



## Full wwPDB EM Validation Report ⓘ

Oct 5, 2025 – 12:16 AM JST

PDB ID : 9VMA / pdb\_00009vma  
EMDB ID : EMD-65181  
Title : Cryo-EM structure of substrate-bound DRT9 hexamer complex  
Authors : Zhang, S.; Zhang, H.  
Deposited on : 2025-06-27  
Resolution : 3.46 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

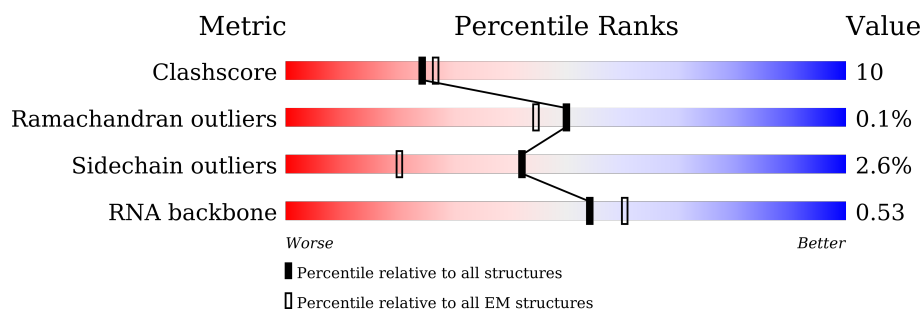
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	499	82% 17% ..
1	B	499	79% 19% ..
1	C	499	79% 20% ..
1	D	499	82% 16% ..
1	E	499	81% 18% .
1	F	499	81% 18% .
2	G	188	35% 40% 11% 13%
2	H	188	33% 43% 9% 15%

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Mol	Chain	Length	Quality of chain
2	I	188	
2	J	188	
2	K	188	
2	L	188	
3	M	4	
3	N	4	
3	O	4	
3	P	4	
3	Q	4	
3	R	4	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called RNA-dependent DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		
1	B	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		
1	C	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		
1	D	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		
1	E	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		
1	F	496	Total	C	N	O	S	0	0
			4080	2626	712	733	9		

- Molecule 2 is a RNA chain called RNA (188-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	163	Total	C	N	O	P	0	0
			3455	1543	584	1165	163		
2	H	160	Total	C	N	O	P	0	0
			3395	1516	578	1141	160		
2	I	160	Total	C	N	O	P	0	0
			3395	1516	578	1141	160		
2	J	160	Total	C	N	O	P	0	0
			3395	1516	578	1141	160		
2	K	160	Total	C	N	O	P	0	0
			3395	1516	578	1141	160		
2	L	160	Total	C	N	O	P	0	0
			3395	1516	578	1141	160		

- Molecule 3 is a DNA chain called DNA (5'-D(P\*AP\*AP\*AP\*A)-3').

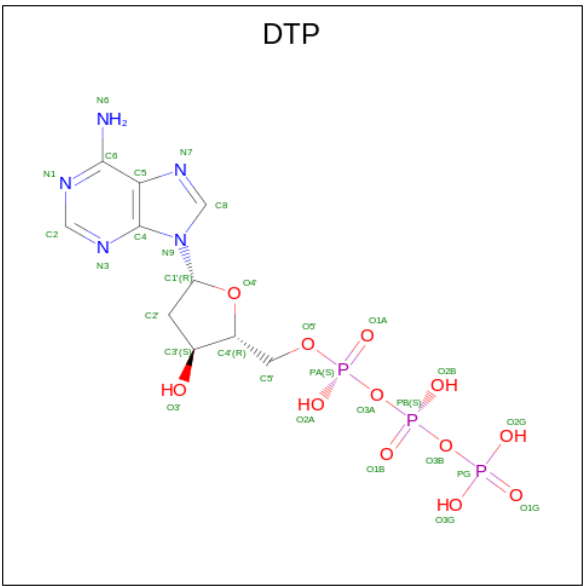
Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	4	Total	C	N	O	P	0	0
			84	40	20	20	4		
3	O	4	Total	C	N	O	P	0	0
			84	40	20	20	4		
3	P	4	Total	C	N	O	P	0	0
			84	40	20	20	4		
3	Q	4	Total	C	N	O	P	0	0
			84	40	20	20	4		
3	R	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>)



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
4	F	1	Total	C	N	O	P	0
			30	10	5	12	3	

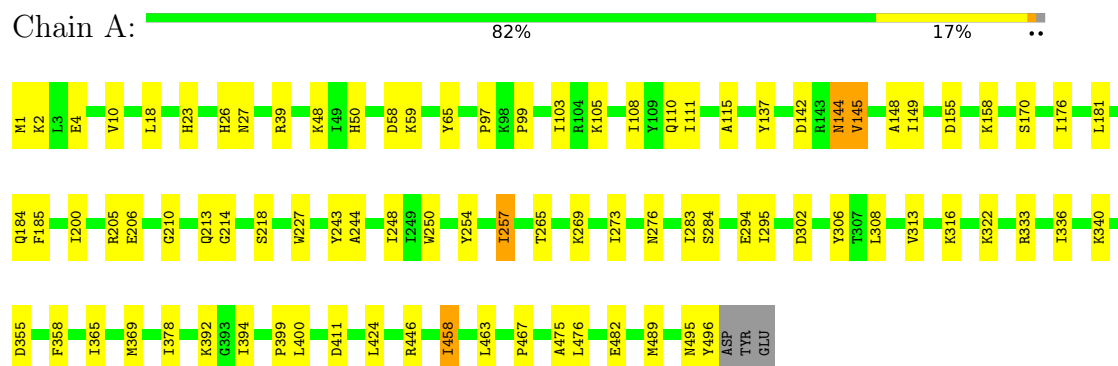
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Mg 1	0
5	B	1	Total 1	Mg 1	0
5	C	1	Total 1	Mg 1	0
5	D	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	F	1	Total 1	Mg 1	0
5	G	1	Total 1	Mg 1	0
5	H	1	Total 1	Mg 1	0
5	I	1	Total 1	Mg 1	0
5	J	1	Total 1	Mg 1	0
5	K	1	Total 1	Mg 1	0
5	L	1	Total 1	Mg 1	0

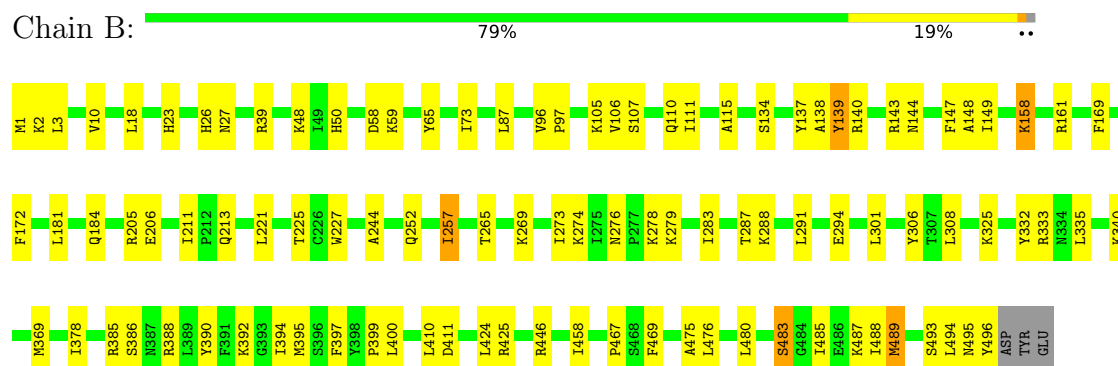
### 3 Residue-property plots

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

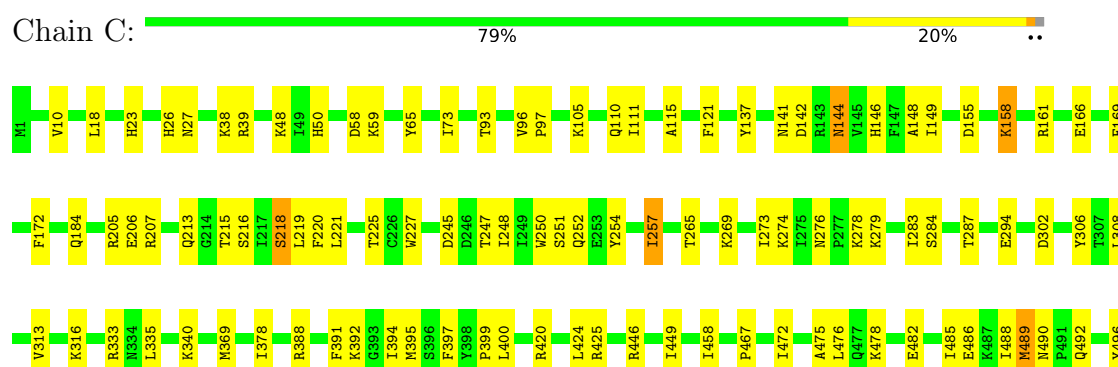
#### • Molecule 1: RNA-dependent DNA polymerase



