



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:30 PM UTC

PDB ID : 1TTT / pdb_00001ttt
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

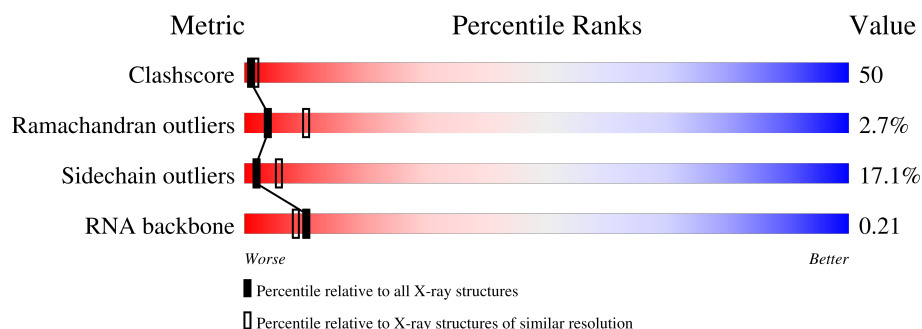
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

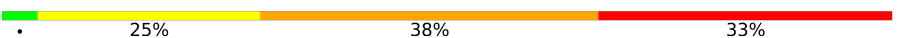
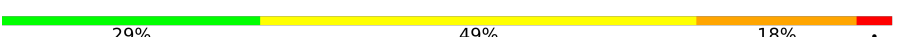
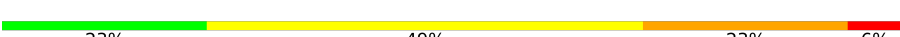
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	76	
1	E	76	
1	F	76	
2	A	405	
2	B	405	
2	C	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

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
1	D	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
1	E	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
1	F	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			

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

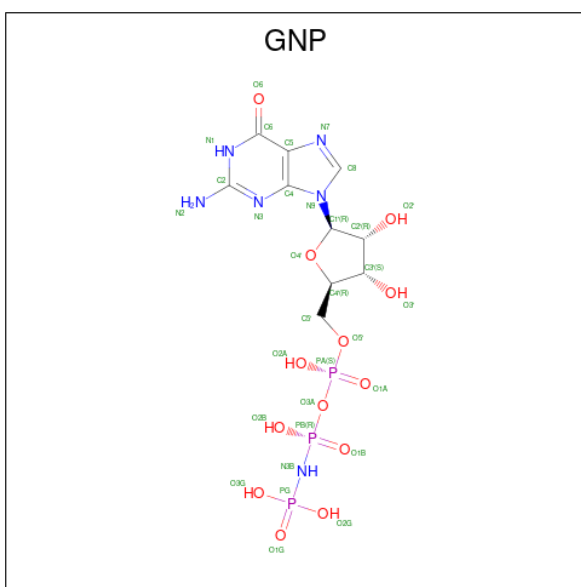
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			
2	B	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			
2	C	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			

- Molecule 3 is MAGNESIUM ION (CCD ID: 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		

-
- Chemical structure of Phenylalanine (PHE) is shown. The structure includes a benzene ring (labeled CE1, CE2, CZ, CD1, CD2, CG) attached to a chiral carbon (CA(S)). The chiral carbon is also bonded to an amino group (N, H2N), a carboxyl group (C, O, OH), and a hydrogen atom (H).

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).



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.

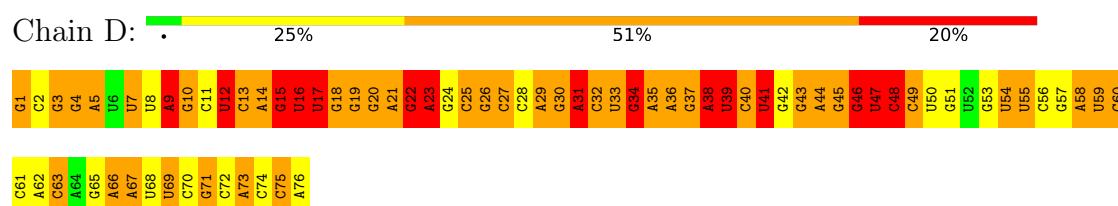
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	6	Total	O	0	0
			6	6		
6	E	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		
6	A	21	Total	O	0	0
			21	21		
6	B	13	Total	O	0	0
			13	13		
6	C	7	Total	O	0	0
			7	7		

3 Residue-property plots

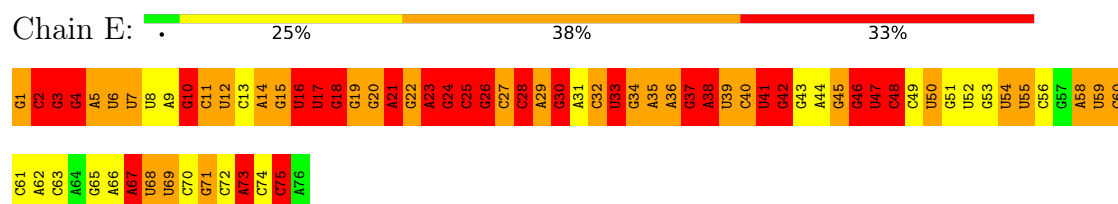
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

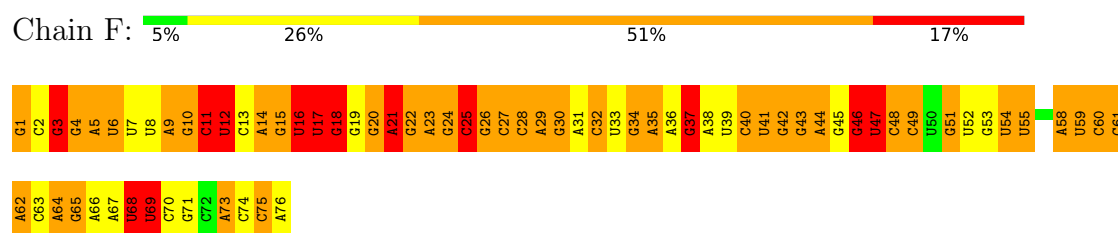
• Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)



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

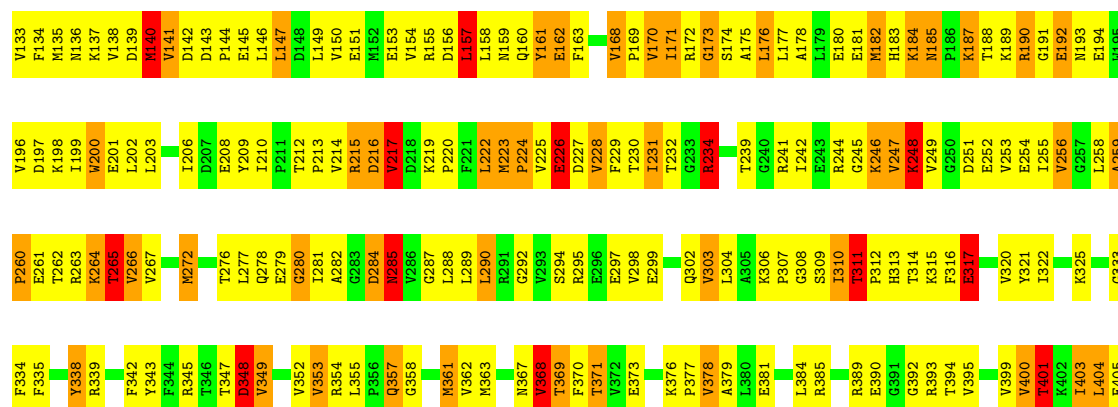


• Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)



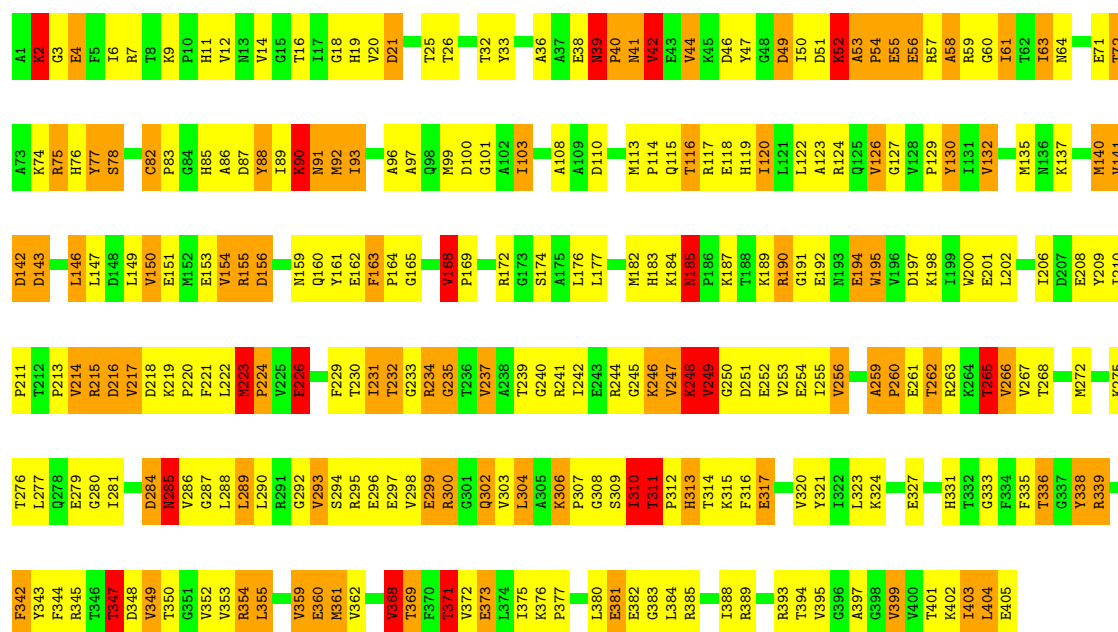
• Molecule 2: OF ELONGATION FACTOR TU (EF-TU)





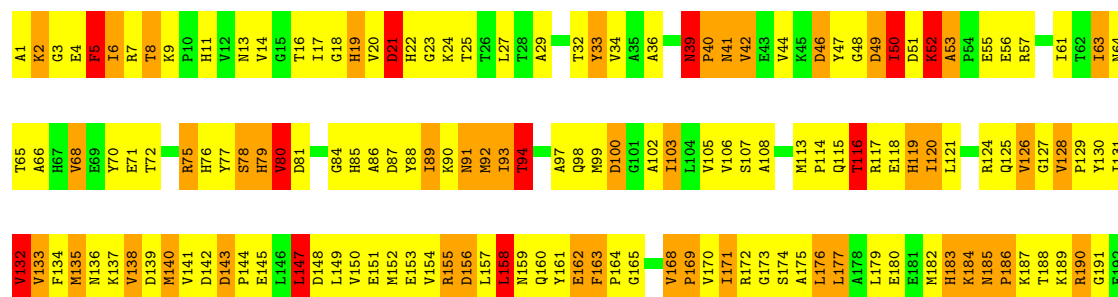
• Molecule 2: OF ELONGATION FACTOR TU (EF-TU)

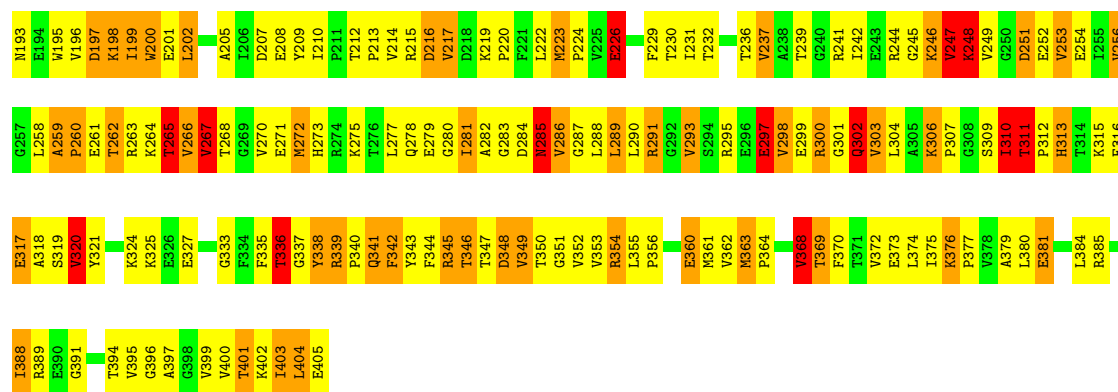
Chain B: 33% 42% 21%



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

Chain C: 23% 49% 23% 6%





4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	14573	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, OMC, M2G, GNP, PSU, 5MC, 2MG, MG, YYG, 7MG, OMG, 5MU, 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	0/1487	1.97	84/2315 (3.6%)
1	E	0.45	0/1487	1.92	82/2315 (3.5%)
1	F	0.47	0/1487	1.94	89/2315 (3.8%)
2	A	1.14	8/3204 (0.2%)	2.00	119/4345 (2.7%)
2	B	1.14	5/3204 (0.2%)	1.95	109/4345 (2.5%)
2	C	1.11	6/3204 (0.2%)	2.02	131/4345 (3.0%)
All	All	0.97	19/14073 (0.1%)	1.97	614/19980 (3.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	2	0
2	A	2	0
All	All	4	0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	VAL	CA-CB	-8.62	1.43	1.54
2	B	61	ILE	CA-CB	-7.06	1.48	1.55
2	C	6	ILE	CA-CB	-6.92	1.45	1.54
2	A	120	ILE	CA-CB	-6.91	1.46	1.54
2	C	388	ILE	CA-CB	-6.84	1.46	1.54
2	C	128	VAL	CA-CB	-6.79	1.45	1.54
2	A	401	THR	CA-CB	-6.54	1.44	1.54
2	C	119	HIS	CA-CB	-5.83	1.44	1.53
2	C	363	MET	SD-CE	5.77	1.94	1.79
2	A	371	THR	CA-C	-5.73	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	ILE	N-CA	-5.58	1.39	1.46
2	C	99	MET	SD-CE	5.58	1.93	1.79
2	B	154	VAL	CA-CB	-5.47	1.47	1.54
2	A	217	VAL	CA-CB	-5.40	1.47	1.54
2	A	63	ILE	CA-CB	5.34	1.62	1.55
2	A	182	MET	SD-CE	5.31	1.92	1.79
2	B	141	VAL	CA-C	-5.22	1.46	1.52
2	A	225	VAL	CA-CB	-5.15	1.48	1.54
2	B	141	VAL	CA-CB	-5.07	1.48	1.54

