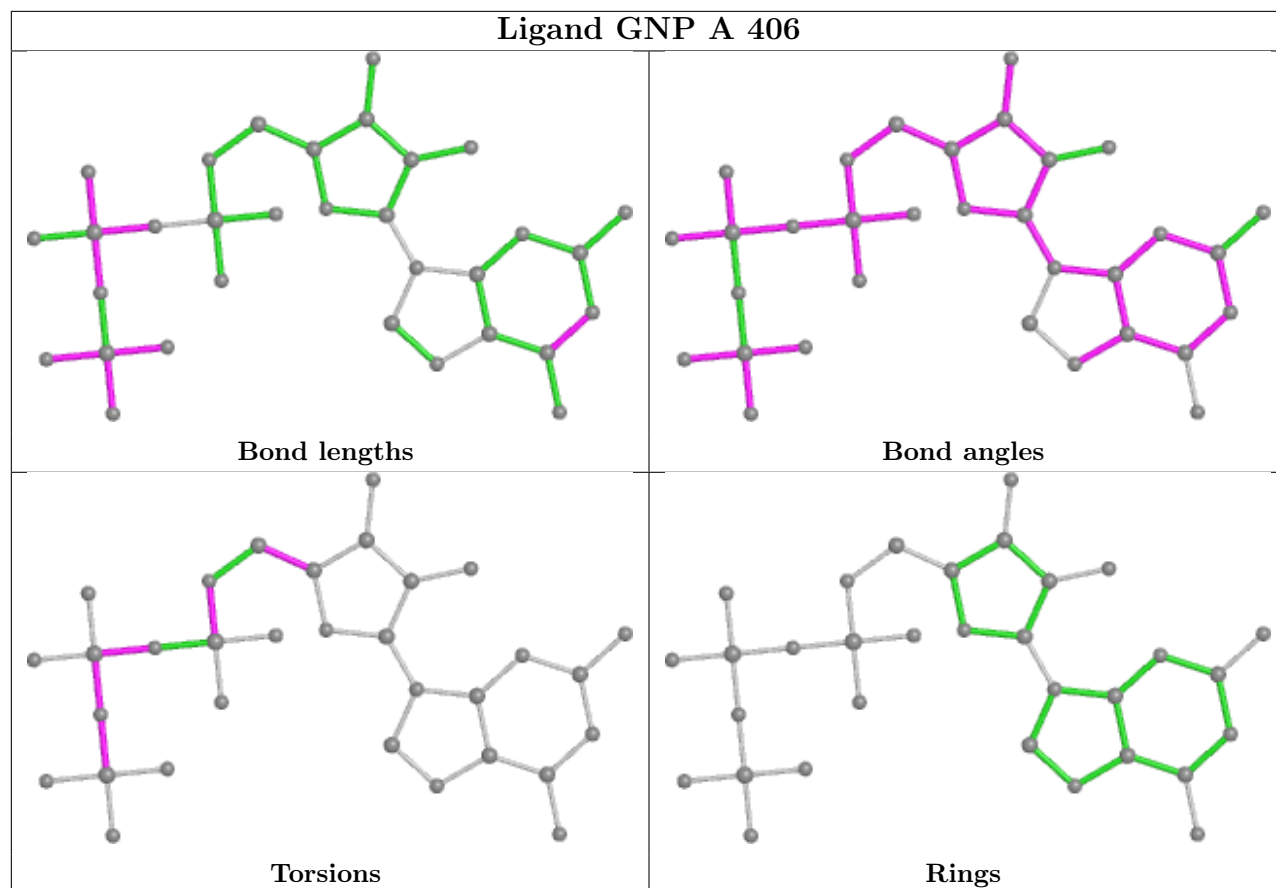
There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	GNP	7	0
5	C	406	GNP	7	0
4	E	77	PHE	1	0
4	F	77	PHE	1	0
4	D	77	PHE	2	0
5	A	406	GNP	6	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.