#### • Molecule 1: RNA-dependent DNA polymerase




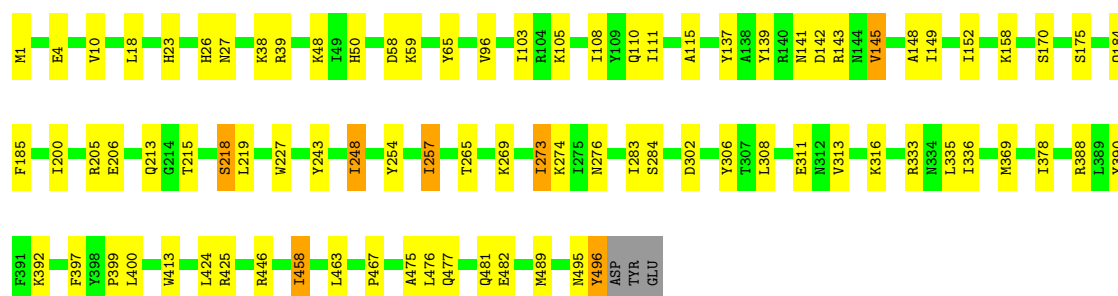
#### • Molecule 1: RNA-dependent DNA polymerase




ASP  
TYR  
GLU

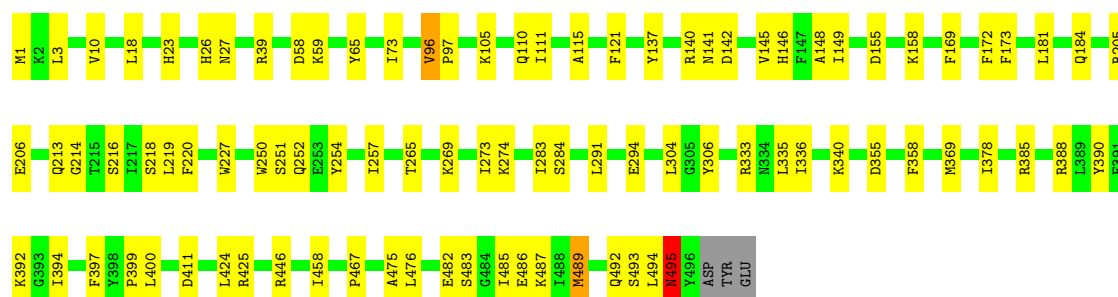
• Molecule 1: RNA-dependent DNA polymerase

Chain D:  82% 16% ..




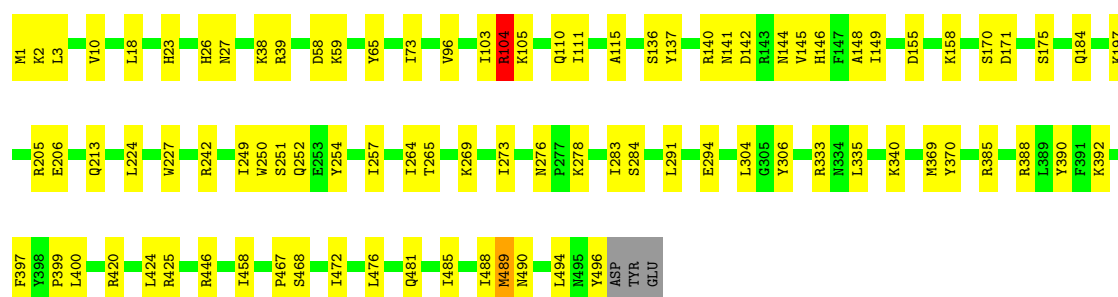
• Molecule 1: RNA-dependent DNA polymerase

Chain E:  81% 18% .



• Molecule 1: RNA-dependent DNA polymerase

Chain F:  81% 18% .

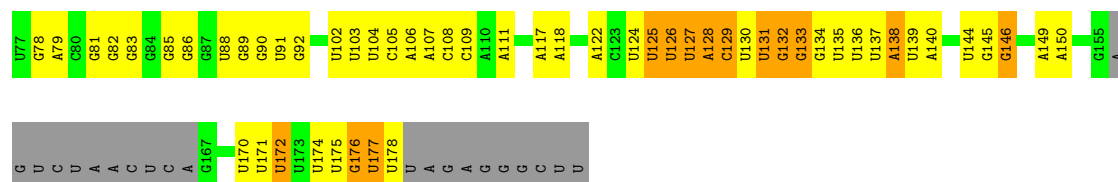


• Molecule 2: RNA (188-MER)

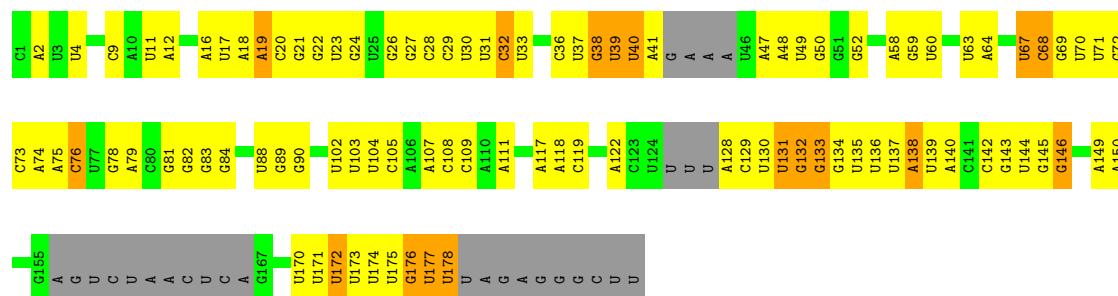
Chain G:  35% 40% 11% 13%



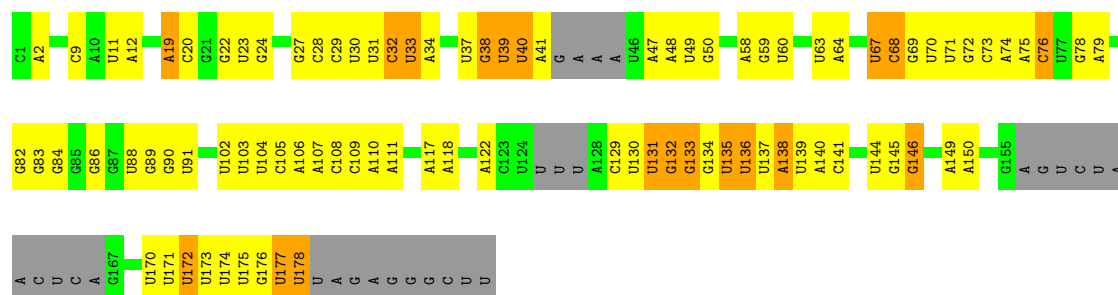
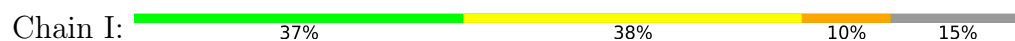




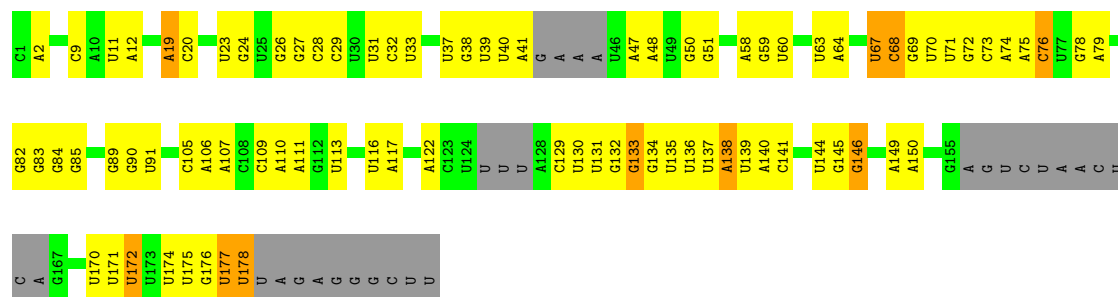
• Molecule 2: RNA (188-MER)



• Molecule 2: RNA (188-MER)

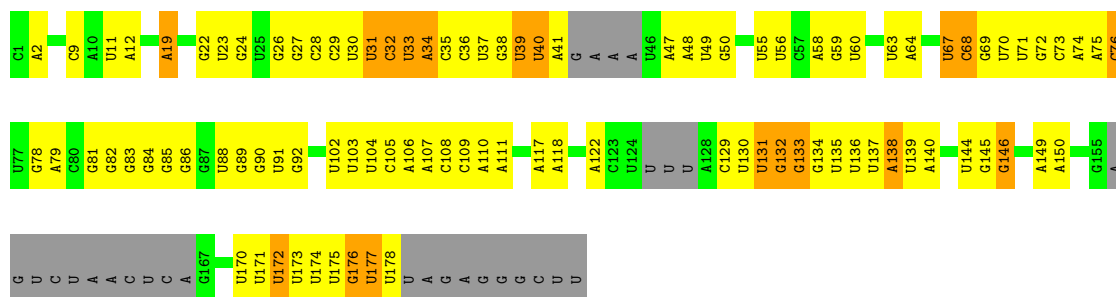


• Molecule 2: RNA (188-MER)