All (614) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	A	N9-C1'-C2'	-16.07	87.90	112.00
1	D	22	G	O4'-C1'-N9	15.49	131.74	108.50
1	D	22	G	N9-C1'-C2'	-15.08	89.38	112.00
1	F	11	C	C3'-C2'-O2'	14.28	132.11	110.70
2	A	163	PHE	N-CA-C	-14.07	90.28	110.40
1	D	21	A	C3'-C2'-O2'	-13.55	90.38	110.70
2	C	208	GLU	N-CA-C	13.43	125.65	111.14
2	B	208	GLU	N-CA-C	13.34	125.84	111.03
1	D	47	U	N1-C1'-C2'	12.72	131.08	112.00
2	B	55	GLU	N-CA-C	-12.41	97.50	112.89
2	A	39	ASN	C-N-CD	-12.11	75.34	125.00
1	F	11	C	C1'-C2'-O2'	12.04	126.45	108.40
2	B	185	ASN	CA-C-N	11.96	131.54	119.82
2	B	185	ASN	C-N-CA	11.96	131.54	119.82
1	E	21	A	N9-C1'-C2'	-11.60	94.59	112.00
2	A	246	LYS	N-CA-C	11.56	125.72	108.14
1	F	21	A	N9-C1'-C2'	-11.40	94.90	112.00
2	C	75	ARG	N-CA-C	11.22	126.12	109.07
2	C	39	ASN	C-N-CD	-11.19	79.10	125.00
1	E	18	G	O4'-C1'-N9	11.04	124.76	108.20
1	D	33	U	N1-C1'-C2'	-11.02	95.46	112.00
2	C	132	VAL	N-CA-C	-11.00	91.91	108.85
2	B	42	VAL	N-CA-C	-10.97	91.89	107.80
2	A	310	ILE	N-CA-C	10.94	126.53	108.81
2	C	141	VAL	N-CA-C	10.90	123.75	107.51
1	D	33	U	O4'-C1'-N1	10.87	124.81	108.50
1	E	69	U	C1'-C2'-O2'	10.86	124.69	108.40
1	D	19	G	N9-C1'-C2'	-10.84	97.74	114.00
1	F	73	A	C3'-C2'-O2'	10.84	126.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	310	ILE	N-CA-C	10.64	124.32	108.46
1	E	35	A	C3'-C2'-O2'	-10.62	94.77	110.70
2	C	338	TYR	CA-C-N	-10.53	108.55	122.98
2	C	338	TYR	C-N-CA	-10.53	108.55	122.98
1	E	15	G	C4'-C3'-O3'	-10.51	97.24	113.00
2	A	209	TYR	CA-C-N	-10.46	115.49	122.60
2	A	209	TYR	C-N-CA	-10.46	115.49	122.60
2	C	103	ILE	CB-CA-C	-10.44	98.41	111.88
2	A	116	THR	N-CA-C	-10.34	100.01	111.07
1	E	15	G	O4'-C1'-N9	-10.32	93.02	108.50
2	B	39	ASN	C-N-CD	-10.21	83.16	125.00
2	B	311	THR	CB-CA-C	10.19	121.86	110.15
2	C	127	GLY	N-CA-C	10.18	128.35	115.42
2	A	63	ILE	N-CA-CB	10.18	119.98	111.64
2	C	53	ALA	N-CA-C	-10.16	97.27	110.07
1	E	3	G	N9-C1'-C2'	-10.12	96.81	112.00
2	A	132	VAL	N-CA-C	-10.09	93.96	108.48
2	A	212	THR	N-CA-C	-10.08	97.12	109.72
1	E	47	U	N1-C1'-C2'	10.04	129.06	114.00
2	C	246	LYS	N-CA-C	10.01	121.99	107.88
2	A	311	THR	CB-CA-C	9.77	121.38	110.15
2	C	142	ASP	N-CA-C	9.72	121.64	111.14
1	D	23	A	N9-C1'-C2'	9.71	126.57	112.00
1	D	7	U	N1-C1'-C2'	-9.68	99.48	114.00
2	B	143	ASP	N-CA-C	-9.64	96.03	109.71
2	B	162	GLU	N-CA-C	9.53	124.85	113.23
1	D	71	G	O4'-C1'-N9	-9.51	94.24	108.50
2	B	235	GLY	N-CA-C	9.50	122.54	110.38
2	B	163	PHE	N-CA-C	-9.46	98.01	110.40
2	A	2	LYS	N-CA-C	9.44	122.54	110.65
1	F	20	G	O3'-P-O5'	-9.42	89.87	104.00
2	A	42	VAL	N-CA-C	-9.42	93.43	107.37
1	F	47	U	N1-C1'-C2'	9.34	126.00	112.00
1	E	69	U	C3'-C2'-O2'	9.29	124.63	110.70
2	B	295	ARG	N-CA-C	-9.27	101.18	111.28
2	A	185	ASN	CA-C-N	9.26	131.41	119.84
2	A	185	ASN	C-N-CA	9.26	131.41	119.84
2	B	183	HIS	N-CA-C	-9.22	101.18	111.14
1	F	13	C	O4'-C1'-N1	9.20	122.29	108.50
1	D	38	A	N9-C1'-C2'	-9.19	98.21	112.00
2	A	208	GLU	N-CA-C	9.16	121.20	111.03
1	F	69	U	C3'-C2'-O2'	9.15	124.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	C	N1-C1'-C2'	9.12	125.67	112.00
1	F	11	C	C2'-C3'-O3'	9.10	127.35	113.70
1	D	22	G	C4'-C3'-O3'	9.06	126.60	113.00
1	E	36	A	N9-C1'-C2'	-9.06	98.40	112.00
2	A	100	ASP	N-CA-C	-9.04	101.96	113.72
2	C	266	VAL	CB-CA-C	-9.00	97.43	110.83
1	D	48	C	C3'-C2'-O2'	-8.93	101.20	114.60
1	E	75	C	C3'-C2'-O2'	-8.86	101.32	114.60
2	A	338	TYR	CA-C-N	-8.84	110.57	123.30
2	A	338	TYR	C-N-CA	-8.84	110.57	123.30
1	F	18	G	O4'-C1'-N9	8.82	121.43	108.20
2	C	310	ILE	N-CA-C	8.81	123.08	108.81
1	F	18	G	N9-C1'-C2'	-8.78	100.83	114.00
1	D	45	G	O4'-C1'-N9	-8.77	95.34	108.50
2	C	116	THR	N-CA-C	-8.75	101.43	110.97
2	B	77	TYR	N-CA-C	8.74	123.14	109.07
2	C	33	TYR	N-CA-C	8.73	120.42	111.07
2	C	6	ILE	N-CA-C	8.69	120.41	107.80
2	B	100	ASP	N-CA-C	-8.69	102.70	113.38
2	A	352	VAL	CB-CA-C	-8.65	100.49	110.96
2	A	214	VAL	N-CA-C	-8.59	95.55	109.12
2	B	285	ASN	N-CA-C	-8.59	93.52	108.20
1	F	62	A	C1'-C2'-O2'	-8.58	95.52	108.40
1	E	13	C	N1-C1'-C2'	8.56	124.85	112.00
1	F	51	G	N9-C1'-C2'	8.56	124.84	112.00
1	E	69	U	C2'-C3'-O3'	8.54	126.52	113.70
1	E	70	C	C3'-C2'-O2'	8.53	123.50	110.70
1	F	73	A	N9-C1'-C2'	-8.53	99.21	112.00
2	C	256	VAL	N-CA-C	8.49	122.14	108.97
1	D	3	G	O3'-P-O5'	8.46	116.69	104.00
1	F	24	G	N9-C1'-C2'	-8.42	99.36	112.00
2	B	92	MET	N-CA-C	-8.42	102.06	111.07
2	C	281	ILE	CB-CA-C	-8.41	98.38	110.82
2	B	395	VAL	CA-C-N	-8.36	111.33	122.03
2	B	395	VAL	C-N-CA	-8.36	111.33	122.03
2	A	367	ASN	N-CA-C	-8.28	93.28	108.02
1	E	19	G	C3'-C2'-O2'	-8.25	102.22	114.60
2	A	51	ASP	N-CA-C	-8.19	94.14	108.23
2	C	52	LYS	N-CA-C	8.18	128.23	110.80
1	F	3	G	N9-C1'-C2'	-8.17	99.75	112.00
1	F	1	G	O4'-C1'-N9	-8.13	96.30	108.50
1	F	51	G	O4'-C1'-N9	-8.12	96.32	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	A	C4'-C3'-O3'	8.12	125.17	113.00
1	D	28	C	O4'-C1'-N1	8.11	120.66	108.50
2	B	247	VAL	N-CA-C	8.08	119.97	108.42
1	D	4	G	C4'-C3'-O3'	-8.07	100.89	113.00
1	D	48	C	O4'-C1'-N1	8.07	120.31	108.20
2	A	317	GLU	N-CA-C	-7.99	98.70	110.52
1	D	25	C	C1'-C2'-O2'	7.97	120.36	108.40
2	A	63	ILE	N-CA-C	-7.93	105.35	111.62
1	D	3	G	N9-C1'-C2'	-7.91	100.14	112.00
1	F	53	G	C3'-C2'-O2'	7.91	122.56	110.70
2	C	105	VAL	CB-CA-C	-7.89	102.71	111.23
1	E	22	G	C1'-C2'-O2'	-7.87	96.59	108.40
2	B	52	LYS	N-CA-C	7.86	122.55	113.19
2	A	53	ALA	N-CA-C	-7.86	99.23	110.08
1	E	71	G	O4'-C1'-N9	-7.86	96.72	108.50
1	E	42	G	C3'-C2'-O2'	7.85	122.48	110.70
2	B	116	THR	N-CA-C	-7.85	102.67	111.07
1	F	42	G	C4'-C3'-O3'	-7.82	101.27	113.00
2	A	74	LYS	N-CA-C	7.81	120.48	111.11
1	D	18	G	N9-C1'-C2'	-7.80	102.30	114.00
2	C	295	ARG	N-CA-C	-7.78	102.75	111.07
2	A	162	GLU	N-CA-C	7.77	122.40	111.52
1	E	61	C	C3'-C2'-O2'	-7.75	99.07	110.70
2	B	349	VAL	CB-CA-C	-7.74	97.32	110.71
2	A	256	VAL	N-CA-C	7.73	120.23	108.71
1	F	71	G	O4'-C1'-N9	-7.72	96.92	108.50
2	B	78	SER	N-CA-C	-7.72	96.65	109.07
2	A	338	TYR	CB-CA-C	-7.70	99.08	110.16
1	D	71	G	C3'-C2'-O2'	7.67	122.20	110.70
2	C	199	ILE	CB-CA-C	-7.66	102.00	112.04
1	D	18	G	O4'-C1'-N9	7.65	119.68	108.20
2	A	34	VAL	N-CA-C	7.63	119.32	110.62
2	C	162	GLU	N-CA-C	7.63	124.61	113.40
1	E	25	C	O4'-C1'-N1	7.62	119.93	108.50
1	F	11	C	N1-C1'-C2'	7.61	123.42	112.00
2	C	339	ARG	CA-C-N	7.60	129.34	119.84
2	C	339	ARG	C-N-CA	7.60	129.34	119.84
1	D	19	G	C3'-C2'-O2'	-7.60	103.20	114.60
1	F	47	U	C4'-C3'-O3'	-7.59	101.62	113.00
2	C	92	MET	N-CA-C	-7.57	102.97	111.07
2	B	226	GLU	N-CA-C	-7.57	104.66	114.04
2	B	51	ASP	N-CA-C	-7.53	100.97	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	11	C	O3'-P-O5'	-7.52	92.72	104.00
1	F	9	A	C3'-C2'-O2'	7.52	125.88	114.60
1	F	21	A	P-O5'-C5'	-7.50	109.66	120.90
1	E	74	C	C4'-C3'-O3'	-7.50	101.76	113.00
1	D	29	A	O3'-P-O5'	-7.49	92.77	104.00
2	A	16	THR	N-CA-C	7.47	121.11	109.07
2	C	2	LYS	N-CA-C	-7.47	94.88	110.80
2	A	185	ASN	O-C-N	7.45	129.88	121.32
1	F	31	A	P-O5'-C5'	-7.42	109.77	120.90
2	C	185	ASN	CA-C-N	7.39	129.08	119.84
2	C	185	ASN	C-N-CA	7.39	129.08	119.84
1	D	1	G	C4'-C3'-O3'	-7.38	101.93	113.00
2	B	150	VAL	CB-CA-C	-7.37	102.38	112.04
2	C	283	GLY	CA-C-N	-7.36	110.90	121.42
2	C	283	GLY	C-N-CA	-7.36	110.90	121.42
1	F	11	C	O4'-C1'-N1	7.33	119.50	108.50
2	A	200	TRP	N-CA-C	-7.32	103.38	111.36
2	A	325	LYS	N-CA-C	-7.32	103.31	111.28
2	C	49	ASP	N-CA-C	-7.30	101.82	111.24
2	C	337	GLY	N-CA-C	-7.29	104.43	114.64
1	D	69	U	O3'-P-O5'	-7.28	93.08	104.00
2	A	39	ASN	CA-C-N	7.26	128.91	119.84
2	A	39	ASN	C-N-CA	7.26	128.91	119.84
1	F	48	C	C1'-C2'-O2'	-7.24	100.94	111.80
2	B	286	VAL	CB-CA-C	-7.24	99.41	111.29
1	E	66	A	C3'-C2'-O2'	-7.24	99.84	110.70
2	A	265	THR	CB-CA-C	-7.22	97.02	111.17
2	C	94	THR	N-CA-CB	7.21	120.46	110.01
1	E	24	G	N9-C1'-C2'	7.21	122.81	112.00
1	F	12	U	N1-C1'-C2'	7.21	122.81	112.00
2	C	200	TRP	N-CA-C	-7.20	103.43	111.28
1	D	31	A	N9-C1'-C2'	-7.19	101.22	112.00
1	E	38	A	N9-C1'-C2'	-7.19	101.22	112.00
1	D	69	U	C2'-C3'-O3'	7.18	124.48	113.70
2	C	247	VAL	N-CA-C	7.18	118.69	108.42
2	C	158	LEU	N-CA-C	-7.18	102.49	111.11
1	D	75	C	C2'-C3'-O3'	-7.18	98.73	109.50
1	D	63	C	C4'-C3'-O3'	-7.16	102.25	113.00
1	E	60	C	N1-C1'-C2'	-7.16	103.26	114.00
2	C	120	ILE	N-CA-C	-7.15	103.70	110.42
1	F	11	C	C4'-C3'-O3'	7.15	123.72	113.00
1	E	73	A	C3'-C2'-O2'	7.14	121.41	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	34	VAL	CB-CA-C	-7.10	102.73	112.04
1	F	68	U	O4'-C1'-N1	7.10	119.15	108.50
2	A	224	PRO	CB-CA-C	-7.10	104.94	111.40
2	B	237	VAL	N-CA-C	7.09	118.51	108.36
1	D	30	G	N9-C1'-C2'	-7.09	101.36	112.00
1	D	15	G	N9-C1'-C2'	7.08	122.63	112.00