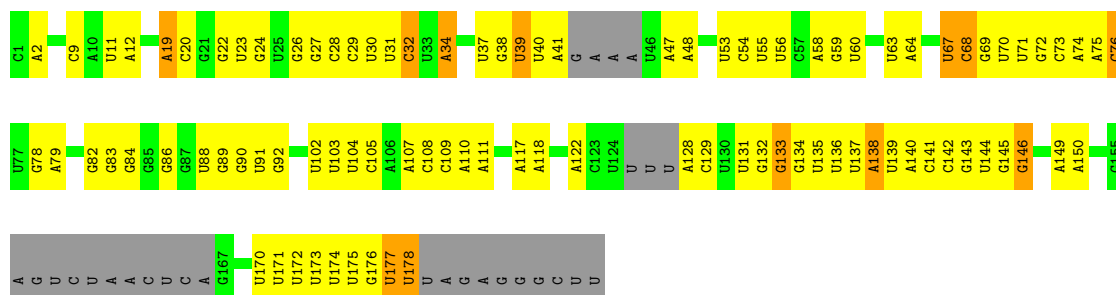
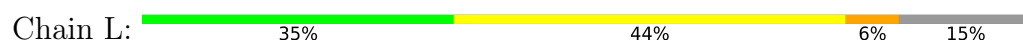


• Molecule 2: RNA (188-MER)





- Molecule 2: RNA (188-MER)



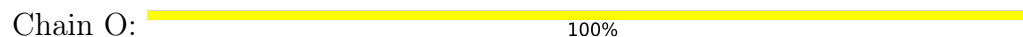
- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')



- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')




- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')



- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')



- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')

Chain Q:  25% 75%

A1  
A2  
A3  
A4

- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*A)-3')

Chain R:  100%

A1  
A2  
A3  
A4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, MG

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	A	0.24	0/4170	0.31	0/5605
1	B	0.29	0/4170	0.36	0/5605
1	C	0.28	0/4170	0.34	0/5605
1	D	0.25	0/4170	0.34	0/5605
1	E	0.25	0/4170	0.32	0/5605
1	F	0.29	0/4170	0.38	0/5605
2	G	0.37	0/3854	0.50	0/5996
2	H	0.32	0/3787	0.41	0/5890
2	I	0.34	0/3787	0.42	0/5890
2	J	0.30	0/3787	0.40	0/5890
2	K	0.33	0/3787	0.43	0/5890
2	L	0.36	0/3787	0.45	0/5890
3	M	0.65	0/95	1.06	0/144
3	N	0.65	0/95	1.21	0/144
3	O	0.60	0/95	1.11	0/144
3	P	0.63	0/95	1.04	0/144
3	Q	0.63	0/95	0.99	0/144
3	R	0.63	0/95	0.92	0/144
All	All	0.31	0/48379	0.41	0/69940

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	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ARG	Sidechain
1	F	104	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4080	0	4147	58	0
1	B	4080	0	4147	79	0
1	C	4080	0	4147	74	0
1	D	4080	0	4147	57	0
1	E	4080	0	4147	65	0
1	F	4080	0	4146	67	0
2	G	3455	0	1739	81	0
2	H	3395	0	1710	91	0
2	I	3395	0	1710	84	0
2	J	3395	0	1710	66	0
2	K	3395	0	1710	79	0
2	L	3395	0	1710	73	0
3	M	84	0	45	3	0
3	N	84	0	45	2	0
3	O	84	0	45	5	0
3	P	84	0	45	8	0
3	Q	84	0	45	5	0
3	R	84	0	45	6	0
4	A	30	0	12	3	0
4	B	30	0	12	0	0
4	C	30	0	12	1	0
4	D	30	0	12	0	0
4	E	30	0	12	5	0
4	F	30	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	45606	0	35512	815	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 10.

All (815) 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:F:399:PRO:HB3	1:F:488:ILE:HG21	1.26	1.10
1:B:399:PRO:HB3	1:B:488:ILE:HG21	1.30	1.09
2:K:63:U:H3	2:K:72:G:H1	1.14	0.96
2:L:63:U:H3	2:L:72:G:H1	1.14	0.93
2:H:63:U:H3	2:H:72:G:H1	1.17	0.92
2:I:63:U:H3	2:I:72:G:H1	1.17	0.92
2:J:37:U:H3	2:J:50:G:H1	1.17	0.91
2:K:86:G:H1	2:K:103:U:H3	1.18	0.91
1:C:146:HIS:CE1	1:C:489:MET:CB	2.55	0.90
2:G:86:G:H1	2:G:103:U:H3	1.20	0.89
2:J:63:U:H3	2:J:72:G:H1	1.17	0.89
1:B:399:PRO:CB	1:B:488:ILE:HG21	2.06	0.85
1:F:399:PRO:CB	1:F:488:ILE:HG21	2.06	0.85
2:L:86:G:H1	2:L:103:U:H3	1.25	0.84
1:F:399:PRO:HB3	1:F:488:ILE:CG2	2.11	0.77
2:H:19:A:H2	2:H:143:G:H22	1.32	0.77
2:I:86:G:H1	2:I:103:U:H3	1.30	0.77
1:C:146:HIS:HE1	1:C:489:MET:HB2	1.50	0.77
1:E:206:GLU:N	1:E:206:GLU:OE1	2.18	0.76
1:B:147:PHE:CE1	1:B:485:ILE:HG21	2.20	0.76
1:B:399:PRO:HB3	1:B:488:ILE:CG2	2.13	0.76
1:C:146:HIS:CE1	1:C:489:MET:HB2	2.19	0.76
1:C:146:HIS:HE1	1:C:489:MET:CB	1.95	0.76
1:B:206:GLU:N	1:B:206:GLU:OE2	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:OE1	1:A:206:GLU:N	2.20	0.75
1:F:206:GLU:N	1:F:206:GLU:OE1	2.19	0.75
1:E:446:ARG:NH2	2:K:82:G:OP2	2.21	0.74
1:A:446:ARG:NH2	2:G:82:G:OP2	2.21	0.74
1:B:105:LYS:HE2	1:B:105:LYS:HA	1.69	0.74
1:F:446:ARG:NH2	2:L:82:G:OP2	2.20	0.74
1:C:446:ARG:NH2	2:I:82:G:OP2	2.21	0.74
1:B:446:ARG:NH2	2:H:82:G:OP2	2.21	0.73
1:C:39:ARG:NH1	1:C:333:ARG:O	2.22	0.73
2:H:146:G:H1	2:H:174:U:H3	0.80	0.73
2:L:144:U:H3	2:L:176:G:H22	1.34	0.73
1:D:446:ARG:NH2	2:J:82:G:OP2	2.21	0.73
1:B:39:ARG:NH1	1:B:333:ARG:O	2.22	0.72
1:B:138:ALA:HB2	1:B:244:ALA:H	1.56	0.70
2:H:22:G:H1	2:H:140:A:H2	1.38	0.69
1:F:144:ASN:ND2	1:F:489:MET:SD	2.66	0.69
1:F:105:LYS:O	1:F:213:GLN:NE2	2.25	0.69
2:L:175:U:H2'	2:L:176:G:C8	2.26	0.69
1:A:399:PRO:HA	1:A:476:LEU:HD13	1.75	0.69
1:B:137:TYR:HA	1:B:143:ARG:HB3	1.75	0.69
2:J:144:U:H3	2:J:176:G:H22	1.38	0.69
1:F:105:LYS:HA	1:F:105:LYS:HE2	1.74	0.68
2:I:22:G:H1	2:I:140:A:H2	1.41	0.68
1:F:399:PRO:HA	1:F:476:LEU:HD13	1.75	0.68
1:E:399:PRO:HA	1:E:476:LEU:HD13	1.74	0.68
1:D:399:PRO:HA	1:D:476:LEU:HD13	1.76	0.68
2:H:144:U:H3	2:H:176:G:H22	1.41	0.68
2:L:146:G:H1	2:L:174:U:H3	0.77	0.67
1:B:184:GLN:OE1	1:B:227:TRP:NE1	2.28	0.67
1:D:219:LEU:HD21	3:P:3:DA:H2	1.58	0.67
1:F:96:VAL:HG13	1:F:104:ARG:HB3	1.75	0.67
1:C:206:GLU:OE2	1:C:206:GLU:N	2.28	0.67
2:J:141:C:H41	2:J:178:U:H5	1.42	0.67
1:D:206:GLU:OE1	1:D:206:GLU:N	2.27	0.66
2:G:175:U:H2'	2:G:176:G:C8	2.30	0.66
1:E:39:ARG:NH1	1:E:333:ARG:O	2.29	0.66
1:F:39:ARG:NH1	1:F:333:ARG:O	2.28	0.66
1:D:108:ILE:HG12	3:P:4:DA:H4'	1.77	0.66
2:H:176:G:O2'	2:H:177:U:OP1	2.13	0.66
1:A:184:GLN:OE1	1:A:227:TRP:NE1	2.28	0.66
2:I:47:A:H2'	2:I:48:A:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:HG23	1:D:283:ILE:HD13	1.78	0.66
1:C:184:GLN:OE1	1:C:227:TRP:NE1	2.26	0.66
1:C:395:MET:HE3	1:C:476:LEU:HD22	1.77	0.65
2:I:146:G:H1	2:I:174:U:H3	0.75	0.65
1:C:391:PHE:CD2	1:C:488:ILE:HD12	2.32	0.65
1:C:141:ASN:HA	3:O:1:DA:H4'	1.78	0.65
1:B:147:PHE:CE1	1:B:485:ILE:CG2	2.80	0.65
1:A:257:ILE:HG23	1:A:283:ILE:HD13	1.78	0.65
1:F:10:VAL:HG12	1:F:115:ALA:HB1	1.79	0.65
1:A:39:ARG:NH1	1:A:333:ARG:O	2.30	0.64
2:I:37:U:H2'	2:I:38:G:H8	1.62	0.64
1:D:184:GLN:OE1	1:D:227:TRP:NE1	2.29	0.64
1:E:10:VAL:HG12	1:E:115:ALA:HB1	1.79	0.64
1:B:388:ARG:HD2	2:H:32:C:C2	2.32	0.64
1:B:257:ILE:HG23	1:B:283:ILE:HD13	1.80	0.64
1:C:257:ILE:HG23	1:C:283:ILE:HD13	1.79	0.64
2:G:47:A:H2'	2:G:48:A:C8	2.32	0.64
1:C:478:LYS:HE3	1:C:482:GLU:OE2	1.97	0.64
1:D:105:LYS:O	1:D:213:GLN:NE2	2.30	0.64
1:C:399:PRO:HA	1:C:476:LEU:HD23	1.80	0.64
2:K:146:G:H1	2:K:174:U:H3	0.76	0.64
1:A:10:VAL:HG12	1:A:115:ALA:HB1	1.80	0.63
2:J:47:A:H2'	2:J:48:A:C8	2.34	0.63
1:B:147:PHE:HE1	1:B:485:ILE:CG2	2.11	0.63
2:G:23:U:H2'	2:G:24:G:H8	1.64	0.63
2:G:144:U:H3	2:G:176:G:H22	1.46	0.63
1:C:10:VAL:HG12	1:C:115:ALA:HB1	1.80	0.63
1:D:105:LYS:HE3	1:D:105:LYS:HA	1.80	0.63
2:J:37:U:O2	2:J:50:G:N2	2.24	0.63
1:E:257:ILE:HG23	1:E:283:ILE:HD13	1.81	0.62
2:L:23:U:H2'	2:L:24:G:H8	1.65	0.62
1:E:214:GLY:HA2	3:Q:4:DA:H62	1.65	0.62
1:B:10:VAL:HG12	1:B:115:ALA:HB1	1.80	0.62
1:D:10:VAL:HG12	1:D:115:ALA:HB1	1.80	0.62
2:H:20:C:H41	2:H:177:U:H1'	1.65	0.62
2:I:141:C:H41	2:I:178:U:H5	1.45	0.62
2:I:144:U:H3	2:I:176:G:H22	1.47	0.62
1:A:99:PRO:HD2	2:G:124:U:H3'	1.81	0.62
2:K:23:U:H2'	2:K:24:G:H8	1.65	0.61
1:F:149:ILE:HG12	1:F:306:TYR:CD1	2.36	0.61
1:F:257:ILE:HG23	1:F:283:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:U:H2'	2:G:24:G:C8	2.36	0.61
2:H:23:U:H2'	2:H:24:G:C8	2.36	0.60
2:I:23:U:H2'	2:I:24:G:H8	1.65	0.60
2:J:175:U:H2'	2:J:176:G:C8	2.36	0.60
1:B:1:MET:HE2	1:B:3:LEU:H	1.66	0.60
1:E:146:HIS:ND1	1:E:489:MET:HG2	2.16	0.60
2:G:37:U:H2'	2:G:38:G:H8	1.67	0.60
2:L:23:U:H2'	2:L:24:G:C8	2.36	0.60
1:E:184:GLN:OE1	1:E:227:TRP:NE1	2.34	0.60
2:H:23:U:H2'	2:H:24:G:H8	1.65	0.60
2:K:23:U:H2'	2:K:24:G:C8	2.37	0.60
2:G:67:U:H5''	2:G:68:C:H5	1.66	0.60
2:I:23:U:H2'	2:I:24:G:C8	2.36	0.60
1:B:480:LEU:CD2	1:B:488:ILE:HG13	2.32	0.60
2:G:39:U:H2'	2:G:40:U:C6	2.36	0.60
2:L:146:G:O6	2:L:174:U:O4	2.20	0.60
2:I:39:U:H2'	2:I:40:U:C6	2.37	0.59
1:E:486:GLU:O	1:E:489:MET:HE2	2.02	0.59
1:D:149:ILE:HG12	1:D:306:TYR:CD1	2.37	0.59
1:B:149:ILE:HG12	1:B:306:TYR:CD1	2.38	0.59
1:A:23:HIS:HA	1:A:26:HIS:CD2	2.38	0.59