1	D	73	A	C4'-C3'-O3'	-7.08	102.38	113.00
1	D	21	A	P-O5'-C5'	-7.08	110.28	120.90
1	F	3	G	O3'-P-O5'	7.07	114.60	104.00
1	E	7	U	O4'-C1'-N1	7.05	118.78	108.20
1	F	15	G	C3'-C2'-O2'	-7.04	100.13	110.70
1	D	13	C	C4'-C3'-O3'	-7.04	102.44	113.00
1	E	3	G	O3'-P-O5'	7.04	114.56	104.00
2	C	5	PHE	N-CA-C	7.04	125.79	110.80
1	F	76	A	C1'-C2'-O2'	-7.02	101.27	111.80
2	C	143	ASP	N-CA-C	7.01	121.84	109.58
2	C	320	VAL	N-CA-C	6.98	119.50	108.89
2	C	42	VAL	N-CA-C	-6.98	97.11	107.51
2	B	75	ARG	N-CA-C	6.97	119.34	108.96
1	E	48	C	O5'-P-OP2	-6.96	87.11	108.00
2	B	39	ASN	CA-C-N	6.96	128.54	119.84
2	B	39	ASN	C-N-CA	6.96	128.54	119.84
2	C	184	LYS	N-CA-C	-6.96	103.63	111.07
1	E	23	A	O4'-C1'-N9	6.94	118.91	108.50
1	D	69	U	C3'-C2'-O2'	6.91	121.07	110.70
2	C	80	VAL	N-CA-CB	6.90	120.15	111.46
1	F	5	A	O4'-C1'-N9	6.89	118.84	108.50
1	F	33	U	C4'-C3'-O3'	-6.86	102.70	113.00
1	D	73	A	N9-C1'-C2'	-6.86	101.71	112.00
1	E	69	U	O3'-P-O5'	-6.86	93.71	104.00
1	E	52	U	C3'-C2'-O2'	6.86	120.98	110.70
1	D	70	C	C3'-C2'-O2'	6.85	120.97	110.70
2	B	403	ILE	N-CA-C	6.82	117.67	107.51
2	A	56	GLU	N-CA-C	-6.82	103.77	111.07
1	D	25	C	N1-C1'-C2'	-6.81	101.78	112.00
2	A	184	LYS	N-CA-C	-6.81	102.93	111.11
1	E	18	G	N9-C1'-C2'	-6.80	103.80	114.00
2	B	103	ILE	N-CA-CB	-6.80	102.89	111.46
1	E	29	A	O3'-P-O5'	-6.79	93.81	104.00
2	C	39	ASN	CA-C-N	6.79	128.33	119.84
2	C	39	ASN	C-N-CA	6.79	128.33	119.84
1	E	42	G	O5'-C5'-C4'	-6.76	101.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	349	VAL	CB-CA-C	-6.76	98.61	110.71
2	C	339	ARG	O-C-N	6.75	127.47	121.32
2	B	317	GLU	N-CA-C	-6.74	99.61	110.32
1	F	44	A	N9-C1'-C2'	6.72	122.08	112.00
1	F	42	G	O4'-C1'-N9	-6.71	98.43	108.50
2	A	77	TYR	N-CA-C	6.71	120.44	109.24
1	E	5	A	C1'-C2'-O2'	6.71	118.46	108.40
2	C	226	GLU	N-CA-C	-6.70	105.39	113.97
2	B	289	LEU	N-CA-C	-6.67	98.83	109.76
2	C	147	LEU	CB-CA-C	-6.66	99.73	110.79
2	A	173	GLY	N-CA-C	6.66	120.19	110.80
1	D	32	OMC	OP1-P-O3'	-6.65	88.04	108.00
2	B	132	VAL	N-CA-C	-6.65	98.91	108.48
2	C	368	VAL	CB-CA-C	-6.64	100.40	111.29
1	E	32	OMC	OP1-P-O3'	-6.63	88.11	108.00
1	D	51	G	N9-C1'-C2'	6.62	121.92	112.00
1	E	30	G	C2'-C3'-O3'	6.61	123.62	113.70
1	F	70	C	O4'-C1'-N1	6.61	118.41	108.50
1	D	47	U	O4'-C1'-N1	6.60	118.40	108.50
2	C	259	ALA	O-C-N	6.60	127.71	121.71
1	D	42	G	O4'-C1'-N9	-6.59	98.62	108.50
1	E	41	U	O4'-C1'-N1	-6.58	98.63	108.50
2	B	184	LYS	CD-CE-NZ	6.56	132.90	111.90
2	A	272	MET	N-CA-C	-6.55	97.12	107.93
2	C	175	ALA	N-CA-C	-6.54	104.33	112.90
1	E	21	A	C3'-C2'-O2'	-6.53	100.90	110.70
1	E	15	G	C1'-C2'-O2'	-6.52	98.62	108.40
2	A	192	GLU	CA-C-N	-6.52	112.17	122.73
2	A	192	GLU	C-N-CA	-6.52	112.17	122.73
2	C	265	THR	CB-CA-C	-6.50	98.42	111.17
2	B	293	VAL	N-CA-C	-6.50	99.36	108.27
1	E	6	U	O4'-C1'-N1	6.49	118.23	108.50
1	D	12	U	C1'-C2'-O2'	6.49	118.13	108.40
1	E	59	U	C4'-C3'-O3'	-6.47	103.29	113.00
1	F	25	C	N1-C1'-C2'	-6.47	102.30	112.00
2	B	382	GLU	N-CA-C	-6.46	101.56	110.35
2	A	259	ALA	CA-C-N	6.45	127.91	119.84
2	A	259	ALA	C-N-CA	6.45	127.91	119.84
2	C	345	ARG	CB-CA-C	-6.44	109.13	116.54
1	D	41	U	O4'-C1'-N1	-6.44	98.84	108.50
2	B	56	GLU	N-CA-C	-6.44	97.09	110.80
1	D	43	G	C3'-C2'-O2'	6.44	120.35	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	G	C4'-C3'-O3'	-6.43	103.35	113.00
2	C	311	THR	N-CA-C	6.43	119.90	109.15
2	A	72	THR	N-CA-C	-6.43	100.05	109.18
2	B	259	ALA	O-C-N	6.42	126.84	121.83
1	F	12	U	O3'-P-O5'	6.42	113.62	104.00
1	E	48	C	O4'-C1'-N1	6.41	117.82	108.20
1	E	28	C	C2'-C3'-O3'	6.41	123.31	113.70
1	F	27	C	C4'-C3'-O3'	-6.39	103.41	113.00
1	F	69	U	O4'-C1'-N1	6.39	118.09	108.50
2	A	175	ALA	N-CA-C	-6.39	104.53	112.90
2	B	284	ASP	CA-C-N	-6.39	114.54	122.84
2	B	284	ASP	C-N-CA	-6.39	114.54	122.84
1	D	9	A	C3'-C2'-O2'	-6.38	105.02	114.60
2	C	65	THR	N-CA-C	-6.38	102.11	110.53
2	B	74	LYS	N-CA-C	6.38	118.31	111.36
2	A	53	ALA	CA-C-N	6.38	125.87	119.24
2	A	53	ALA	C-N-CA	6.38	125.87	119.24
2	A	170	VAL	N-CA-C	6.37	116.04	106.42
1	D	63	C	C2'-C3'-O3'	-6.37	104.14	113.70
2	B	185	ASN	CA-C-O	6.37	128.88	120.16
1	E	59	U	O4'-C1'-N1	6.36	118.05	108.50
1	E	47	U	C2'-C3'-O3'	6.35	119.03	109.50
1	D	30	G	C3'-C2'-O2'	6.35	120.22	110.70
1	F	68	U	C1'-C2'-O2'	6.34	117.92	108.40
2	A	285	ASN	N-CA-C	-6.34	95.96	107.75
2	A	226	GLU	N-CA-C	-6.33	106.20	114.04
1	F	12	U	C4'-C3'-O3'	6.31	122.47	113.00
2	A	162	GLU	CB-CA-C	-6.30	103.41	111.86
1	E	4	G	C4'-C3'-O3'	-6.29	103.56	113.00
2	A	209	TYR	N-CA-C	6.29	118.13	111.28
2	C	346	THR	CB-CA-C	-6.27	98.75	110.36
2	C	253	VAL	CB-CA-C	-6.26	102.62	111.19
2	C	402	LYS	CA-C-N	-6.24	115.45	123.19
2	C	402	LYS	C-N-CA	-6.24	115.45	123.19
1	E	30	G	O4'-C1'-N9	6.22	117.83	108.50
2	A	311	THR	N-CA-C	6.22	119.54	109.15
2	B	338	TYR	CA-C-N	-6.22	114.77	122.42
2	B	338	TYR	C-N-CA	-6.22	114.77	122.42
2	B	300	ARG	CA-C-N	-6.21	116.12	123.08
2	B	300	ARG	C-N-CA	-6.21	116.12	123.08
2	C	285	ASN	N-CA-C	-6.20	96.32	107.98
2	C	163	PHE	N-CA-C	-6.20	101.02	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	61	C	C3'-C2'-O2'	-6.18	101.42	110.70
1	D	69	U	C1'-C2'-O2'	6.17	117.66	108.40
1	D	33	U	C2'-C3'-O3'	-6.16	104.46	113.70
2	A	348	ASP	CB-CA-C	6.15	119.62	110.14
2	C	283	GLY	N-CA-C	-6.15	106.54	114.85
1	F	20	G	O5'-C5'-C4'	-6.14	102.29	111.50
1	F	48	C	O4'-C1'-N1	6.14	117.41	108.20
2	B	265	THR	CB-CA-C	-6.13	99.21	110.62
1	D	63	C	OP1-P-O3'	-6.13	89.60	108.00
2	B	246	LYS	N-CA-C	6.12	116.65	108.38
1	F	65	G	O4'-C1'-N9	-6.12	99.31	108.50
2	A	368	VAL	CB-CA-C	-6.12	101.26	111.29
1	E	43	G	N9-C1'-C2'	6.11	121.17	112.00
2	A	6	ILE	N-CA-C	6.10	117.49	107.24
2	A	266	VAL	CB-CA-C	-6.09	101.76	110.83
2	C	251	ASP	N-CA-C	-6.08	102.50	110.53
2	C	169	PRO	CA-N-CD	-6.08	103.49	112.00
2	B	218	ASP	N-CA-C	6.06	119.15	111.69
1	D	38	A	C4'-C3'-O3'	-6.05	103.92	113.00
1	F	9	A	O4'-C1'-N9	6.05	117.27	108.20
2	C	183	HIS	N-CA-C	-6.04	104.25	111.69
1	D	25	C	C3'-C2'-O2'	6.04	119.76	110.70
1	F	15	G	C4'-C3'-O3'	-6.04	103.94	113.00
1	D	23	A	C3'-C2'-O2'	-6.04	101.65	110.70
2	A	140	MET	CA-C-N	-6.03	114.02	122.71
2	A	140	MET	C-N-CA	-6.03	114.02	122.71
2	C	293	VAL	N-CA-C	-6.03	99.43	108.12
2	C	360	GLU	N-CA-C	6.03	120.77	113.41
2	A	82	CYS	CA-C-N	6.03	126.50	119.99
2	A	82	CYS	C-N-CA	6.03	126.50	119.99
2	B	248	LYS	N-CA-C	-6.03	99.89	109.23
2	C	344	PHE	N-CA-C	-6.01	98.48	108.34
1	E	50	U	C3'-C2'-O2'	-5.98	101.73	110.70
2	B	256	VAL	N-CA-C	5.97	118.46	109.20
2	C	147	LEU	N-CA-C	-5.97	104.78	111.28
1	F	69	U	C2'-C3'-O3'	5.96	122.65	113.70
2	C	397	ALA	N-CA-C	-5.95	98.12	110.80
2	A	353	VAL	CB-CA-C	-5.95	102.89	111.34
2	A	292	GLY	N-CA-C	5.95	124.46	113.76
1	F	30	G	C3'-C2'-O2'	5.94	119.61	110.70
2	A	378	VAL	N-CA-C	5.94	116.08	107.88
2	C	325	LYS	N-CA-C	-5.93	103.99	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	ILE	CB-CA-C	-5.93	104.38	111.97
2	B	249	VAL	N-CA-C	-5.92	101.04	109.51
2	C	78	SER	N-CA-C	-5.91	98.88	108.52
1	F	28	C	O4'-C1'-N1	5.90	117.36	108.50
2	A	26	THR	N-CA-C	-5.90	104.54	110.97
2	A	247	VAL	CB-CA-C	-5.90	99.86	110.48
2	A	163	PHE	CA-C-N	5.90	127.21	119.84
2	A	163	PHE	C-N-CA	5.90	127.21	119.84
2	A	232	THR	N-CA-C	5.90	123.36	110.80
2	C	168	VAL	N-CA-C	5.90	115.44	108.96
1	D	31	A	C2'-C3'-O3'	-5.89	104.87	113.70
2	A	120	ILE	CB-CA-C	-5.88	104.44	111.97
1	D	35	A	C3'-C2'-O2'	-5.88	101.88	110.70
2	C	185	ASN	N-CA-C	5.88	122.80	109.81
1	D	60	C	C3'-C2'-O2'	-5.87	105.80	114.60
2	B	2	LYS	N-CA-C	-5.87	98.30	110.80
2	C	79	HIS	CA-C-N	-5.87	115.50	123.12
2	C	79	HIS	C-N-CA	-5.87	115.50	123.12
2	C	300	ARG	CA-C-N	-5.86	116.47	123.44
2	C	300	ARG	C-N-CA	-5.86	116.47	123.44
2	B	250	GLY	N-CA-C	-5.86	106.63	114.25
2	C	133	VAL	CB-CA-C	-5.86	101.80	110.82
1	D	59	U	O4'-C1'-N1	5.86	117.28	108.50
2	B	276	THR	N-CA-C	5.85	118.72	110.23
2	C	105	VAL	N-CA-C	5.85	116.82	107.98
1	D	1	G	O3'-P-O5'	-5.85	95.23	104.00
1	D	71	G	C2'-C3'-O3'	5.85	122.47	113.70
1	E	2	C	OP2-P-O3'	5.85	125.54	108.00
2	C	202	LEU	N-CA-C	-5.84	104.61	110.97
1	E	47	U	C4'-C3'-O3'	-5.83	100.66	109.40
1	F	31	A	C1'-C2'-O2'	5.81	117.12	108.40
2	B	266	VAL	N-CA-C	-5.81	100.04	108.17
2	A	369	THR	CB-CA-C	-5.80	98.87	110.42
1	E	34	OMG	O3'-P-O5'	-5.80	95.30	104.00
2	C	313	HIS	N-CA-C	5.80	117.60	108.96
2	C	311	THR	CB-CA-C	5.80	116.82	110.15
1	E	15	G	C3'-C2'-O2'	-5.77	102.04	110.70
1	E	21	A	C4'-C3'-O3'	5.77	121.65	113.00
2	A	392	GLY	CA-C-N	-5.76	112.42	121.87
2	A	392	GLY	C-N-CA	-5.76	112.42	121.87
1	E	66	A	O4'-C1'-N9	-5.76	99.86	108.50
1	D	50	U	C3'-C2'-O2'	-5.75	102.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	THR	N-CA-C	-5.75	101.41	109.69
1	E	46	7MG	O3'-P-O5'	5.75	112.62	104.00
1	F	66	A	O4'-C1'-N9	-5.75	99.88	108.50
2	A	295	ARG	N-CA-C	-5.75	105.15	111.82
2	A	325	LYS	CA-C-N	5.75	127.98	120.28
2	A	325	LYS	C-N-CA	5.75	127.98	120.28
2	B	142	ASP	O-C-N	5.75	128.62	121.84
2	B	344	PHE	N-CA-C	-5.73	99.55	108.90
2	B	336	THR	N-CA-C	-5.73	102.56	110.35
2	B	259	ALA	CA-C-N	5.73	127.00	119.84
2	B	259	ALA	C-N-CA	5.73	127.00	119.84
2	C	99	MET	N-CA-C	5.73	119.15	109.76
1	D	61	C	O4'-C1'-N1	5.72	117.08	108.50
1	E	75	C	N1-C1'-C2'	-5.72	105.42	114.00
2	C	155	ARG	N-CA-C	5.72	118.29	111.71
2	B	39	ASN	O-C-N	5.71	126.18	121.44
2	C	174	SER	N-CA-C	-5.71	99.88	109.07
2	C	197	ASP	N-CA-C	5.71	119.05	111.75
2	A	171	ILE	CB-CA-C	-5.70	103.74	111.15
2	A	234	ARG	N-CA-C	5.70	118.59	111.24
2	A	126	VAL	CB-CA-C	5.69	120.92	111.37
2	A	157	LEU	N-CA-C	-5.69	105.08	111.28
2	B	393	ARG	N-CA-C	5.68	117.71	109.07
1	F	21	A	C3'-C2'-O2'	-5.68	102.18	110.70
2	C	376	LYS	N-CA-C	-5.68	100.78	108.11
1	E	14	A	C1'-C2'-O2'	5.67	116.91	108.40
1	F	12	U	C3'-C2'-O2'	-5.67	102.19	110.70
2	C	237	VAL	N-CA-C	5.66	116.10	108.17
1	D	20	G	O5'-C5'-C4'	-5.66	103.01	111.50
2	C	289	LEU	N-CA-C	-5.66	100.46	109.96
2	A	39	ASN	O-C-N	5.65	125.18	121.23
2	B	195	TRP	N-CA-CB	-5.64	101.53	109.94
1	F	30	G	O3'-P-O5'	-5.63	95.56	104.00
2	A	231	ILE	N-CA-C	5.63	117.09	108.71
2	A	264	LYS	N-CA-C	5.62	119.22	110.17
2	A	176	LEU	N-CA-C	-5.62	104.84	110.97
2	C	325	LYS	O-C-N	5.62	127.93	122.09
1	E	29	A	C4'-C3'-O3'	-5.61	104.58	113.00
2	A	59	ARG	NH1-CZ-NH2	5.61	126.59	119.30
2	A	228	VAL	N-CA-C	5.60	116.81	108.46
2	A	284	ASP	CA-C-N	-5.60	115.07	122.85
2	A	284	ASP	C-N-CA	-5.60	115.07	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	A	C1'-C2'-O2'	5.60	116.80	108.40
2	C	341	GLN	N-CA-C	5.59	118.93	109.76
2	B	397	ALA	N-CA-C	-5.59	98.80	108.69
1	E	74	C	C3'-C2'-O2'	5.58	119.08	110.70
2	C	207	ASP	N-CA-C	-5.57	105.11	111.07
2	C	297	GLU	N-CA-C	5.57	120.18	113.17
2	C	185	ASN	O-C-N	5.55	127.71	121.32
2	C	310	ILE	CB-CA-C	-5.54	100.79	110.71
2	C	306	LYS	N-CA-C	-5.51	101.39	109.50
2	C	152	MET	N-CA-C	-5.51	105.18	111.07
1	E	24	G	O4'-C1'-N9	-5.50	100.25	108.50
1	E	1	G	C2'-C3'-O3'	5.49	121.94	113.70
2	C	298	VAL	CB-CA-C	-5.49	101.21	110.71
2	A	395	VAL	CA-C-O	5.46	123.71	118.90
2	B	373	GLU	N-CA-C	-5.46	98.29	108.02
2	C	5	PHE	CA-C-N	-5.46	116.02	123.12
2	C	5	PHE	C-N-CA	-5.46	116.02	123.12
1	F	73	A	O4'-C1'-N9	-5.46	100.31	108.50
2	A	310	ILE	CB-CA-C	-5.46	100.94	110.71
2	B	49	ASP	N-CA-C	-5.45	106.22	112.92
1	E	67	A	OP2-P-O3'	5.44	124.32	108.00
1	F	73	A	O3'-P-O5'	-5.44	95.85	104.00
2	C	278	GLN	CA-C-O	5.42	126.48	120.90
1	F	64	A	P-O5'-C5'	-5.41	112.78	120.90
1	E	68	U	N1-C1'-C2'	-5.41	103.89	112.00
2	A	259	ALA	O-C-N	5.41	127.54	121.32
1	F	22	G	C1'-C2'-O2'	-5.40	100.30	108.40
1	D	37	YYG	OP1-P-O3'	5.40	124.20	108.00
2	C	100	ASP	N-CA-C	-5.39	105.83	112.90
1	E	33	U	C3'-C2'-O2'	5.39	118.78	110.70
2	C	177	LEU	N-CA-C	5.39	116.83	111.07
1	E	20	G	O4'-C1'-N9	-5.38	100.43	108.50
1	E	20	G	O5'-C5'-C4'	-5.38	103.43	111.50
2	A	59	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	D	56	C	C4'-C3'-O3'	-5.38	104.94	113.00
1	D	23	A	O4'-C1'-N9	5.37	116.55	108.50
1	E	61	C	O5'-C5'-C4'	-5.37	103.45	111.50
2	B	304	LEU	CA-C-N	-5.36	113.59	122.11
2	B	304	LEU	C-N-CA	-5.36	113.59	122.11
1	E	29	A	O4'-C1'-N9	5.35	116.53	108.50
2	C	336	THR	N-CA-C	-5.35	102.38	110.24
2	C	135	MET	CG-SD-CE	5.35	112.66	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	193	ASN	N-CA-C	5.34	118.16	109.24
1	F	1	G	C3'-C2'-O2'	5.34	118.72	110.70
2	B	313	HIS	N-CA-C	5.34	117.09	109.14
1	D	5	A	C1'-C2'-O2'	5.33	116.40	108.40
2	B	130	TYR	CA-C-N	-5.33	115.58	122.99
2	B	130	TYR	C-N-CA	-5.33	115.58	122.99
1	E	35	A	C2'-C3'-O3'	-5.33	105.71	113.70
1	F	25	C	C1'-C2'-O2'	5.32	116.39	108.40
2	C	212	THR	N-CA-C	-5.32	103.37	110.07
1	F	35	A	O4'-C1'-N9	-5.31	100.53	108.50
2	B	75	ARG	CB-CA-C	-5.31	99.03	111.09
1	F	42	G	C3'-C2'-O2'	-5.30	102.74	110.70
1	F	28	C	C3'-C2'-O2'	5.30	118.65	110.70
1	F	1	G	O3'-P-O5'	-5.30	96.06	104.00
1	D	65	G	C2'-C3'-O3'	5.29	121.64	113.70
1	D	27	C	C2'-C3'-O3'	-5.29	105.77	113.70
1	E	73	A	N9-C1'-C2'	-5.29	104.07	112.00
1	D	70	C	P-O5'-C5'	-5.28	112.98	120.90
2	C	143	ASP	O-C-N	5.28	125.90	121.31
1	F	21	A	C2'-C3'-O3'	-5.27	105.79	113.70
1	E	65	G	OP2-P-O3'	-5.27	92.19	108.00
2	C	325	LYS	CA-C-N	5.27	127.34	120.28
2	C	325	LYS	C-N-CA	5.27	127.34	120.28
1	D	29	A	C3'-C2'-O2'	5.27	118.60	110.70
2	B	347	THR	CB-CA-C	-5.26	100.51	109.51
2	A	141	VAL	N-CA-C	5.26	116.24	108.45
2	C	396	GLY	N-CA-C	-5.26	100.74	110.73
2	C	21	ASP	N-CA-C	5.25	121.97	110.80
2	B	223	MET	C-N-CD	-5.24	103.50	125.00
1	D	75	C	C3'-C2'-O2'	-5.24	106.74	114.60
1	F	60	C	C3'-C2'-O2'	-5.24	106.74	114.60
2	A	73	ALA	N-CA-C	-5.24	105.26	110.97
2	B	93	ILE	CB-CA-C	-5.23	105.08	112.14
2	C	267	VAL	CB-CA-C	5.22	119.20	111.26
1	F	42	G	C1'-C2'-O2'	-5.22	100.57	108.40
2	A	168	VAL	CA-C-N	5.22	125.47	119.83
2	A	168	VAL	C-N-CA	5.22	125.47	119.83
2	C	198	LYS	N-CA-C	-5.22	105.50	111.14
2	A	105	VAL	CB-CA-C	-5.22	104.44	110.91
1	D	30	G	O5'-C5'-C4'	-5.21	103.68	111.50
2	B	168	VAL	CA-C-N	5.21	126.02	120.13
2	B	168	VAL	C-N-CA	5.21	126.02	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	29	A	C3'-C2'-O2'	5.20	118.50	110.70
2	B	234	ARG	CA-C-N	-5.20	113.38	121.97
2	B	234	ARG	C-N-CA	-5.20	113.38	121.97
2	B	342	PHE	CA-C-O	5.20	126.05	120.38
2	C	348	ASP	CA-C-N	-5.20	114.09	122.25
2	C	348	ASP	C-N-CA	-5.20	114.09	122.25
2	A	185	ASN	N-CA-C	5.20	121.29	109.81
2	B	299	GLU	O-C-N	5.20	129.20	123.33
1	F	61	C	O4'-C1'-N1	5.19	116.29	108.50
1	F	25	C	O4'-C1'-N1	5.18	116.28	108.50
2	A	133	VAL	CB-CA-C	-5.18	102.94	110.81
1	E	3	G	O4'-C1'-N9	5.17	116.26	108.50
2	C	248	LYS	N-CA-C	-5.17	101.43	109.24
1	D	51	G	C3'-C2'-O2'	5.17	118.45	110.70
2	C	93	ILE	CA-C-N	-5.17	113.72	120.44
2	C	93	ILE	C-N-CA	-5.17	113.72	120.44
1	D	27	C	O4'-C1'-N1	5.16	116.24	108.50
2	A	255	ILE	CB-CA-C	-5.16	105.22	111.88
2	B	311	THR	N-CA-CB	5.16	119.29	110.05
1	D	66	A	O4'-C1'-N9	-5.16	100.77	108.50
1	F	60	C	N1-C1'-C2'	-5.16	106.27	114.00
1	F	33	U	O5'-C5'-C4'	-5.15	103.78	111.50
2	A	87	ASP	CB-CA-C	-5.15	99.67	110.17
1	F	35	A	C3'-C2'-O2'	-5.14	102.98	110.70
2	B	371	THR	CB-CA-C	-5.14	99.55	109.37
1	F	46	7MG	P-O3'-C3'	5.13	127.90	120.20
2	A	248	LYS	N-CA-C	-5.13	100.65	108.76
1	F	33	U	C1'-C2'-O2'	5.13	116.10	108.40
2	B	185	ASN	N-CA-C	5.13	121.14	109.81
2	C	339	ARG	N-CA-C	5.13	120.55	108.40
2	A	101	GLY	N-CA-C	-5.12	102.98	110.87
2	B	372	VAL	N-CA-C	-5.12	100.96	108.85
2	A	187	LYS	N-CA-C	5.12	119.24	113.15
1	F	64	A	C1'-C2'-O2'	5.12	116.08	108.40
2	C	302	GLN	N-CA-CB	5.12	117.76	110.44
1	E	43	G	C2'-C3'-O3'	5.12	121.38	113.70
2	C	301	GLY	N-CA-C	-5.12	107.80	113.79
2	B	384	LEU	N-CA-C	-5.12	102.71	110.28
2	A	278	GLN	N-CA-C	-5.11	105.36	111.03
2	B	82	CYS	O-C-N	5.10	124.81	121.14
1	E	38	A	O5'-P-OP1	-5.10	92.69	108.00
2	A	222	LEU	CB-CA-C	-5.10	102.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	GLU	CA-C-N	-5.10	114.59	122.49
2	B	296	GLU	C-N-CA	-5.10	114.59	122.49
1	E	73	A	O4'-C1'-N9	-5.10	100.86	108.50
2	A	77	TYR	CA-C-N	5.10	129.55	122.77
2	A	77	TYR	C-N-CA	5.10	129.55	122.77
2	B	82	CYS	CA-C-N	5.10	127.13	120.25
2	B	82	CYS	C-N-CA	5.10	127.13	120.25
1	D	35	A	O4'-C1'-N9	-5.09	100.87	108.50
1	E	56	C	O4'-C1'-N1	-5.08	100.88	108.50
2	B	143	ASP	CA-C-O	5.08	124.01	119.59
1	F	23	A	N9-C1'-C2'	-5.08	104.38	112.00
2	A	249	VAL	CA-C-N	-5.08	114.63	122.86
2	A	249	VAL	C-N-CA	-5.08	114.63	122.86
2	A	280	GLY	N-CA-C	-5.08	103.45	112.54
2	B	339	ARG	O-C-N	5.08	125.33	121.27
1	F	44	A	C1'-C2'-O2'	5.08	116.01	108.40
2	B	25	THR	N-CA-C	5.08	116.50	110.97
2	B	26	THR	CB-CA-C	-5.08	102.69	110.81
2	B	130	TYR	N-CA-C	5.08	117.52	109.50
2	B	110	ASP	N-CA-C	5.07	119.59	113.41
2	B	360	GLU	N-CA-C	5.07	120.11	113.88
1	E	42	G	C5'-C4'-O4'	-5.07	102.20	109.80
2	C	219	LYS	CA-C-N	5.06	124.97	119.76
2	C	219	LYS	C-N-CA	5.06	124.97	119.76
1	E	1	G	O3'-P-O5'	-5.05	96.42	104.00
1	F	59	U	C3'-C2'-O2'	5.05	118.28	110.70
2	C	8	THR	N-CA-C	5.05	117.52	111.71
2	C	310	ILE	N-CA-CB	-5.05	102.48	111.92
1	D	56	C	O4'-C1'-N1	-5.04	100.93	108.50
1	F	43	G	N9-C1'-C2'	-5.04	104.44	112.00
2	C	169	PRO	CB-CA-C	-5.04	103.75	110.85
1	D	36	A	N9-C1'-C2'	-5.02	104.47	112.00
2	B	306	LYS	N-CA-C	-5.02	103.27	109.64
2	B	4	GLU	CB-CA-C	-5.02	105.30	113.37
1	D	4	G	P-O5'-C5'	-5.01	113.38	120.90
2	C	272	MET	N-CA-CB	5.01	118.72	110.90
2	B	90	LYS	CD-CE-NZ	5.00	127.92	111.90
1	F	47	U	C1'-C2'-O2'	-5.00	100.90	108.40
2	A	161	TYR	N-CA-C	-5.00	107.02	112.72