1:C:149:ILE:HG12	1:C:306:TYR:CD1	2.38	0.59
2:J:39:U:H2'	2:J:40:U:C6	2.38	0.59
2:H:146:G:O6	2:H:174:U:O4	2.20	0.59
2:K:39:U:H2'	2:K:40:U:C6	2.38	0.59
1:C:58:ASP:OD2	1:C:110:GLN:NE2	2.36	0.59
1:B:269:LYS:NZ	1:D:158:LYS:O	2.36	0.58
1:C:23:HIS:HA	1:C:26:HIS:CD2	2.38	0.58
1:B:144:ASN:ND2	1:B:489:MET:SD	2.76	0.58
1:F:385:ARG:HD3	2:L:34:A:C8	2.38	0.58
1:D:39:ARG:NH1	1:D:333:ARG:O	2.34	0.58
2:I:146:G:O6	2:I:174:U:O4	2.22	0.58
1:B:58:ASP:OD2	1:B:110:GLN:NE2	2.36	0.58
1:E:485:ILE:HG22	1:E:489:MET:SD	2.43	0.58
1:F:146:HIS:CE1	1:F:489:MET:HB3	2.37	0.58
1:F:171:ASP:O	1:F:175:SER:OG	2.20	0.58
2:I:175:U:H2'	2:I:176:G:C8	2.39	0.58
2:J:23:U:H2'	2:J:24:G:H8	1.67	0.58
4:E:501:DTP:H5'1	4:E:501:DTP:H8	1.86	0.58
2:H:39:U:H2'	2:H:40:U:C6	2.38	0.58
1:F:23:HIS:HA	1:F:26:HIS:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:23:U:H2'	2:J:24:G:C8	2.38	0.57
1:A:158:LYS:O	1:C:269:LYS:NZ	2.36	0.57
1:D:23:HIS:HA	1:D:26:HIS:CD2	2.39	0.57
1:D:58:ASP:OD2	1:D:110:GLN:NE2	2.38	0.57
2:I:27:G:N1	2:I:136:U:N3	2.52	0.57
1:A:58:ASP:OD2	1:A:110:GLN:NE2	2.38	0.57
2:K:67:U:H5''	2:K:68:C:H5	1.70	0.57
1:F:205:ARG:O	2:K:67:U:N3	2.38	0.57
2:G:124:U:N3	2:G:128:A:OP2	2.36	0.57
2:H:29:C:H2'	2:H:30:U:C6	2.40	0.57
2:H:67:U:H5''	2:H:68:C:H5	1.69	0.57
2:L:67:U:H5''	2:L:68:C:H5	1.70	0.57
1:B:23:HIS:HA	1:B:26:HIS:CD2	2.38	0.57
2:K:37:U:H2'	2:K:38:G:H8	1.69	0.57
1:B:158:LYS:O	1:F:269:LYS:NZ	2.37	0.57
2:K:146:G:O6	2:K:174:U:O4	2.21	0.57
1:A:149:ILE:HG12	1:A:306:TYR:CD2	2.39	0.57
1:E:205:ARG:O	2:L:67:U:N3	2.38	0.57
1:E:485:ILE:O	1:E:489:MET:HG3	2.04	0.57
2:I:47:A:H2'	2:I:48:A:H8	1.69	0.57
1:E:23:HIS:HA	1:E:26:HIS:CD2	2.39	0.57
1:E:149:ILE:HG12	1:E:306:TYR:CD2	2.40	0.57
1:F:58:ASP:OD2	1:F:110:GLN:NE2	2.38	0.57
1:B:105:LYS:O	1:B:213:GLN:NE2	2.35	0.56
1:A:205:ARG:O	2:H:67:U:N3	2.39	0.56
2:H:37:U:H2'	2:H:38:G:H8	1.68	0.56
2:H:47:A:H2'	2:H:48:A:C8	2.41	0.56
2:I:67:U:H5''	2:I:68:C:H5	1.70	0.56
2:K:47:A:H2'	2:K:48:A:C8	2.40	0.56
1:E:58:ASP:OD2	1:E:110:GLN:NE2	2.38	0.56
2:G:26:G:H2'	2:G:27:G:H8	1.71	0.56
1:F:184:GLN:OE1	1:F:227:TRP:NE1	2.36	0.56
1:C:146:HIS:CE1	1:C:489:MET:HB3	2.38	0.56
1:A:355:ASP:OD1	1:A:358:PHE:N	2.30	0.56
1:D:269:LYS:NZ	1:F:158:LYS:O	2.38	0.56
2:J:67:U:H5''	2:J:68:C:H5	1.70	0.56
1:B:480:LEU:HD23	1:B:488:ILE:HG13	1.87	0.55
1:E:385:ARG:HD3	2:K:34:A:C8	2.41	0.55
2:L:37:U:H2'	2:L:38:G:H8	1.70	0.55
1:A:269:LYS:NZ	1:E:158:LYS:O	2.37	0.55
1:B:169:PHE:HB2	1:B:172:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:ARG:HD2	2:K:32:C:N3	2.21	0.55
2:L:175:U:H2'	2:L:176:G:H8	1.67	0.55
1:F:224:LEU:O	1:F:227:TRP:HD1	1.89	0.55
2:K:175:U:H2'	2:K:176:G:C8	2.41	0.55
1:C:205:ARG:O	2:J:67:U:N3	2.40	0.55
2:L:26:G:H2'	2:L:27:G:H8	1.71	0.55
2:J:26:G:H2'	2:J:27:G:H8	1.71	0.55
3:P:3:DA:H2''	3:P:4:DA:H3'	1.88	0.55
3:R:2:DA:H1'	3:R:3:DA:N7	2.21	0.55
1:E:105:LYS:O	1:E:213:GLN:NE2	2.40	0.55
2:G:47:A:H2'	2:G:48:A:H8	1.72	0.55
2:G:71:U:H2'	2:G:72:G:H8	1.72	0.55
2:G:175:U:H2'	2:G:176:G:H8	1.72	0.55
1:C:213:GLN:OE1	4:C:501:DTP:H2'2	2.07	0.54
2:I:88:U:H2'	2:I:89:G:H8	1.71	0.54
1:D:495:ASN:O	1:D:496:TYR:C	2.50	0.54
1:B:147:PHE:CD1	1:B:485:ILE:HG21	2.42	0.54
1:C:158:LYS:O	1:E:269:LYS:NZ	2.37	0.54
1:E:355:ASP:OD1	1:E:358:PHE:N	2.33	0.54
2:L:39:U:H2'	2:L:40:U:C6	2.43	0.54
1:F:388:ARG:HD2	2:L:32:C:C6	2.42	0.54
2:K:29:C:H2'	2:K:30:U:C6	2.44	0.54
1:D:205:ARG:O	2:I:67:U:N3	2.41	0.53
1:D:369:MET:CE	1:D:467:PRO:HB2	2.37	0.53
1:B:483:SER:HB3	1:B:487:LYS:HG3	1.90	0.53
2:J:85:G:O6	2:J:105:C:N4	2.41	0.53
1:C:155:ASP:OD2	1:C:250:TRP:NE1	2.31	0.53
1:F:340:LYS:NZ	2:L:118:A:OP1	2.33	0.53
1:E:340:LYS:NZ	2:K:118:A:OP1	2.33	0.53
1:E:96:VAL:HG22	1:E:97:PRO:HD2	1.91	0.53
2:H:28:C:H2'	2:H:29:C:C6	2.43	0.53
1:F:390:TYR:HD1	1:F:392:LYS:HG2	1.74	0.53
2:I:29:C:H2'	2:I:30:U:C6	2.43	0.53
2:J:174:U:H2'	2:J:175:U:C6	2.44	0.53
1:A:99:PRO:CD	2:G:124:U:H3'	2.39	0.53
1:D:175:SER:OG	1:D:273:ILE:HG22	2.09	0.53
1:E:369:MET:SD	1:E:467:PRO:HB2	2.49	0.53
2:G:174:U:H2'	2:G:175:U:C6	2.44	0.52
2:K:38:G:N3	2:K:38:G:H2'	2.24	0.52
2:L:88:U:H2'	2:L:89:G:H8	1.74	0.52
3:P:3:DA:C8	3:P:4:DA:H2'	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:PHE:HE1	1:F:494:LEU:CB	2.22	0.52
2:H:38:G:N3	2:H:38:G:H2'	2.25	0.52
2:H:88:U:H2'	2:H:89:G:H8	1.74	0.52
2:K:28:C:H2'	2:K:29:C:C6	2.44	0.52
1:A:144:ASN:OD1	1:A:144:ASN:N	2.43	0.52
2:I:28:C:H2'	2:I:29:C:C6	2.44	0.52
1:C:392:LYS:HZ1	2:I:131:U:H5'	1.75	0.52
2:G:22:G:H1	2:G:140:A:H2	1.58	0.52
2:K:88:U:H2'	2:K:89:G:H8	1.75	0.52
1:A:99:PRO:HG2	2:G:124:U:H5''	1.92	0.52
1:B:205:ARG:HB3	2:G:67:U:H3	1.75	0.52
2:G:71:U:H2'	2:G:72:G:C8	2.45	0.52
2:G:63:U:H2'	2:G:64:A:C8	2.45	0.52
1:C:388:ARG:HD2	2:I:32:C:N3	2.25	0.52
1:E:27:ASN:ND2	2:K:23:U:O4'	2.43	0.52
1:F:27:ASN:ND2	2:L:23:U:O4'	2.43	0.52
1:C:369:MET:SD	1:C:467:PRO:HB2	2.50	0.52
1:E:494:LEU:O	1:E:495:ASN:C	2.52	0.52
1:F:494:LEU:HA	2:L:128:A:O2'	2.10	0.52
2:H:129:C:O2'	2:H:130:U:O4'	2.21	0.51
2:J:171:U:H2'	2:J:172:U:H6	1.75	0.51
1:B:27:ASN:ND2	2:H:23:U:O4'	2.43	0.51
1:B:340:LYS:NZ	2:H:118:A:OP1	2.32	0.51
1:F:144:ASN:HD21	3:R:2:DA:H62	1.58	0.51
1:C:27:ASN:ND2	2:I:23:U:O4'	2.42	0.51
1:C:340:LYS:NZ	2:I:118:A:OP1	2.32	0.51
2:K:129:C:O2'	2:K:130:U:O4'	2.20	0.51
1:A:369:MET:SD	1:A:467:PRO:HB2	2.51	0.51
2:G:88:U:H2'	2:G:89:G:H8	1.76	0.51
2:I:171:U:H2'	2:I:172:U:H6	1.76	0.51