All (4) chirality outliers are listed below:

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

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1652	0	856	118	0
1	E	1652	0	855	115	0
1	F	1652	0	856	110	0
2	A	3144	0	3161	294	0
2	B	3144	0	3160	314	0
2	C	3144	0	3162	370	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
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	1294	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 50.

All (1294) 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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:363:MET:HE3	2:C:364:PRO:HD2	1.58	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	1.41	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:A:272:MET:HE3	2:A:285:ASN:H	1.39	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
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
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:39:PSU:H4'	2:C:360:GLU:CD	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:A:335:PHE:CE1	2:A:361:MET:HE3	2.19	0.78
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:C:287:GLY:C	2:C:288:LEU:HD23	2.09	0.78
2:B:299:GLU:O	2:B:302:GLN:HG3	1.84	0.78
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:335:PHE:CE1	2:B:361:MET:HE3	2.22	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
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:272:MET:HE3	2:B:285:ASN:H	1.54	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
1:E:37:YYG:H31	1:E:37:YYG:H1'	1.71	0.73
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:YYG:H31	1:F:37:YYG:H1'	1.73	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
2:C:272:MET:HE3	2:C:285:ASN:N	2.05	0.70
1:D:26:M2G:N3	1:D:26:M2G:H2'	2.04	0.70
2:C:355:LEU:HD22	2:C:362:VAL:HG23	1.72	0.70
2:A:74:LYS:HG3	6:A:428:HOH:O	1.91	0.70
2:B:354:ARG:HH12	2:B:373:GLU:CD	1.99	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:B:277:LEU:CD2	2:B:280:GLY:HA2	2.22	0.69
2:A:335:PHE:HA	2:A:355:LEU:HD11	1.73	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: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:52:LYS:HB2	2:B:52:LYS:HZ3	1.57	0.68
2:C:303:VAL:C	2:C:304:LEU:HD23	2.19	0.68
1:F:37:YYG:H103	1:F:37:YYG:N20	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:MET:HE1	2:C:151:GLU:HB2	1.76	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
1:F:37:YYG:HN20	1:F:37:YYG:C10	2.08	0.66
2:A:7:ARG:HH22	2:A:284:ASP:CG	2.03	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:140:MET:HE2	2:B:140:MET:HA	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:333:GLY:HA3	2:B:361:MET:HE2	1.81	0.63
2:A:335:PHE:CE1	2:A:361:MET:HB2	2.33	0.63
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:A:9:LYS:NZ	2:A:72:THR:O	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:247:VAL:C	2:B:248:LYS:HD3	2.26	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
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:37:YYG:H1'	1:D:37:YYG:H33	1.84	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:189:LYS:HG2	2:B:192:GLU:OE2	2.02	0.60
2:C:223:MET:O	2:C:223:MET:HG3	1.98	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
2:B:87:ASP:C	2:B:88:TYR:HD1	2.10	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:A:96:ALA:HA	2:A:99:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:53:G:H3'	1:E:54:5MU:H73	1.84	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
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:333:GLY:CA	2:B:361:MET:HE2	2.33	0.58
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
1:F:37:YYG:H103	1:F:37:YYG:HN20	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:223:MET:HE3	2:B:240:GLY:HA3	1.84	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
2:C:176:LEU:HB2	5:C:406:GNP:C5	2.35	0.57
2:A:92:MET:HE3	2:A:119:HIS:CG	2.40	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:7:ARG:HH22	2:B:284:ASP:CG	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:B:140:MET:CE	2.36	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:C:380:LEU:C	2:C:381:GLU:HG2	2.26	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
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:B:254:GLU:CD	2:B:308:GLY:H	2.14	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:A:92:MET:HE3	2:A:119:HIS:HA	1.88	0.55
2:C:299:GLU:O	2:C:302:GLN:HG3	2.06	0.55
2:C:335:PHE:CE1	2:C:361:MET:HE3	2.41	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:92:MET:HE3	2:B:119:HIS:HA	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:140:MET:HE3	2:A:140:MET:HA	1.89	0.54
2:A:335:PHE:CZ	2:A:361:MET:HE3	2.42	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
2:C:56:GLU:CD	2:C:63:ILE:H	2.15	0.54
1:D:45:G:O5'	1:D:45:G:H8	1.91	0.54
1:F:65:G:HO2'	2:C:350:THR:HG1	1.54	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:140:MET:HE2	2:C:140:MET:HA	1.89	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
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
2:C:135:MET:CE	2:C:151:GLU:HB2	2.36	0.54
2:A:38:GLU:HG3	2:A:200:TRP:CZ2	2.43	0.54
2:A:38:GLU:OE2	2:A:190:ARG:HG3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:27:LEU:HG	2:A:27:LEU:O	2.06	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
1:F:11:C:HO2'	1:F:12:U:H6	1.56	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
1:E:37:YYG:H31	1:E:37:YYG:C1'	2.38	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
2:C:92:MET:HE3	2:C:119:HIS:CG	2.43	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
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:B:335:PHE:CZ	2:B:361:MET:HE3	2.44	0.53
2:C:399:VAL:HG22	2:C:400:VAL:N	2.23	0.53
1:F:37:YYG:H31	1:F:37:YYG:C1'	2.39	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:247:VAL:C	2:C:248:LYS:HD3	2.33	0.52
1:D:25:C:N3	1:D:26:M2G:C8	2.78	0.52
1:D:37:YYG:H33	1:D:37:YYG:C1'	2.39	0.52
2:A:46:ASP:H	2:A:49:ASP:CG	2.16	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
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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLU:OE1	2:B:308:GLY:N	2.36	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
2:C:11:HIS:CE1	2:C:272:MET:HE2	2.45	0.51
1:D:25:C:C2	1:D:26:M2G:C8	2.98	0.51
2:B:345:ARG:HH22	2:B:381:GLU:CD	2.18	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:63:ILE:HG13	2:C:64:ASN:N	2.22	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:66:A:O2'	1:D:67:A:H5'	2.11	0.51
2:A:46:ASP:HB2	2:A:49:ASP:CG	2.36	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:A:140:MET:HA	2:A:140:MET:CE	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:C:333:GLY:HA3	2:C:361:MET:HE2	1.93	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
2:A:69:GLU:O	2:A:70:TYR:HB3	2.10	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: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
2:A:40:PRO:HG2	2:A:41:ASN:OD1	2.11	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:A:202:LEU:HD12	2:A:202:LEU:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:MET:HE2	2:C:150:VAL:HG12	1.94	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: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: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:B:285:ASN:C	2:B:285:ASN:HD22	2.20	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: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:249:VAL:HG13	2:B:268:THR:C	2.37	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
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: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:D:37:YYG:H1'	1:D:37:YYG:C3	2.42	0.49
1:E:7:U:H4'	1:E:8:U:OP2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:72:THR:HB	6:A:428:HOH:O	2.12	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:A:188:THR:HG22	2:A:189:LYS:N	2.28	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:248:LYS:HE3	2:C:251:ASP:CG	2.39	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
1:F:36:A:HO2'	1:F:37:YYG:H5'	1.78	0.48
2:A:180:GLU:O	2:A:183:HIS:HB2	2.14	0.48
2:A:191:GLY:H	2:A:197:ASP:CG	2.21	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:37:YYG:H103	1:F:37:YYG:C21	2.45	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
2:A:136:ASN:CG	2:A:137:LYS:H	2.23	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
2:C:338:TYR:C	2:C:340:PRO:HD3	2.40	0.47
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:C:21:ASP:CG	5:C:406:GNP:H5'2	2.40	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:O	2:C:214:VAL:HG12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:LEU:N	2:A:177:LEU:CD1	2.79	0.46
2:A:316:PHE:C	2:A:404:LEU:HD22	2.39	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
1:F:37:YYG:N20	1:F:37:YYG:C10	2.72	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
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:B:191:GLY:H	2:B:197:ASP:CG	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:ASP:C	2:C:23:GLY:H	2.23	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:B:230:THR:C	2:B:231:ILE:HD13	2.41	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:281:ILE:O	2:A:281:ILE:HG13	2.12	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: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
2:A:177:LEU:N	2:A:177:LEU:HD12	2.30	0.45
2:B:118:GLU:OE2	2:B:389:ARG:NH1	2.49	0.45
2:B:176:LEU:C	2:B:176:LEU:HD12	2.40	0.45
2:C:39:ASN:HA	2:C:40:PRO:HD3	1.47	0.45
2:C:136:ASN:CG	2:C:137:LYS:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:222:LEU:HD12	2:A:222:LEU:C	2.40	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
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: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
2:A:16:THR:O	2:A:82:CYS:HB2	2.17	0.45
2:A:92:MET:CE	2:A:119:HIS:HA	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:ILE:O	2:A:6:ILE:HG22	2.17	0.44
2:A:160:GLN:C	2:A:162:GLU:H	2.25	0.44
2:A:254:GLU:CD	2:A:307:PRO:HA	2.41	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: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:A:289:LEU:C	2:A:290:LEU:HG	2.42	0.44
2:B:320:VAL:CG1	2:B:321:TYR:N	2.79	0.44
1:E:15:G:O2'	1:E:16:H2U:O5'	2.29	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:202:LEU:HD12	2:B:202:LEU:C	2.42	0.44
2:B:289:LEU:C	2:B:290:LEU:HG	2.42	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:A:384:LEU:C	2:A:399:VAL:HG23	2.43	0.43
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
2:C:375:ILE:C	2:C:376:LYS:HG3	2.42	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:VAL:HG13	2:C:126:VAL:O	2.18	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:6:ILE:C	2:C:8:THR:H	2.24	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:B:83:PRO:O	2:B:83:PRO:HG2	2.18	0.43
2:B:140:MET:HE2	2:B:140:MET:CA	2.43	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
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
1:D:39:PSU:H4'	2:B:360:GLU:CD	2.43	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
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:A:272:MET:HE3	2:A:285:ASN:N	2.20	0.43
2:B:117:ARG:NH1	2:B:160:GLN:HE22	2.17	0.43
2:B:129:PRO:C	2:B:130:TYR:CD1	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:272:MET:HE3	2:B:285:ASN:N	2.30	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
2:C:136:ASN:CG	2:C:137:LYS:N	2.77	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:HD12	2:B:176:LEU:O	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:D:12:U:O2'	1:D:13:C:O5'	2.29	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
2:C:171:ILE:CG2	2:C:172:ARG:N	2.80	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
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:11:HIS:C	2:B:12:VAL:HG23	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:79:HIS:CD2	2:A:79:HIS:C	2.98	0.42
2:A:234:ARG:HB3	2:A:289:LEU:HD22	2.02	0.42
2:B:215:ARG:N	2:B:215:ARG:CD	2.80	0.42
2:C:143:ASP:HA	2:C:144:PRO:HD2	1.53	0.42
1:D:12:U:HO2'	1:D:13:C:P	2.42	0.42
1:F:37:YYG:C1'	1:F:37:YYG:C3	2.98	0.42
2:A:184:LYS:O	2:A:185:ASN:HB3	2.19	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:F:55:PSU:C6	1:F:55:PSU:C3'	3.02	0.41
2:A:129:PRO:C	2:A:130:TYR:CD1	2.98	0.41
2:B:383:GLY:C	2:B:399:VAL:HG23	2.44	0.41
2:C:13:ASN:N	2:C:100:ASP:OD2	2.44	0.41
2:C:321:TYR:CD2	2:C:321:TYR:C	2.96	0.41
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:287:GLY:C	2:A:288:LEU:HD23	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:185:ASN:C	2:B:187:LYS:N	2.78	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:B:146:LEU:HD12	2:B:146:LEU:HA	1.72	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:F:15:G:H2'	1:F:16:H2U:H62	2.02	0.41
2:A:188:THR:C	2:A:189:LYS:HD3	2.46	0.41
2:A:229:PHE:CD1	2:A:229:PHE:N	2.89	0.41
2:B:60:GLY:C	2:B:61:ILE:HG23	2.46	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
2:C:403:ILE:C	2:C:404:LEU:HD13	2.46	0.41
1:F:37:YYG:H141	1:F:37:YYG:O22	2.20	0.41
2:B:176:LEU:CB	5:B:406:GNP:C6	2.99	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:191:GLY:H	2:C:197:ASP:CG	2.28	0.41
2:C:341:GLN:CD	2:C:341:GLN:N	2.79	0.41
2:C:376:LYS:HA	2:C:377:PRO:HD3	1.77	0.41
2:A:96:ALA:CA	2:A:99:MET:HE3	2.50	0.41
2:B:176:LEU:HB3	5:B:406:GNP:C6	2.51	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:A:C5	1:D:22:G:N2	2.89	0.41
1:D:18:G:OP2	1:D:58:1MA:HM13	2.21	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: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:232:THR:C	2:B:234:ARG:N	2.79	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: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:39:PSU:H4'	2:C:360:GLU:OE2	2.19	0.41
1:E:59:U:C4	1:E:60:C:N3	2.89	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
1:D:37:YYG:C1'	1:D:37:YYG:C3	2.99	0.40
1:F:37:YYG:C10	2:A:335:PHE:CE2	3.05	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
2:C:2:LYS:HB2	2:C:3:GLY:H	1.50	0.40
2:C:16:THR:C	2:C:17:ILE:HG23	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:PRO:C	2:C:168:VAL:HG23	2.46	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:136:ASN:CG	2:A:137:LYS:N	2.80	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:B:232:THR:C	2:B:234:ARG:H	2.30	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:37:YYG:H101	2:A:335:PHE:CE2	2.56	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:115:GLN:N	2:A:115:GLN:CD	2.80	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%)	8 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	403/405 (100%)	359 (89%)	31 (8%)	13 (3%)	3	7
2	C	403/405 (100%)	353 (88%)	36 (9%)	14 (4%)	3	6
All	All	1209/1215 (100%)	1074 (89%)	102 (8%)	33 (3%)	4	10

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%)	283 (84%)	55 (16%)	2	6
2	B	338/338 (100%)	281 (83%)	57 (17%)	2	6
2	C	338/338 (100%)	276 (82%)	62 (18%)	2	5
All	All	1014/1014 (100%)	840 (83%)	174 (17%)	2	6

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	ILE
2	A	9	LYS
2	A	16	THR
2	A	17	ILE
2	A	21	ASP
2	A	26	THR
2	A	39	ASN
2	A	44	VAL
2	A	46	ASP
2	A	57	ARG
2	A	59	ARG
2	A	63	ILE
2	A	80	VAL
2	A	105	VAL
2	A	107	SER
2	A	114	PRO
2	A	119	HIS
2	A	126	VAL
2	A	140	MET
2	A	141	VAL
2	A	147	LEU
2	A	156	ASP
2	A	157	LEU
2	A	190	ARG
2	A	215	ARG
2	A	216	ASP

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Mol	Chain	Res	Type
2	A	217	VAL
2	A	223	MET
2	A	226	GLU
2	A	230	THR
2	A	231	ILE
2	A	234	ARG
2	A	241	ARG
2	A	242	ILE
2	A	247	VAL
2	A	248	LYS
2	A	265	THR
2	A	267	VAL
2	A	285	ASN
2	A	290	LEU
2	A	298	VAL
2	A	303	VAL
2	A	311	THR
2	A	314	THR
2	A	317	GLU
2	A	339	ARG
2	A	348	ASP
2	A	349	VAL
2	A	357	GLN
2	A	361	MET
2	A	378	VAL
2	A	381	GLU
2	A	401	THR
2	A	403	ILE
2	A	404	LEU
2	B	6	ILE
2	B	16	THR
2	B	21	ASP
2	B	39	ASN
2	B	42	VAL
2	B	44	VAL
2	B	52	LYS
2	B	63	ILE
2	B	88	TYR
2	B	90	LYS
2	B	91	ASN
2	B	126	VAL
2	B	140	MET

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Mol	Chain	Res	Type
2	B	146	LEU
2	B	155	ARG
2	B	156	ASP
2	B	168	VAL
2	B	182	MET
2	B	185	ASN
2	B	190	ARG
2	B	214	VAL
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	241	ARG
2	B	248	LYS
2	B	249	VAL
2	B	262	THR
2	B	265	THR
2	B	267	VAL
2	B	285	ASN
2	B	298	VAL
2	B	302	GLN
2	B	307	PRO
2	B	310	ILE
2	B	311	THR
2	B	314	THR
2	B	317	GLU
2	B	323	LEU
2	B	347	THR
2	B	349	VAL
2	B	354	ARG
2	B	355	LEU
2	B	361	MET
2	B	368	VAL
2	B	369	THR
2	B	371	THR
2	B	381	GLU
2	B	388	ILE
2	B	399	VAL
2	B	401	THR

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Mol	Chain	Res	Type
2	B	404	LEU
2	B	405	GLU
2	C	5	PHE
2	C	21	ASP
2	C	39	ASN
2	C	46	ASP
2	C	50	ILE
2	C	52	LYS
2	C	63	ILE
2	C	68	VAL
2	C	78	SER
2	C	80	VAL
2	C	89	ILE
2	C	91	ASN
2	C	94	THR
2	C	116	THR
2	C	126	VAL
2	C	132	VAL
2	C	138	VAL
2	C	140	MET
2	C	147	LEU
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	231	ILE
2	C	232	THR
2	C	247	VAL
2	C	248	LYS
2	C	249	VAL
2	C	262	THR
2	C	265	THR
2	C	267	VAL
2	C	285	ASN
2	C	286	VAL
2	C	297	GLU

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Mol	Chain	Res	Type
2	C	298	VAL
2	C	302	GLN
2	C	303	VAL
2	C	307	PRO
2	C	310	ILE
2	C	311	THR
2	C	317	GLU
2	C	319	SER
2	C	320	VAL
2	C	336	THR
2	C	342	PHE
2	C	347	THR
2	C	349	VAL
2	C	354	ARG
2	C	368	VAL
2	C	369	THR
2	C	381	GLU
2	C	388	ILE
2	C	395	VAL
2	C	401	THR
2	C	403	ILE
2	C	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	A	357	GLN
2	B	19	HIS
2	B	39	ASN
2	B	64	ASN

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Mol	Chain	Res	Type
2	B	85	HIS
2	B	115	GLN
2	B	119	HIS
2	B	160	GLN
2	B	183	HIS
2	B	185	ASN
2	B	331	HIS
2	B	341	GLN
2	B	367	ASN
2	C	19	HIS
2	C	39	ASN
2	C	67	HIS
2	C	85	HIS
2	C	119	HIS
2	C	160	GLN
2	C	183	HIS
2	C	341	GLN
2	C	367	ASN

5.3.3 RNA ⓘ

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%)	26 (34%)	6 (8%)
All	All	225/228 (98%)	85 (37%)	22 (9%)

All (85) 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

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Mol	Chain	Res	Type
1	D	31	A
1	D	34	OMG
1	D	38	A
1	D	39	PSU
1	D	41	U
1	D	44	A
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

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Mol	Chain	Res	Type
1	E	48	C
1	E	67	A
1	E	68	U
1	E	69	U
1	E	73	A
1	E	75	C
1	F	3	G
1	F	4	G
1	F	5	A
1	F	6	U
1	F	11	C
1	F	12	U
1	F	16	H2U
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

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Mol	Chain	Res	Type
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
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 ⓘ

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	1MA	D	58	1	21,25,26	0.80	1 (4%)	30,37,40	0.89	3 (10%)
1	2MG	E	10	1	23,26,27	0.39	0	33,38,41	0.90	2 (6%)
1	M2G	D	26	1	24,27,28	0.36	0	33,40,43	1.42	5 (15%)
1	H2U	F	17	1	18,21,22	1.13	1 (5%)	19,30,33	1.41	4 (21%)
1	OMG	F	34	1	23,26,27	0.40	0	32,38,41	1.15	2 (6%)
1	7MG	E	46	1	23,26,27	2.69	3 (13%)	27,39,42	2.10	4 (14%)
1	1MA	E	58	1	21,25,26	0.76	1 (4%)	30,37,40	0.97	3 (10%)
1	2MG	F	10	1	23,26,27	0.38	0	33,38,41	0.84	2 (6%)
1	OMC	D	32	1	19,22,23	0.38	0	25,31,34	1.02	2 (8%)
1	OMC	F	32	1	19,22,23	0.37	0	25,31,34	0.86	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	D	40	1	19,22,23	1.93	1 (5%)	26,32,35	1.35	4 (15%)
1	OMC	E	32	1	19,22,23	0.35	0	25,31,34	1.21	2 (8%)
1	PSU	D	39	1	18,21,22	0.66	0	21,30,33	1.07	2 (9%)
1	5MC	E	49	1	19,22,23	0.47	0	26,32,35	0.86	2 (7%)
1	PSU	E	55	1	18,21,22	0.64	0	21,30,33	1.17	2 (9%)
1	5MC	F	40	1	19,22,23	2.92	1 (5%)	26,32,35	3.64	4 (15%)
1	M2G	E	26	1	24,27,28	0.41	0	33,40,43	2.75	7 (21%)
1	YYG	E	37	1	38,42,43	1.62	8 (21%)	45,62,65	2.24	17 (37%)
1	M2G	F	26	1	24,27,28	0.34	0	33,40,43	0.55	0
1	7MG	D	46	1	23,26,27	3.01	4 (17%)	27,39,42	2.06	6 (22%)
1	PSU	E	39	1	18,21,22	0.87	1 (5%)	21,30,33	1.04	1 (4%)
1	H2U	D	16	1	18,21,22	0.74	0	19,30,33	1.96	4 (21%)
1	5MC	E	40	1	19,22,23	2.57	1 (5%)	26,32,35	1.33	3 (11%)
1	1MA	F	58	1	21,25,26	0.79	1 (4%)	30,37,40	0.66	1 (3%)
1	5MC	F	49	1	19,22,23	1.04	1 (5%)	26,32,35	0.98	2 (7%)
1	OMG	D	34	1	23,26,27	0.42	0	32,38,41	0.88	2 (6%)
1	H2U	E	17	1	18,21,22	1.16	2 (11%)	19,30,33	2.91	5 (26%)
1	PSU	F	39	1	18,21,22	0.82	0	21,30,33	1.58	2 (9%)
1	H2U	E	16	1	18,21,22	0.62	0	19,30,33	2.98	8 (42%)
1	H2U	D	17	1	18,21,22	0.72	1 (5%)	19,30,33	1.49	4 (21%)
1	5MC	D	49	1	19,22,23	0.59	1 (5%)	26,32,35	2.09	5 (19%)
1	5MU	D	54	1	19,22,23	4.53	1 (5%)	27,32,35	3.58	5 (18%)
1	YYG	D	37	1	38,42,43	1.73	7 (18%)	45,62,65	2.77	17 (37%)
1	H2U	F	16	1	18,21,22	1.10	1 (5%)	19,30,33	2.90	10 (52%)
1	PSU	D	55	1	18,21,22	0.75	0	21,30,33	1.04	2 (9%)
1	7MG	F	46	1	23,26,27	2.71	3 (13%)	27,39,42	2.14	5 (18%)
1	5MU	E	54	1	19,22,23	1.93	1 (5%)	27,32,35	0.91	2 (7%)
1	OMG	E	34	1	23,26,27	0.38	0	32,38,41	1.47	4 (12%)
1	YYG	F	37	1	38,42,43	1.50	5 (13%)	45,62,65	2.48	17 (37%)
1	2MG	D	10	1	23,26,27	0.34	0	33,38,41	0.71	1 (3%)
1	5MU	F	54	1	19,22,23	1.51	1 (5%)	27,32,35	0.71	1 (3%)
1	PSU	F	55	1	18,21,22	0.78	0	21,30,33	1.00	1 (4%)

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	1MA	D	58	1	-	2/7/25/26	0/3/3/3
1	2MG	E	10	1	-	1/9/27/28	0/3/3/3
1	M2G	D	26	1	-	0/11/29/30	0/3/3/3
1	H2U	F	17	1	-	4/7/38/39	0/2/2/2
1	OMG	F	34	1	-	1/9/27/28	0/3/3/3
1	7MG	E	46	1	-	1/7/37/38	0/3/3/3
1	1MA	E	58	1	-	0/7/25/26	0/3/3/3
1	2MG	F	10	1	-	0/9/27/28	0/3/3/3
1	OMC	D	32	1	-	1/9/27/28	0/2/2/2
1	OMC	F	32	1	-	0/9/27/28	0/2/2/2
1	5MC	D	40	1	-	0/7/25/26	0/2/2/2
1	OMC	E	32	1	-	2/9/27/28	0/2/2/2
1	PSU	D	39	1	-	4/7/25/26	0/2/2/2
1	5MC	E	49	1	-	0/7/25/26	0/2/2/2
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	M2G	E	26	1	-	3/11/29/30	0/3/3/3
1	YYG	E	37	1	-	14/24/42/43	0/4/4/4
1	M2G	F	26	1	-	1/11/29/30	0/3/3/3
1	7MG	D	46	1	-	2/7/37/38	0/3/3/3
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	H2U	D	16	1	-	6/7/38/39	0/2/2/2
1	5MC	E	40	1	-	2/7/25/26	0/2/2/2
1	1MA	F	58	1	-	2/7/25/26	0/3/3/3
1	5MC	F	49	1	-	0/7/25/26	0/2/2/2
1	OMG	D	34	1	-	2/9/27/28	0/3/3/3
1	H2U	E	17	1	-	2/7/38/39	0/2/2/2
1	PSU	F	39	1	-	0/7/25/26	0/2/2/2
1	H2U	E	16	1	-	5/7/38/39	0/2/2/2
1	H2U	D	17	1	-	6/7/38/39	0/2/2/2
1	5MC	D	49	1	-	0/7/25/26	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	YYG	D	37	1	-	9/24/42/43	0/4/4/4
1	H2U	F	16	1	-	0/7/38/39	0/2/2/2
1	PSU	D	55	1	-	1/7/25/26	0/2/2/2
1	7MG	F	46	1	-	0/7/37/38	0/3/3/3
1	5MU	E	54	1	-	0/7/25/26	0/2/2/2
1	OMG	E	34	1	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YYG	F	37	1	-	4/24/42/43	0/4/4/4
1	2MG	D	10	1	-	2/9/27/28	0/3/3/3
1	5MU	F	54	1	-	0/7/25/26	0/2/2/2
1	PSU	F	55	1	-	1/7/25/26	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	5MU	C5M-C5	-19.68	1.02	1.50
1	D	46	7MG	C8-N9	-13.33	1.37	1.45
1	F	40	5MC	CM5-C5	-12.66	1.19	1.50
1	F	46	7MG	C8-N9	-12.34	1.37	1.45
1	E	46	7MG	C8-N9	-12.31	1.37	1.45
1	E	40	5MC	CM5-C5	-11.04	1.23	1.50
1	D	40	5MC	CM5-C5	-8.25	1.30	1.50
1	E	54	5MU	C5M-C5	-8.20	1.30	1.50
1	F	54	5MU	C5M-C5	-6.38	1.35	1.50
1	D	37	YYG	O23-C21	-5.16	1.25	1.34
1	F	37	YYG	O23-C21	-4.93	1.26	1.34
1	E	37	YYG	O23-C21	-4.56	1.26	1.34
1	F	49	5MC	CM5-C5	4.03	1.60	1.50
1	D	37	YYG	C2-N3	-3.90	1.32	1.38
1	F	16	H2U	C2-N1	3.84	1.40	1.35
1	E	37	YYG	C2-N3	-3.77	1.32	1.38
1	D	37	YYG	O17-C16	3.74	1.30	1.21
1	F	37	YYG	O18-C16	-3.69	1.24	1.33
1	E	37	YYG	O18-C16	-3.65	1.24	1.33
1	F	37	YYG	C2-N3	-3.65	1.32	1.38
1	F	17	H2U	C2-N1	3.62	1.40	1.35
1	E	17	H2U	C2-N1	3.62	1.40	1.35
1	D	46	7MG	CM7-N7	3.55	1.58	1.45
1	D	37	YYG	C13-C12	3.51	1.54	1.50
1	D	37	YYG	O22-C21	3.48	1.28	1.21
1	E	37	YYG	C13-C12	3.18	1.54	1.50
1	E	37	YYG	C15-N20	3.04	1.52	1.45
1	D	46	7MG	C5-N7	3.00	1.39	1.35
1	F	46	7MG	C5-N7	2.93	1.39	1.35
1	E	46	7MG	C5-N7	2.80	1.39	1.35
1	E	37	YYG	O22-C21	2.75	1.26	1.21
1	D	37	YYG	C15-N20	2.68	1.51	1.45
1	D	58	1MA	C6-N6	2.67	1.34	1.28
1	F	37	YYG	C12-N1	-2.60	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	58	1MA	C6-N6	2.48	1.34	1.28
1	F	58	1MA	C6-N6	2.46	1.33	1.28
1	D	46	7MG	C8-N7	-2.41	1.30	1.42
1	E	37	YYG	C12-N1	-2.35	1.35	1.40
1	D	17	H2U	C2-N1	2.34	1.38	1.35
1	E	46	7MG	C8-N7	-2.33	1.31	1.42
1	F	46	7MG	C8-N7	-2.33	1.31	1.42
1	D	37	YYG	C11-N2	-2.31	1.33	1.38
1	E	17	H2U	O2-C2	2.23	1.27	1.23
1	E	39	PSU	O4'-C1'	-2.22	1.40	1.43
1	E	37	YYG	C21-N20	2.12	1.40	1.34
1	D	49	5MC	CM5-C5	-2.04	1.45	1.50
1	F	37	YYG	C11-N2	-2.02	1.34	1.38