2:J:106:A:O2'	2:J:107:A:H5''	2.11	0.51
2:K:171:U:H2'	2:K:172:U:H6	1.76	0.51
2:L:38:G:N3	2:L:38:G:H2'	2.25	0.51
2:H:103:U:H2'	2:H:104:U:H6	1.76	0.51
2:H:142:C:H2'	2:H:143:G:C8	2.45	0.51
2:J:89:G:H2'	2:J:90:G:H8	1.75	0.51
1:F:369:MET:HE3	1:F:467:PRO:HB2	1.93	0.51
2:G:171:U:H2'	2:G:172:U:H6	1.76	0.51
3:R:4:DA:H8	3:R:4:DA:H5''	1.76	0.51
2:L:142:C:H2'	2:L:143:G:C8	2.46	0.51
2:L:171:U:H2'	2:L:172:U:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:O	1:A:213:GLN:NE2	2.43	0.51
1:B:369:MET:SD	1:B:467:PRO:HB2	2.51	0.51
1:D:27:ASN:ND2	2:J:23:U:O4'	2.43	0.51
2:H:174:U:H2'	2:H:175:U:H6	1.75	0.51
1:A:244:ALA:HB3	2:G:126:U:O4	2.11	0.50
1:C:105:LYS:O	1:C:213:GLN:NE2	2.44	0.50
2:G:38:G:H2'	2:G:38:G:N3	2.26	0.50
2:J:89:G:H2'	2:J:90:G:C8	2.46	0.50
1:A:27:ASN:ND2	2:G:23:U:O4'	2.43	0.50
2:G:28:C:H2'	2:G:29:C:C6	2.46	0.50
3:O:2:DA:H2''	3:O:3:DA:H5''	1.93	0.50
2:H:146:G:N2	2:H:174:U:O2	2.34	0.50
1:A:145:VAL:HG12	1:A:243:TYR:CE1	2.47	0.50
1:B:424:LEU:HD22	2:H:107:A:H5'	1.94	0.50
4:E:501:DTP:N1	3:Q:4:DA:N6	2.60	0.50
2:G:63:U:H2'	2:G:64:A:H8	1.76	0.50
2:J:28:C:H2'	2:J:29:C:C6	2.47	0.50
1:B:48:LYS:HG3	1:B:50:HIS:NE2	2.27	0.50
2:K:49:U:H2'	2:K:50:G:H8	1.77	0.50
2:J:24:G:H22	2:J:138:A:H2	1.59	0.50
4:A:501:DTP:C8	4:A:501:DTP:H5'1	2.41	0.50
1:C:48:LYS:HG3	1:C:50:HIS:NE2	2.27	0.50
2:H:49:U:H2'	2:H:50:G:H8	1.77	0.49
1:A:170:SER:HA	1:A:276:ASN:HB2	1.94	0.49
1:D:145:VAL:HG12	1:D:243:TYR:CE1	2.47	0.49
1:F:1:MET:HE1	1:F:3:LEU:HB3	1.94	0.49
2:G:129:C:H2'	2:G:130:U:C6	2.47	0.49
1:D:458:ILE:HG23	1:D:463:LEU:HD13	1.94	0.49
2:L:73:C:H2'	2:L:74:A:C8	2.48	0.49
2:L:109:C:OP2	2:L:110:A:O2'	2.22	0.49
2:G:31:U:H2'	2:G:32:C:O2	2.12	0.49
2:G:145:G:H3'	2:G:146:G:H8	1.78	0.49
1:A:108:ILE:HG12	3:M:4:DA:H2''	1.94	0.49
1:C:369:MET:HA	1:C:394:ILE:HG22	1.95	0.49
1:D:219:LEU:HD21	3:P:3:DA:C2	2.45	0.49
2:H:171:U:H2'	2:H:172:U:H6	1.76	0.49
2:K:131:U:H4'	2:K:132:G:OP2	2.11	0.49
2:H:19:A:C5	2:H:176:G:N2	2.81	0.49
2:K:22:G:H1	2:K:140:A:H2	1.61	0.49
2:K:47:A:H2'	2:K:48:A:H8	1.77	0.49
2:K:73:C:H2'	2:K:74:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:73:C:H2'	2:L:74:A:H8	1.78	0.49
1:A:340:LYS:NZ	2:G:118:A:OP1	2.33	0.49
1:B:278:LYS:HD2	1:B:279:LYS:HG2	1.95	0.49
1:F:140:ARG:NH2	1:F:142:ASP:OD2	2.43	0.49
2:I:24:G:H22	2:I:138:A:H2	1.61	0.49
2:I:49:U:H2'	2:I:50:G:C8	2.47	0.49
2:I:108:C:H2'	2:I:109:C:C6	2.47	0.49
2:L:63:U:O2	2:L:72:G:N2	2.35	0.49
1:C:420:ARG:NH2	2:I:82:G:O6	2.41	0.49
2:H:63:U:H2'	2:H:64:A:H8	1.78	0.49
2:I:63:U:H2'	2:I:64:A:H8	1.78	0.49
2:K:63:U:H2'	2:K:64:A:H8	1.78	0.49
2:K:171:U:H2'	2:K:172:U:C6	2.48	0.49
3:O:3:DA:H1'	3:O:4:DA:H5'	1.94	0.49
1:D:215:THR:O	1:D:218:SER:OG	2.29	0.49
2:H:84:G:H1	2:H:105:C:H42	1.60	0.49
2:J:171:U:H2'	2:J:172:U:C6	2.48	0.49
1:A:142:ASP:N	1:A:142:ASP:OD1	2.46	0.49
1:B:134:SER:HB2	1:B:143:ARG:HH21	1.78	0.49
2:G:24:G:H22	2:G:138:A:H2	1.60	0.49
2:G:64:A:C6	2:G:72:G:C6	3.01	0.49
2:I:171:U:H2'	2:I:172:U:C6	2.48	0.49
2:I:175:U:H2'	2:I:176:G:H8	1.77	0.49
2:J:73:C:H2'	2:J:74:A:H8	1.78	0.49
1:B:385:ARG:HG2	2:H:33:U:H1'	1.94	0.48
1:D:388:ARG:NH1	2:J:31:U:O2	2.46	0.48
1:E:141:ASN:HA	3:Q:1:DA:H4'	1.94	0.48
2:J:71:U:H2'	2:J:72:G:H8	1.77	0.48
2:L:63:U:H2'	2:L:64:A:H8	1.79	0.48
1:A:48:LYS:HE3	1:A:50:HIS:NE2	2.28	0.48
2:I:38:G:N3	2:I:38:G:H2'	2.27	0.48
2:J:175:U:H2'	2:J:176:G:H8	1.77	0.48
2:K:73:C:H2'	2:K:74:A:C8	2.48	0.48
2:H:24:G:H22	2:H:138:A:H2	1.62	0.48
2:I:32:C:H1'	2:I:33:U:C5	2.48	0.48
2:J:38:G:N3	2:J:38:G:H2'	2.28	0.48
2:J:47:A:H2'	2:J:48:A:H8	1.78	0.48
2:L:108:C:H2'	2:L:109:C:C6	2.48	0.48
4:A:501:DTP:H5'2	2:G:126:U:H3	1.79	0.48
2:H:47:A:H2'	2:H:48:A:H8	1.78	0.48
2:H:171:U:H2'	2:H:172:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:G:C2	2:I:136:U:C2	3.01	0.48
2:I:73:C:H2'	2:I:74:A:H8	1.79	0.48
1:F:335:LEU:O	1:F:425:ARG:NH1	2.46	0.48
1:F:369:MET:CE	1:F:467:PRO:HB2	2.43	0.48
2:H:73:C:H2'	2:H:74:A:H8	1.79	0.48
2:H:139:U:H2'	2:H:140:A:O4'	2.13	0.48
2:J:82:G:H2'	2:J:83:G:O4'	2.14	0.48
1:C:278:LYS:HD2	1:C:279:LYS:HG2	1.96	0.48
2:G:108:C:H2'	2:G:109:C:C6	2.49	0.48
2:I:73:C:H2'	2:I:74:A:C8	2.49	0.48
2:I:139:U:H2'	2:I:140:A:O4'	2.13	0.48
2:K:24:G:H22	2:K:138:A:H2	1.62	0.48
1:E:18:LEU:HD12	1:E:111:ILE:HD11	1.95	0.48
2:G:171:U:H2'	2:G:172:U:C6	2.48	0.48
2:J:73:C:H2'	2:J:74:A:C8	2.49	0.48
1:D:142:ASP:OD1	1:D:142:ASP:N	2.46	0.48
1:E:369:MET:HA	1:E:394:ILE:HG22	1.96	0.48
2:H:63:U:O2	2:H:72:G:N2	2.37	0.48
2:H:175:U:H2'	2:H:176:G:H8	1.78	0.48
2:I:49:U:H2'	2:I:50:G:H8	1.79	0.48
2:J:63:U:H2'	2:J:64:A:H8	1.79	0.48
2:K:32:C:H1'	2:K:33:U:H3	1.79	0.48
1:E:489:MET:HA	1:E:492:GLN:CB	2.44	0.48
2:I:20:C:N4	2:I:177:U:O2'	2.47	0.48
2:I:109:C:OP2	2:I:110:A:O2'	2.22	0.48
2:J:145:G:H3'	2:J:146:G:H8	1.79	0.48
1:E:1:MET:HE1	1:E:3:LEU:HB3	1.96	0.47
2:I:89:G:H2'	2:I:90:G:H8	1.79	0.47
2:I:146:G:N2	2:I:174:U:O2	2.28	0.47
2:L:71:U:H2'	2:L:72:G:H8	1.78	0.47
2:L:171:U:H2'	2:L:172:U:C6	2.48	0.47
1:A:458:ILE:HG23	1:A:463:LEU:HD13	1.97	0.47
2:H:108:C:H2'	2:H:109:C:C6	2.48	0.47
3:O:3:DA:H4'	3:O:4:DA:OP1	2.14	0.47
1:A:1:MET:HG3	1:A:4:GLU:H	1.79	0.47
1:B:335:LEU:O	1:B:425:ARG:NH1	2.47	0.47
1:F:18:LEU:HD12	1:F:111:ILE:HD11	1.95	0.47
2:K:71:U:H2'	2:K:72:G:H8	1.78	0.47
2:K:139:U:H2'	2:K:140:A:O4'	2.14	0.47
1:C:247:THR:C	1:C:248:ILE:HD13	2.39	0.47