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	40	5MC	CM5-C5-C6	-14.23	103.59	122.85
1	D	54	5MU	C5M-C5-C4	12.85	132.50	118.78
1	D	54	5MU	C5M-C5-C6	-11.18	107.72	122.85
1	F	40	5MC	CM5-C5-C4	11.06	138.68	120.51
1	E	26	M2G	CM1-N2-C2	9.34	139.72	120.61
1	E	17	H2U	O4'-C1'-N1	9.30	121.96	109.30
1	E	16	H2U	O2-C2-N1	-7.89	113.62	123.10
1	E	26	M2G	O4'-C1'-N9	7.67	125.74	108.36
1	D	49	5MC	CM5-C5-C6	7.02	132.35	122.85
1	F	46	7MG	N9-C8-N7	6.87	113.09	103.37
1	D	46	7MG	N9-C8-N7	6.83	113.05	103.37
1	E	46	7MG	N9-C8-N7	6.81	113.01	103.37
1	F	37	YYG	C14-C15-C16	-6.78	91.39	110.38
1	E	16	H2U	O4'-C1'-N1	6.43	118.06	109.30
1	D	49	5MC	CM5-C5-C4	-6.33	110.11	120.51
1	F	16	H2U	N3-C2-N1	6.30	122.98	116.65
1	D	37	YYG	C14-C15-C16	-6.28	92.79	110.38
1	D	37	YYG	C16-C15-N20	6.02	124.52	110.65
1	D	37	YYG	C2'-C1'-N9	-5.99	96.58	113.25
1	D	54	5MU	O2'-C2'-C3'	-5.74	93.43	111.82
1	E	17	H2U	O3'-C3'-C2'	-5.74	93.43	111.82
1	D	37	YYG	C5-C4-N3	5.68	128.61	123.99
1	F	37	YYG	C16-C15-N20	5.64	123.65	110.65
1	E	37	YYG	C5-C4-N3	5.58	128.53	123.99
1	F	37	YYG	C5-C4-N3	5.48	128.44	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	16	H2U	O2-C2-N3	-5.42	111.49	121.49
1	F	39	PSU	O2'-C2'-C3'	-5.34	94.70	111.82
1	F	16	H2U	O2-C2-N1	-5.30	116.73	123.10
1	D	37	YYG	C19-O18-C16	5.26	127.85	115.92
1	E	37	YYG	O18-C16-O17	-5.22	113.69	123.85
1	E	26	M2G	CM2-N2-C2	-5.16	110.06	120.61
1	D	37	YYG	N3-C2-N2	-5.11	119.58	126.62
1	D	37	YYG	C13-C14-C15	5.08	122.53	113.16
1	E	26	M2G	O3'-C3'-C4'	5.06	125.63	111.08
1	D	16	H2U	O4'-C1'-N1	5.01	116.13	109.30
1	F	37	YYG	N3-C2-N2	-5.00	119.73	126.62
1	F	34	OMG	CM2-O2'-C2'	-4.94	101.80	114.47
1	E	40	5MC	CM5-C5-C6	-4.91	116.21	122.85
1	D	26	M2G	C2'-C1'-N9	-4.89	99.64	113.25
1	D	16	H2U	O2-C2-N1	-4.78	117.36	123.10
1	F	37	YYG	C14-C13-C12	-4.72	103.70	113.36
1	E	37	YYG	N3-C2-N2	-4.64	120.22	126.62
1	E	46	7MG	O3'-C3'-C4'	-4.64	97.75	111.08
1	D	40	5MC	O4'-C1'-N1	4.59	118.77	108.36
1	E	34	OMG	O2'-C2'-C1'	-4.56	100.32	108.99
1	D	37	YYG	C15-N20-C21	4.56	132.27	120.93
1	E	46	7MG	C4-C5-N7	4.55	110.75	105.38
1	F	46	7MG	C4-C5-N7	4.48	110.67	105.38
1	E	17	H2U	C5-C4-N3	4.44	121.41	116.69
1	F	46	7MG	O4'-C1'-N9	4.42	115.32	109.30
1	D	46	7MG	C4-C5-N7	4.38	110.55	105.38
1	E	34	OMG	O4'-C1'-N9	-4.38	98.44	108.36
1	D	46	7MG	O4'-C1'-N9	4.28	115.13	109.30
1	E	34	OMG	CM2-O2'-C2'	-4.13	103.88	114.47
1	E	16	H2U	O4-C4-C5	-4.12	113.76	122.20
1	F	37	YYG	O23-C21-N20	4.11	117.69	110.77
1	E	26	M2G	O2'-C2'-C1'	4.04	124.03	110.10
1	F	37	YYG	C14-C15-N20	-3.90	103.18	110.91
1	E	32	OMC	CM2-O2'-C2'	-3.87	104.54	114.47
1	E	26	M2G	O2'-C2'-C3'	3.86	124.20	111.82
1	D	37	YYG	O23-C21-O22	-3.84	119.03	124.62
1	D	37	YYG	C2-N1-C12	-3.84	103.03	109.94
1	E	37	YYG	O18-C16-C15	3.79	121.14	111.49
1	E	32	OMC	C2'-C1'-N1	-3.75	107.12	114.24
1	F	37	YYG	C2-N1-C12	-3.62	103.43	109.94
1	D	17	H2U	N3-C2-N1	3.58	120.25	116.65
1	F	46	7MG	O3'-C3'-C2'	3.58	123.28	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	YYG	C3-N3-C4	3.52	129.95	123.11
1	E	37	YYG	C13-C14-C15	3.51	119.62	113.16
1	E	40	5MC	CM5-C5-C4	3.50	126.27	120.51
1	D	37	YYG	C14-C13-C12	3.48	120.47	113.36
1	E	37	YYG	C2'-C1'-N9	-3.40	103.78	113.25
1	F	49	5MC	O3'-C3'-C4'	3.38	120.80	111.08
1	F	17	H2U	N3-C2-N1	3.34	120.00	116.65
1	D	32	OMC	C2'-C1'-N1	-3.33	107.92	114.24
1	F	32	OMC	O2'-C2'-C1'	-3.33	102.66	108.99
1	E	37	YYG	C15-N20-C21	3.33	129.21	120.93
1	E	37	YYG	O4'-C1'-N9	-3.27	100.94	108.36
1	E	37	YYG	C14-C15-C16	-3.26	101.26	110.38
1	D	40	5MC	O2'-C2'-C3'	-3.22	101.48	111.82
1	E	55	PSU	O2'-C2'-C1'	-3.17	103.68	111.21
1	D	17	H2U	O2-C2-N1	-3.14	119.33	123.10
1	D	26	M2G	O4'-C1'-N9	3.08	115.33	108.36
1	F	16	H2U	O3'-C3'-C4'	3.07	119.90	111.08
1	E	16	H2U	N3-C2-N1	3.07	119.73	116.65
1	D	54	5MU	O4'-C1'-N1	-3.05	101.44	108.36
1	E	37	YYG	C10-C11-N2	3.04	125.41	119.32
1	F	16	H2U	O4'-C1'-N1	-3.03	105.17	109.30
1	E	16	H2U	O3'-C3'-C2'	-2.99	102.23	111.82
1	E	10	2MG	O3'-C3'-C4'	2.97	119.62	111.08
1	E	46	7MG	O4'-C1'-N9	-2.93	105.30	109.30
1	F	10	2MG	C2'-C1'-N9	2.90	121.33	113.25
1	F	37	YYG	C2'-C1'-N9	-2.87	105.25	113.25
1	E	58	1MA	N1-C2-N3	2.87	129.41	126.00
1	F	16	H2U	O3'-C3'-C2'	2.87	121.02	111.82
1	D	37	YYG	O23-C21-N20	2.86	115.58	110.77
1	D	34	OMG	CM2-O2'-C2'	-2.85	107.16	114.47
1	D	58	1MA	C2'-C1'-N9	2.83	121.12	113.25
1	F	34	OMG	O2'-C2'-C1'	-2.81	103.66	108.99
1	F	55	PSU	C6-C5-C4	2.80	120.06	118.17
1	D	26	M2G	CM2-N2-CM1	2.79	124.79	115.87
1	E	37	YYG	C16-C15-N20	2.77	117.04	110.65
1	E	37	YYG	C24-O23-C21	2.77	118.84	115.63
1	E	49	5MC	O2'-C2'-C3'	2.75	120.63	111.82
1	D	46	7MG	O3'-C3'-C4'	2.73	118.92	111.08
1	F	37	YYG	O3'-C3'-C2'	2.72	120.55	111.82
1	D	16	H2U	O4-C4-C5	-2.72	116.64	122.20
1	F	16	H2U	O2'-C2'-C3'	2.72	120.53	111.82
1	F	39	PSU	C6-C5-C4	2.70	120.00	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	1MA	N1-C2-N3	2.66	129.16	126.00
1	E	54	5MU	O3'-C3'-C4'	-2.63	103.53	111.08
1	E	16	H2U	O3'-C3'-C4'	-2.62	103.55	111.08
1	D	17	H2U	O3'-C3'-C4'	-2.62	103.56	111.08
1	E	58	1MA	O2'-C2'-C1'	2.62	119.11	110.10
1	F	58	1MA	N1-C2-N3	2.61	129.10	126.00
1	F	17	H2U	O2-C2-N3	-2.60	116.70	121.49
1	E	17	H2U	N3-C2-N1	-2.59	114.05	116.65
1	F	16	H2U	O4-C4-N3	-2.59	116.31	120.30
1	E	10	2MG	O4'-C1'-N9	2.59	114.22	108.36
1	F	37	YYG	O22-C21-N20	-2.56	120.66	124.86
1	D	26	M2G	CM2-N2-C2	-2.56	115.37	120.61
1	E	37	YYG	C3-N3-C4	2.55	128.07	123.11
1	F	16	H2U	O4-C4-C5	-2.55	116.98	122.20
1	F	17	H2U	O2-C2-N1	-2.53	120.06	123.10
1	D	26	M2G	O2'-C2'-C1'	2.53	118.81	110.10
1	D	46	7MG	O3'-C3'-C2'	-2.49	103.83	111.82
1	E	17	H2U	O2-C2-N3	-2.44	116.99	121.49
1	D	55	PSU	C6-C5-C4	2.43	119.81	118.17
1	E	37	YYG	C2-N2-C11	-2.42	101.72	106.31
1	D	10	2MG	CM2-N2-C2	-2.41	118.46	123.65
1	E	16	H2U	O2-C2-N3	-2.41	117.05	121.49
1	F	37	YYG	O2'-C2'-C1'	-2.41	101.82	110.10
1	E	37	YYG	O23-C21-N20	2.37	114.76	110.77
1	D	39	PSU	O2'-C2'-C3'	-2.36	104.25	111.82
1	E	55	PSU	C6-C5-C4	2.36	119.77	118.17
1	F	16	H2U	C5-C4-N3	2.35	119.19	116.69
1	E	39	PSU	C6-C5-C4	2.33	119.75	118.17
1	D	46	7MG	O2'-C2'-C1'	2.33	118.12	110.10
1	D	34	OMG	O3'-C3'-C2'	2.33	117.70	111.19
1	D	40	5MC	C2'-C1'-N1	-2.32	106.79	113.25
1	F	17	H2U	C5-C4-N3	2.32	119.15	116.69
1	F	10	2MG	O2'-C2'-C3'	2.32	119.24	111.82
1	D	49	5MC	C5-C6-N1	-2.28	120.84	123.31
1	F	37	YYG	C11-C12-N1	2.26	106.90	105.31
1	D	39	PSU	C6-C5-C4	2.25	119.69	118.17
1	D	37	YYG	O4'-C1'-N9	2.23	113.41	108.36
1	F	37	YYG	C19-O18-C16	2.22	120.94	115.92
1	D	17	H2U	O4-C4-C5	-2.21	117.67	122.20
1	E	16	H2U	C5-C6-N1	2.21	118.21	111.52
1	D	32	OMC	O3'-C3'-C2'	-2.20	105.03	111.19
1	F	54	5MU	C6-C5-C4	2.19	119.83	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	YYG	O23-C21-O22	-2.19	121.44	124.62
1	E	37	YYG	C2-N1-C12	-2.17	106.04	109.94
1	F	46	7MG	O3'-C3'-C4'	2.16	117.28	111.08
1	F	40	5MC	C5-C6-N1	-2.15	120.98	123.31
1	F	40	5MC	O3'-C3'-C4'	2.15	117.25	111.08
1	D	49	5MC	O3'-C3'-C4'	2.14	117.23	111.08
1	D	54	5MU	C6-C5-C4	2.13	119.78	118.02
1	D	40	5MC	C5-C6-N1	-2.13	121.00	123.31
1	F	37	YYG	N9-C4-N3	-2.13	126.00	129.45
1	D	37	YYG	N9-C4-N3	-2.13	126.01	129.45
1	E	54	5MU	C6-C5-C4	2.12	119.77	118.02
1	D	16	H2U	C5-C6-N1	-2.10	105.16	111.52
1	D	37	YYG	C24-O23-C21	-2.09	113.21	115.63
1	E	40	5MC	C5-C6-N1	-2.08	121.06	123.31
1	F	37	YYG	C2-N2-C11	-2.07	102.39	106.31
1	E	58	1MA	O2'-C2'-C3'	-2.07	105.18	111.82
1	E	49	5MC	C5-C6-N1	-2.06	121.08	123.31
1	D	49	5MC	O2'-C2'-C3'	2.06	118.42	111.82
1	D	58	1MA	O2'-C2'-C1'	2.06	117.19	110.10
1	D	37	YYG	O3'-C3'-C4'	-2.05	105.20	111.08
1	E	34	OMG	C2'-C1'-N9	-2.04	110.36	114.24
1	D	55	PSU	C6-N1-C2	-2.04	120.80	122.69
1	F	37	YYG	O23-C21-O22	-2.04	121.65	124.62
1	F	49	5MC	C5-C6-N1	-2.03	121.11	123.31
1	E	26	M2G	O3'-C3'-C2'	2.02	118.28	111.82

There are no chirality outliers.

All (83) 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	32	OMC	C3'-C2'-O2'-CM2
1	D	37	YYG	O23-C21-N20-C15
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	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'

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Mol	Chain	Res	Type	Atoms
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	N1-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	D	37	YYG	O22-C21-N20-C15
1	E	37	YYG	O23-C21-N20-C15
1	D	17	H2U	C3'-C4'-C5'-O5'
1	D	34	OMG	O4'-C4'-C5'-O5'
1	D	46	7MG	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	D	37	YYG	C16-C15-N20-C21
1	F	37	YYG	C16-C15-N20-C21
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	E	37	YYG	C3'-C4'-C5'-O5'
1	F	37	YYG	C3'-C4'-C5'-O5'
1	D	17	H2U	C2'-C1'-N1-C6
1	E	17	H2U	C2'-C1'-N1-C6
1	E	40	5MC	C3'-C4'-C5'-O5'
1	E	37	YYG	C13-C14-C15-C16
1	D	39	PSU	O4'-C4'-C5'-O5'
1	E	16	H2U	C3'-C4'-C5'-O5'
1	E	37	YYG	O4'-C4'-C5'-O5'
1	F	58	1MA	C3'-C4'-C5'-O5'
1	F	37	YYG	O4'-C4'-C5'-O5'
1	D	37	YYG	N20-C15-C16-O18
1	E	37	YYG	N20-C15-C16-O18
1	D	37	YYG	C13-C14-C15-C16
1	D	58	1MA	C3'-C4'-C5'-O5'
1	D	34	OMG	C3'-C4'-C5'-O5'
1	E	37	YYG	N20-C15-C16-O17
1	D	37	YYG	C14-C15-C16-O18
1	E	37	YYG	C14-C15-C16-O18

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Mol	Chain	Res	Type	Atoms
1	D	37	YYG	N20-C15-C16-O17
1	E	37	YYG	C14-C15-C16-O17
1	F	37	YYG	C12-C13-C14-C15
1	E	46	7MG	C3'-C4'-C5'-O5'
1	F	17	H2U	O4'-C4'-C5'-O5'
1	D	10	2MG	C3'-C4'-C5'-O5'
1	E	37	YYG	C12-C13-C14-C15
1	D	37	YYG	C14-C15-C16-O17
1	F	17	H2U	C3'-C4'-C5'-O5'
1	D	16	H2U	C2'-C1'-N1-C6
1	D	17	H2U	C4'-C5'-O5'-P
1	E	16	H2U	C4'-C5'-O5'-P
1	F	26	M2G	C4'-C5'-O5'-P
1	D	55	PSU	O4'-C1'-C5-C4
1	E	55	PSU	O4'-C1'-C5-C4
1	E	34	OMG	C3'-C4'-C5'-O5'
1	D	10	2MG	O4'-C4'-C5'-O5'
1	E	34	OMG	O4'-C4'-C5'-O5'
1	E	37	YYG	C11-C12-C13-C14
1	D	17	H2U	O4'-C1'-N1-C2
1	E	10	2MG	C4'-C5'-O5'-P
1	E	26	M2G	C4'-C5'-O5'-P
1	D	17	H2U	C2'-C1'-N1-C2
1	E	55	PSU	O4'-C1'-C5-C6
1	F	55	PSU	O4'-C1'-C5-C6
1	E	32	OMC	C3'-C2'-O2'-CM2
1	D	37	YYG	C13-C14-C15-N20
1	D	16	H2U	O4'-C1'-N1-C2
1	E	16	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 152 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	58	1MA	2	0
1	E	10	2MG	9	0
1	D	26	M2G	11	0
1	F	17	H2U	1	0
1	F	34	OMG	4	0
1	E	46	7MG	2	0
1	E	58	1MA	1	0
1	F	10	2MG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	32	OMC	2	0
1	F	32	OMC	1	0
1	D	40	5MC	4	0
1	E	32	OMC	3	0
1	D	39	PSU	6	0
1	E	55	PSU	1	0
1	F	40	5MC	3	0
1	E	26	M2G	9	0
1	E	37	YYG	10	0
1	F	26	M2G	7	0
1	D	46	7MG	2	0
1	E	39	PSU	2	0
1	D	16	H2U	5	0
1	F	49	5MC	1	0
1	D	34	OMG	2	0
1	E	17	H2U	3	0
1	E	16	H2U	5	0
1	D	17	H2U	3	0
1	D	49	5MC	1	0
1	D	54	5MU	1	0
1	D	37	YYG	8	0
1	F	16	H2U	5	0
1	D	55	PSU	1	0
1	F	46	7MG	4	0
1	E	54	5MU	2	0
1	E	34	OMG	3	0
1	F	37	YYG	20	0
1	D	10	2MG	4	0
1	F	54	5MU	1	0
1	F	55	PSU	3	0

5.5 Carbohydrates

There are no oligosaccharides 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	34,34,34	1.86	3 (8%)	47,54,54	1.70	8 (17%)
4	PHE	D	77	1	10,11,12	1.18	1 (10%)	8,13,15	0.41	0
4	PHE	F	77	1	10,11,12	1.35	2 (20%)	8,13,15	0.30	0
4	PHE	E	77	1	10,11,12	1.09	1 (10%)	8,13,15	0.64	0
5	GNP	A	406	3	34,34,34	2.03	7 (20%)	47,54,54	2.84	15 (31%)
5	GNP	C	406	3	34,34,34	2.53	4 (11%)	47,54,54	3.10	13 (27%)