2:G:126:U:H1'	2:G:127:U:P	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:139:U:H2'	2:G:140:A:O4'	2.14	0.47
2:I:129:C:H2'	2:I:130:U:C6	2.50	0.47
1:C:215:THR:OG1	1:C:218:SER:OG	2.24	0.47
2:G:36:C:H2'	2:G:37:U:C6	2.50	0.47
2:H:73:C:H2'	2:H:74:A:C8	2.50	0.47
2:H:78:G:H2'	2:H:79:A:H8	1.79	0.47
1:A:97:PRO:HG3	2:G:124:U:OP2	2.15	0.47
1:B:205:ARG:O	2:G:67:U:N3	2.48	0.47
1:F:142:ASP:N	1:F:142:ASP:OD1	2.47	0.47
2:G:128:A:N3	2:G:128:A:H2'	2.30	0.47
1:B:332:TYR:OH	2:H:119:C:OP2	2.28	0.47
1:C:166:GLU:HG2	1:C:248:ILE:HD12	1.97	0.47
1:C:485:ILE:HG22	1:C:489:MET:HG2	1.96	0.47
1:D:254:TYR:OH	1:F:294:GLU:OE2	2.27	0.47
1:E:169:PHE:HB2	1:E:172:PHE:HB2	1.97	0.47
1:F:146:HIS:ND1	1:F:489:MET:HG2	2.30	0.47
1:F:155:ASP:OD2	1:F:250:TRP:NE1	2.39	0.47
2:H:49:U:H2'	2:H:50:G:C8	2.50	0.47
2:I:78:G:H2'	2:I:79:A:H8	1.79	0.47
2:L:139:U:H2'	2:L:140:A:O4'	2.14	0.47
2:I:19:A:N7	2:I:177:U:H4'	2.29	0.47
2:L:173:U:H2'	2:L:174:U:H6	1.78	0.47
1:C:216:SER:HA	1:C:219:LEU:HG	1.97	0.47
2:I:71:U:H2'	2:I:72:G:H8	1.79	0.47
1:D:96:VAL:HG21	3:P:4:DA:C2	2.50	0.47
2:H:71:U:H2'	2:H:72:G:H8	1.80	0.47
2:I:63:U:O2	2:I:72:G:N2	2.37	0.47
2:K:74:A:H2'	2:K:75:A:C8	2.50	0.47
2:L:74:A:H2'	2:L:75:A:C8	2.50	0.47
1:F:141:ASN:C	3:R:1:DA:C2	2.93	0.46
2:J:170:U:H2'	2:J:171:U:C6	2.51	0.46
2:K:49:U:H2'	2:K:50:G:C8	2.51	0.46
2:H:170:U:H2'	2:H:171:U:C6	2.51	0.46
2:I:74:A:H2'	2:I:75:A:C8	2.50	0.46
2:K:64:A:C6	2:K:72:G:C6	3.04	0.46
2:L:24:G:H22	2:L:138:A:H2	1.62	0.46
1:B:369:MET:HA	1:B:394:ILE:HG22	1.98	0.46
1:E:145:VAL:HG23	1:E:304:LEU:HD12	1.97	0.46
1:C:142:ASP:OD1	1:C:142:ASP:N	2.48	0.46
1:D:397:PHE:HE2	2:J:129:C:C2	2.33	0.46
1:E:73:ILE:HG23	2:K:11:U:H1'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:70:U:H2'	2:G:71:U:C6	2.51	0.46
2:G:133:G:H2'	2:G:134:G:H8	1.81	0.46
2:I:89:G:H2'	2:I:90:G:C8	2.50	0.46
2:J:63:U:O2	2:J:72:G:N2	2.36	0.46
2:H:64:A:C6	2:H:72:G:C6	3.04	0.46
2:I:170:U:H2'	2:I:171:U:C6	2.51	0.46
2:J:139:U:H2'	2:J:140:A:O4'	2.15	0.46
2:K:78:G:H2'	2:K:79:A:H8	1.80	0.46
1:A:155:ASP:OD2	1:A:250:TRP:NE1	2.39	0.46
1:C:335:LEU:O	1:C:425:ARG:NH1	2.48	0.46
1:C:378:ILE:HG23	1:C:475:ALA:HB2	1.97	0.46
1:D:1:MET:HG3	1:D:4:GLU:H	1.81	0.46
1:D:18:LEU:HD12	1:D:111:ILE:HD11	1.98	0.46
2:L:170:U:H2'	2:L:171:U:C6	2.50	0.46
4:A:501:DTP:H8	4:A:501:DTP:O1A	2.16	0.46
1:C:169:PHE:HB2	1:C:172:PHE:HB2	1.98	0.46
2:G:125:U:H1'	2:G:127:U:OP2	2.15	0.46
2:H:102:U:H2'	2:H:103:U:H6	1.80	0.46
2:J:64:A:C6	2:J:72:G:C6	3.03	0.46
1:B:397:PHE:HE2	2:H:129:C:C2	2.33	0.46
1:E:489:MET:HG3	1:E:489:MET:H	1.38	0.46
2:J:20:C:N4	2:J:177:U:O2'	2.48	0.46
2:J:74:A:H2'	2:J:75:A:C8	2.51	0.46
2:L:22:G:H1	2:L:140:A:H2	1.61	0.46
1:A:18:LEU:HD12	1:A:111:ILE:HD11	1.98	0.46
1:B:107:SER:OG	1:B:213:GLN:O	2.30	0.46
1:D:413:TRP:HD1	2:J:82:G:C2	2.34	0.46
2:H:74:A:H2'	2:H:75:A:C8	2.50	0.46
2:I:173:U:H2'	2:I:174:U:H6	1.81	0.46
2:K:105:C:O2'	2:K:106:A:H5'	2.16	0.46
2:K:170:U:H2'	2:K:171:U:C6	2.51	0.46
1:A:369:MET:HA	1:A:394:ILE:HG22	1.97	0.46
1:A:495:ASN:HB3	3:M:2:DA:C5	2.51	0.46
1:E:397:PHE:HE2	2:K:129:C:C2	2.33	0.46
2:G:106:A:O2'	2:G:107:A:H5''	2.16	0.46
2:K:71:U:H2'	2:K:72:G:C8	2.51	0.46
2:L:78:G:H2'	2:L:79:A:H8	1.80	0.46
2:G:146:G:H2'	2:G:146:G:N3	2.31	0.45
2:H:133:G:H2'	2:H:134:G:H8	1.82	0.45
2:J:146:G:N3	2:J:146:G:H2'	2.31	0.45
2:K:133:G:H2'	2:K:134:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:A:C6	2:L:72:G:C6	3.03	0.45
1:B:73:ILE:HG23	2:H:11:U:H1'	1.99	0.45
1:D:170:SER:HA	1:D:276:ASN:HB2	1.97	0.45
2:L:34:A:H61	2:L:53:U:H3	1.64	0.45
2:L:103:U:H2'	2:L:104:U:H6	1.81	0.45
1:C:294:GLU:OE2	1:E:254:TYR:OH	2.26	0.45
4:E:501:DTP:H5'1	4:E:501:DTP:C8	2.46	0.45
2:G:89:G:H2'	2:G:90:G:C8	2.52	0.45
2:G:102:U:H2'	2:G:103:U:H6	1.82	0.45
2:I:84:G:H1	2:I:105:C:H42	1.65	0.45
2:I:103:U:H2'	2:I:104:U:H6	1.81	0.45
1:A:2:LYS:HD2	1:A:2:LYS:HA	1.81	0.45
1:A:185:PHE:HZ	1:A:200:ILE:HG21	1.81	0.45
1:C:39:ARG:NH1	1:C:333:ARG:HG3	2.32	0.45
1:D:149:ILE:HG22	1:D:400:LEU:HD13	1.98	0.45
1:F:73:ILE:HG23	2:L:11:U:H1'	1.98	0.45
2:G:105:C:O2'	2:G:106:A:H5'	2.16	0.45
2:G:170:U:H2'	2:G:171:U:C6	2.51	0.45
2:I:64:A:C6	2:I:72:G:C6	3.03	0.45
2:J:71:U:H2'	2:J:72:G:C8	2.50	0.45
2:L:71:U:H2'	2:L:72:G:C8	2.51	0.45
1:C:276:ASN:OD1	1:C:276:ASN:N	2.49	0.45
1:D:335:LEU:O	1:D:425:ARG:NH1	2.48	0.45
2:I:133:G:H2'	2:I:134:G:H8	1.82	0.45
2:L:19:A:N7	2:L:177:U:H4'	2.31	0.45
1:A:149:ILE:HG22	1:A:400:LEU:HD13	1.99	0.45
1:B:390:TYR:HD1	1:B:392:LYS:HG2	1.81	0.45
1:C:485:ILE:O	1:C:486:GLU:C	2.59	0.45
1:E:155:ASP:OD2	1:E:250:TRP:NE1	2.40	0.45
1:E:390:TYR:CD1	1:E:392:LYS:HG2	2.51	0.45
1:F:249:ILE:HD11	1:F:264:ILE:HD11	1.98	0.45
1:F:278:LYS:HE3	1:F:278:LYS:HB3	1.71	0.45
2:J:145:G:H1	2:J:175:U:H3	1.63	0.45
2:L:28:C:H2'	2:L:29:C:C6	2.51	0.45
1:C:73:ILE:HG23	2:I:11:U:H1'	1.99	0.45
2:G:89:G:H2'	2:G:90:G:H8	1.82	0.45
2:G:170:U:H2'	2:G:171:U:H6	1.82	0.45
2:H:75:A:H2'	2:H:76:C:C6	2.52	0.45
1:B:496:TYR:HA	2:H:128:A:C8	2.51	0.45
1:C:18:LEU:HD12	1:C:111:ILE:HD11	1.99	0.45
1:F:145:VAL:HG23	1:F:304:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:130:U:O2'	2:G:131:U:H5	1.99	0.45
2:H:58:A:H2'	2:H:59:G:H8	1.82	0.45
2:H:89:G:H2'	2:H:90:G:H8	1.82	0.45
2:I:131:U:H4'	2:I:132:G:OP2	2.16	0.45
2:K:146:G:N2	2:K:174:U:O2	2.29	0.45
2:K:170:U:H2'	2:K:171:U:H6	1.82	0.45
1:A:378:ILE:HG23	1:A:475:ALA:HB2	1.99	0.45
1:C:221:LEU:O	1:C:225:THR:OG1	2.34	0.45