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	-	9/18/38/38	0/3/3/3
4	PHE	D	77	1	-	0/5/6/8	0/1/1/1
4	PHE	F	77	1	-	1/5/6/8	0/1/1/1
4	PHE	E	77	1	-	1/5/6/8	0/1/1/1
5	GNP	A	406	3	-	9/18/38/38	0/3/3/3
5	GNP	C	406	3	-	5/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	406	GNP	PA-O3A	-9.80	1.48	1.59
5	C	406	GNP	PB-O3A	-8.02	1.49	1.59
5	A	406	GNP	PA-O3A	-7.82	1.51	1.59
5	B	406	GNP	PA-O3A	-7.45	1.51	1.59
5	B	406	GNP	PB-O3A	-6.27	1.51	1.59
5	C	406	GNP	PG-O1G	5.26	1.54	1.46
5	A	406	GNP	PB-O3A	-4.80	1.53	1.59
5	A	406	GNP	PB-O2B	-3.71	1.46	1.56
5	C	406	GNP	PG-O2G	-3.55	1.47	1.56
4	D	77	PHE	CA-N	-3.22	1.39	1.48
5	B	406	GNP	PG-O2G	-3.14	1.48	1.56
4	F	77	PHE	CA-N	-3.06	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	GNP	PG-O2G	-3.00	1.48	1.56
4	E	77	PHE	CA-N	-2.67	1.40	1.48
5	A	406	GNP	PG-O1G	2.36	1.49	1.46
4	F	77	PHE	O-C	2.22	1.28	1.20
5	A	406	GNP	PB-N3B	-2.18	1.57	1.63
5	A	406	GNP	PG-O3G	-2.18	1.51	1.56

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	406	GNP	O2B-PB-O1B	10.89	133.22	109.87
5	A	406	GNP	C1'-N9-C8	-10.22	97.70	126.73
5	A	406	GNP	C1'-N9-C4	9.51	154.59	126.49
5	C	406	GNP	C1'-N9-C8	9.09	152.55	126.73
5	C	406	GNP	C1'-N9-C4	-8.65	100.94	126.49
5	C	406	GNP	C2'-C1'-N9	-6.08	96.32	113.25
5	A	406	GNP	O2B-PB-O1B	6.01	122.77	109.87
5	C	406	GNP	O3A-PB-N3B	5.18	120.97	106.59
5	A	406	GNP	O2G-PG-O3G	4.83	120.58	107.59
5	B	406	GNP	O2A-PA-O3A	4.72	120.03	107.27
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	A	406	GNP	O3A-PA-O1A	-4.31	97.73	110.70
5	B	406	GNP	O3A-PA-O1A	-4.04	98.55	110.70
5	C	406	GNP	O3A-PA-O1A	-3.86	99.08	110.70
5	A	406	GNP	O4'-C1'-C2'	-3.63	98.86	106.62
5	A	406	GNP	O5'-C5'-C4'	-3.32	97.68	108.99
5	A	406	GNP	O3'-C3'-C4'	-3.32	101.55	111.08
5	B	406	GNP	O1B-PB-N3B	-3.26	106.97	111.77
5	B	406	GNP	C1'-N9-C8	3.08	135.49	126.73
5	C	406	GNP	O5'-C5'-C4'	2.98	119.14	108.99
5	A	406	GNP	O2A-PA-O5'	-2.83	94.72	107.57
5	C	406	GNP	O2'-C2'-C3'	2.83	120.88	111.82
5	A	406	GNP	C3'-C2'-C1'	-2.80	96.16	101.46
5	C	406	GNP	O5'-PA-O1A	2.76	119.86	108.94
5	A	406	GNP	O3G-PG-O1G	-2.72	106.64	113.45
5	C	406	GNP	O2A-PA-O1A	2.62	124.62	112.44
5	B	406	GNP	C2'-C1'-N9	-2.51	106.26	113.25
5	B	406	GNP	O2B-PB-O3A	2.45	112.82	104.64
5	A	406	GNP	O4'-C4'-C5'	2.40	117.01	109.33
5	A	406	GNP	O2A-PA-O1A	2.40	123.59	112.44
5	B	406	GNP	C1'-N9-C4	-2.32	119.64	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	GNP	O3'-C3'-C2'	-2.12	105.02	111.82
5	C	406	GNP	N2-C2-N3	-2.12	115.54	119.67
5	A	406	GNP	O2A-PA-O3A	2.05	112.82	107.27
5	C	406	GNP	PA-O5'-C5'	2.05	133.09	121.35

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-O2B
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-O2B
5	C	406	GNP	PB-N3B-PG-O1G
5	C	406	GNP	PG-N3B-PB-O1B
5	C	406	GNP	C5'-O5'-PA-O3A
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	C3'-C4'-C5'-O5'
5	A	406	GNP	C5'-O5'-PA-O3A
5	A	406	GNP	C5'-O5'-PA-O2A
5	B	406	GNP	C5'-O5'-PA-O3A
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	C	406	GNP	C4'-C5'-O5'-PA
5	A	406	GNP	PA-O3A-PB-O1B
5	B	406	GNP	PA-O3A-PB-O1B

There are no ring outliers.

6 monomers are involved in 24 short contacts:

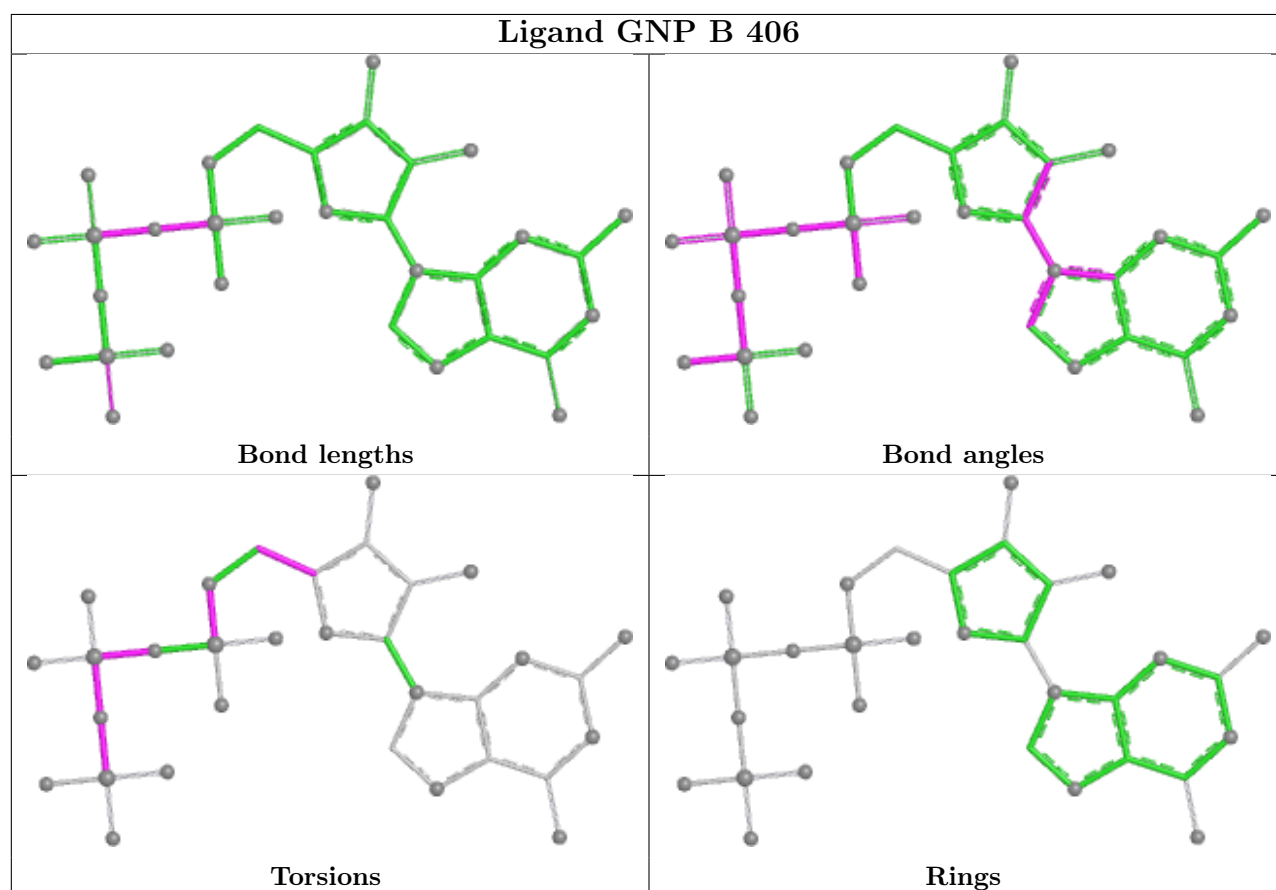
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	GNP	7	0
4	D	77	PHE	2	0

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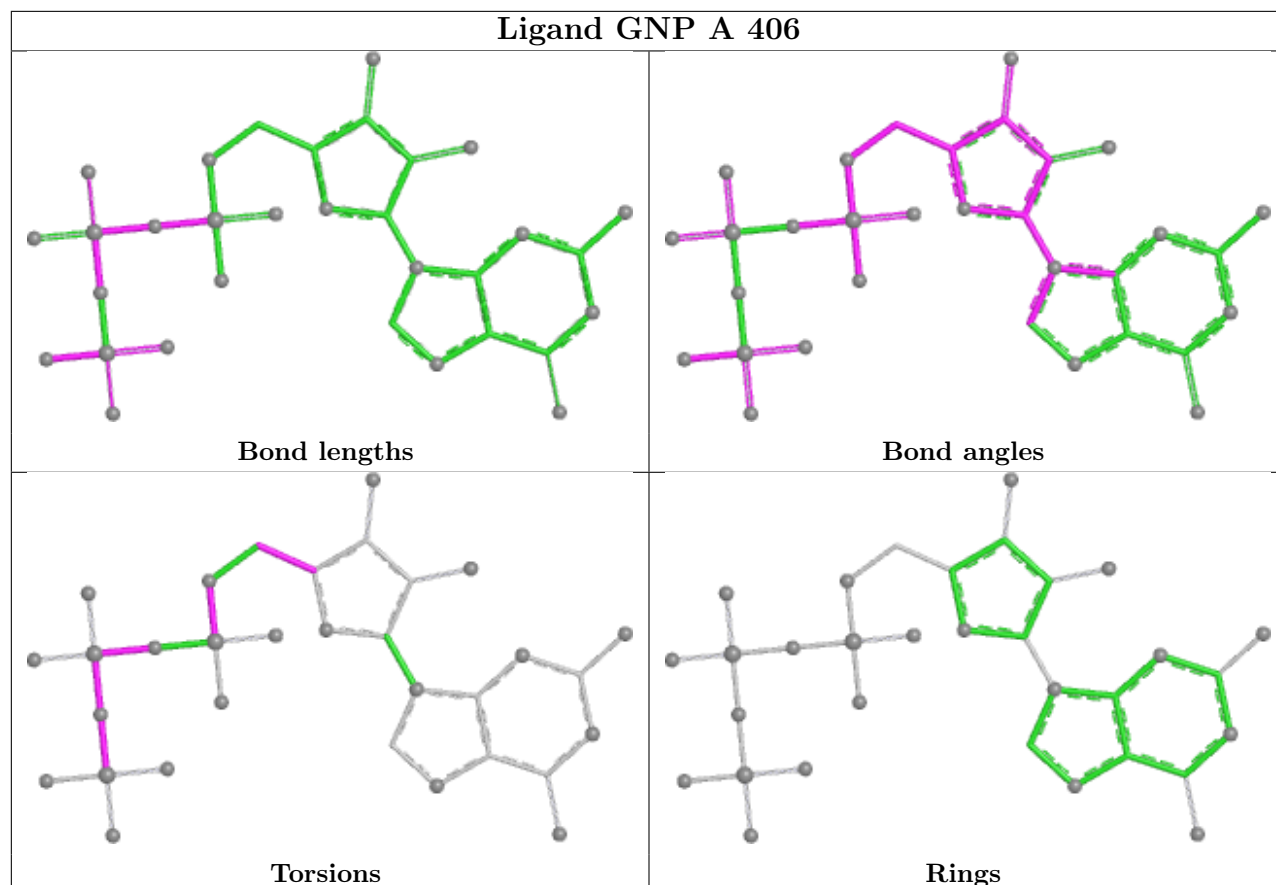
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	77	PHE	1	0
4	E	77	PHE	1	0
5	A	406	GNP	6	0
5	C	406	GNP	7	0

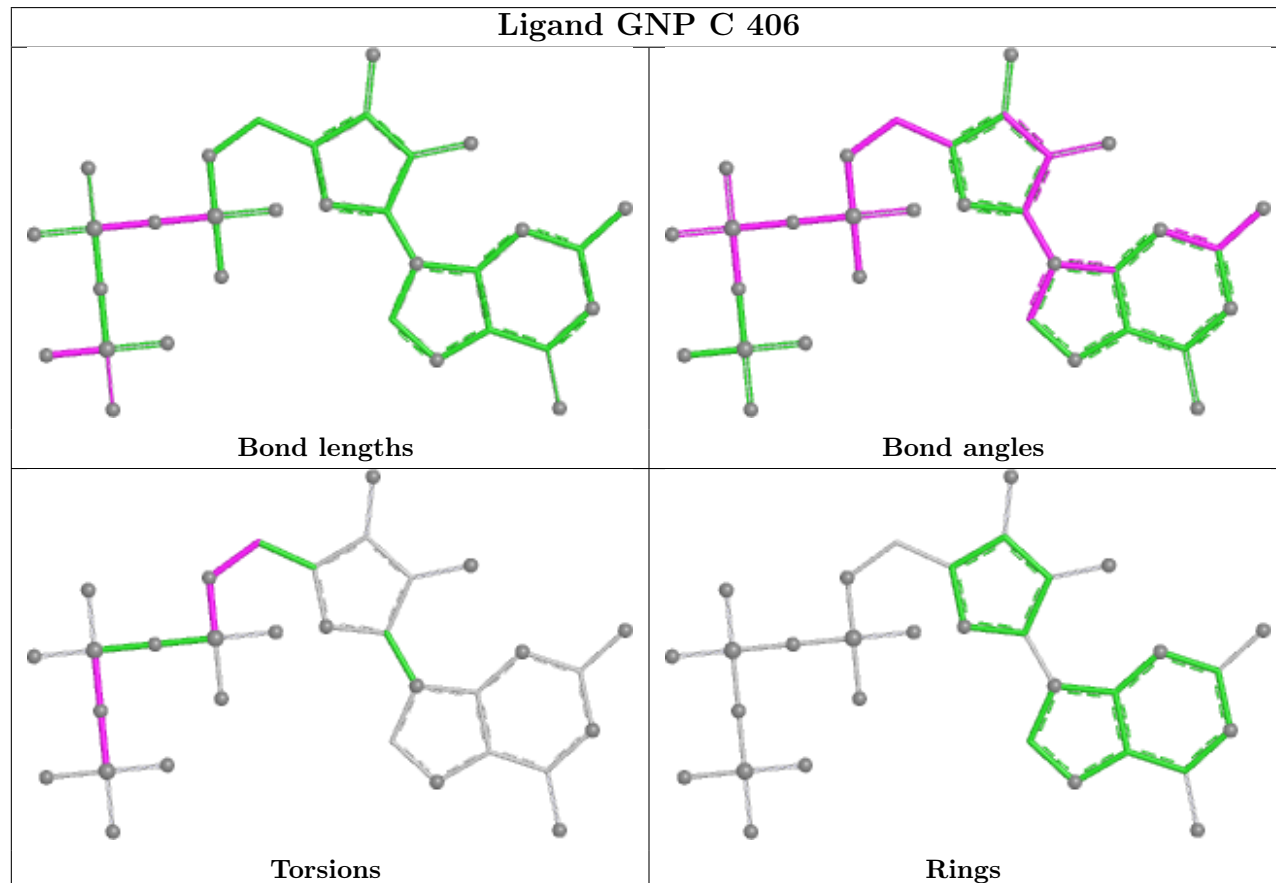
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand GNP A 406



Ligand GNP C 406



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.