2:H:26:G:H2'	2:H:27:G:H8	1.82	0.45
2:K:75:A:H2'	2:K:76:C:C6	2.52	0.45
2:L:170:U:H2'	2:L:171:U:H6	1.82	0.45
1:B:39:ARG:NH1	1:B:333:ARG:HG3	2.30	0.45
1:D:274:LYS:HA	1:D:274:LYS:HD3	1.87	0.45
1:E:137:TYR:CD1	1:E:148:ALA:HB2	2.52	0.45
2:G:103:U:H2'	2:G:104:U:H6	1.82	0.45
2:H:16:A:H2'	2:H:17:U:O4'	2.17	0.45
2:H:89:G:H2'	2:H:90:G:C8	2.52	0.45
2:H:131:U:H4'	2:H:132:G:OP2	2.17	0.45
2:H:173:U:H2'	2:H:174:U:H6	1.82	0.45
2:I:75:A:H2'	2:I:76:C:C6	2.52	0.45
2:K:89:G:H2'	2:K:90:G:H8	1.82	0.45
1:E:173:PHE:H	4:E:501:DTP:HO3'	1.65	0.44
2:H:58:A:H2'	2:H:59:G:C8	2.53	0.44
2:H:170:U:H2'	2:H:171:U:H6	1.82	0.44
2:I:102:U:H2'	2:I:103:U:H6	1.82	0.44
2:J:170:U:H2'	2:J:171:U:H6	1.81	0.44
2:L:89:G:H2'	2:L:90:G:C8	2.52	0.44
2:L:133:G:H2'	2:L:134:G:H8	1.82	0.44
1:A:294:GLU:HG2	1:A:295:ILE:HG23	1.98	0.44
1:B:147:PHE:HE1	1:B:485:ILE:HB	1.82	0.44
1:C:424:LEU:HD22	2:I:107:A:H5'	1.99	0.44
1:D:477:GLN:O	1:D:481:GLN:HG2	2.17	0.44
2:J:19:A:N7	2:J:177:U:H4'	2.31	0.44
2:J:75:A:H2'	2:J:76:C:C6	2.52	0.44
2:J:129:C:H2'	2:J:130:U:C6	2.52	0.44
2:K:144:U:H2'	2:K:145:G:O4'	2.17	0.44
1:A:365:ILE:O	1:A:369:MET:HG2	2.18	0.44
1:C:395:MET:HE3	1:C:395:MET:HB3	1.90	0.44
1:F:39:ARG:NH1	1:F:333:ARG:HG3	2.33	0.44
2:G:176:G:HO2'	2:G:177:U:P	2.41	0.44
2:K:89:G:H2'	2:K:90:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:75:A:H2'	2:L:76:C:C6	2.52	0.44
1:B:18:LEU:HD12	1:B:111:ILE:HD11	2.00	0.44
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.81	0.44
1:E:39:ARG:NH1	1:E:333:ARG:HG3	2.33	0.44
2:K:108:C:H2'	2:K:109:C:C6	2.52	0.44
2:L:91:U:H2'	2:L:92:G:H8	1.83	0.44
1:B:294:GLU:OE2	1:F:254:TYR:OH	2.26	0.44
2:L:82:G:H2'	2:L:83:G:O4'	2.18	0.44
3:Q:3:DA:H2'	3:Q:4:DA:C2	2.53	0.44
1:D:308:LEU:HD23	1:D:313:VAL:HG22	2.00	0.44
1:E:378:ILE:HG23	1:E:475:ALA:HB2	1.99	0.44
2:J:78:G:H2'	2:J:79:A:H8	1.82	0.44
2:K:35:C:H2'	2:K:36:C:C6	2.52	0.44
2:K:86:G:N2	2:K:103:U:O2	2.37	0.44
2:K:102:U:H2'	2:K:103:U:H6	1.82	0.44
2:K:173:U:H2'	2:K:174:U:H6	1.82	0.44
1:A:39:ARG:NH1	1:A:333:ARG:HG3	2.33	0.44
1:B:378:ILE:HG23	1:B:475:ALA:HB2	1.99	0.44
1:C:392:LYS:NZ	2:I:131:U:H5'	2.31	0.44
1:F:420:ARG:NH2	2:L:82:G:O6	2.47	0.44
2:H:129:C:H2'	2:H:130:U:C6	2.53	0.44
2:I:58:A:H2'	2:I:59:G:H8	1.83	0.44
2:J:133:G:H2'	2:J:134:G:H8	1.82	0.44
1:A:496:TYR:C	2:G:127:U:H5'	2.43	0.44
1:D:378:ILE:HG23	1:D:475:ALA:HB2	1.99	0.44
2:H:175:U:C2	2:H:176:G:N7	2.86	0.44
2:I:170:U:H2'	2:I:171:U:H6	1.82	0.44
2:K:88:U:H2'	2:K:89:G:C8	2.53	0.44
2:K:91:U:H2'	2:K:92:G:H8	1.83	0.44
1:F:137:TYR:CD1	1:F:148:ALA:HB2	2.53	0.44
2:I:58:A:H2'	2:I:59:G:C8	2.53	0.44
2:I:71:U:H2'	2:I:72:G:C8	2.52	0.44
2:L:102:U:H2'	2:L:103:U:H6	1.81	0.44
1:D:185:PHE:HZ	1:D:200:ILE:HG21	1.83	0.43
2:G:58:A:H2'	2:G:59:G:H8	1.83	0.43
2:H:71:U:H2'	2:H:72:G:C8	2.53	0.43
2:I:32:C:H4'	2:I:33:U:H5'	2.00	0.43
2:K:129:C:H2'	2:K:130:U:C6	2.52	0.43
1:B:147:PHE:HE1	1:B:485:ILE:CB	2.31	0.43
1:B:386:SER:HB2	2:H:33:U:O2	2.17	0.43
1:C:121:PHE:HD1	1:C:220:PHE:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:LYS:HD2	1:F:2:LYS:HA	1.83	0.43
2:G:78:G:H2'	2:G:79:A:H8	1.83	0.43
2:K:106:A:O2'	2:K:107:A:H5''	2.17	0.43
1:A:308:LEU:HD23	1:A:313:VAL:HG22	1.99	0.43
1:B:2:LYS:HD2	1:B:2:LYS:HA	1.82	0.43
1:C:472:ILE:HD12	1:C:472:ILE:HA	1.87	0.43
1:E:149:ILE:HG22	1:E:400:LEU:HD13	2.00	0.43
1:E:489:MET:HE3	1:E:489:MET:HB2	1.91	0.43
2:H:70:U:H2'	2:H:71:U:C6	2.54	0.43
2:I:82:G:H2'	2:I:83:G:O4'	2.19	0.43
2:K:31:U:H5'	2:K:32:C:OP2	2.18	0.43
2:K:70:U:H2'	2:K:71:U:C6	2.54	0.43
2:L:89:G:H2'	2:L:90:G:H8	1.82	0.43
1:B:276:ASN:OD1	1:B:276:ASN:N	2.49	0.43
1:B:278:LYS:HE3	1:B:278:LYS:HB3	1.83	0.43
1:B:325:LYS:NZ	2:H:119:C:N3	2.62	0.43
1:C:161:ARG:HG2	1:C:287:THR:HG22	2.00	0.43
1:D:39:ARG:NH1	1:D:333:ARG:HG3	2.33	0.43
1:E:146:HIS:CE1	1:E:489:MET:HB3	2.54	0.43
1:E:335:LEU:O	1:E:425:ARG:NH1	2.48	0.43
2:H:19:A:C6	2:H:176:G:N2	2.87	0.43
2:H:82:G:H2'	2:H:83:G:O4'	2.19	0.43
2:J:58:A:H2'	2:J:59:G:H8	1.83	0.43
2:J:70:U:H2'	2:J:71:U:C6	2.53	0.43
2:J:113:U:N3	2:J:116:U:OP2	2.36	0.43
2:K:82:G:H2'	2:K:83:G:O4'	2.18	0.43
2:L:63:U:H2'	2:L:64:A:C8	2.54	0.43
1:B:221:LEU:O	1:B:225:THR:OG1	2.31	0.43
2:H:88:U:H2'	2:H:89:G:C8	2.52	0.43
2:I:70:U:H2'	2:I:71:U:C6	2.53	0.43
1:B:274:LYS:HA	1:B:274:LYS:HD3	1.85	0.43
1:E:394:ILE:HD12	1:E:394:ILE:HA	1.87	0.43
1:F:424:LEU:HD22	2:L:107:A:H5'	2.01	0.43
2:L:146:G:N2	2:L:174:U:O2	2.32	0.43
1:A:294:GLU:OE2	1:C:254:TYR:OH	2.26	0.43
2:J:105:C:O2'	2:J:106:A:H5'	2.18	0.43
3:N:3:DA:H2''	3:N:4:DA:OP2	2.18	0.43
1:A:103:ILE:HD12	1:A:103:ILE:HA	1.87	0.43
1:A:336:ILE:HD13	1:A:424:LEU:HD23	1.99	0.43
1:C:274:LYS:HA	1:C:274:LYS:HD3	1.85	0.43
2:G:73:C:H2'	2:G:74:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:129:C:O2'	2:J:130:U:O4'	2.22	0.43
2:K:63:U:H2'	2:K:64:A:C8	2.54	0.43
2:L:20:C:N4	2:L:177:U:O2'	2.50	0.43
1:C:38:LYS:HE2	1:C:38:LYS:HB3	1.94	0.43
1:C:397:PHE:CE1	1:C:492:GLN:CB	3.02	0.43
1:E:140:ARG:NH2	1:E:142:ASP:OD2	2.52	0.43
2:H:174:U:H2'	2:H:175:U:C6	2.54	0.43
2:J:58:A:H2'	2:J:59:G:C8	2.54	0.43
2:J:63:U:H2'	2:J:64:A:C8	2.53	0.43
1:B:390:TYR:CD1	1:B:392:LYS:HG2	2.53	0.42
2:G:49:U:H2'	2:G:50:G:H8	1.82	0.42
2:J:50:G:H2'	2:J:51:G:H8	1.84	0.42
2:K:103:U:H2'	2:K:104:U:H6	1.83	0.42
2:L:70:U:H2'	2:L:71:U:C6	2.54	0.42
1:A:214:GLY:HA2	3:M:4:DA:C2	2.54	0.42
1:B:1:MET:CE	1:B:3:LEU:H	2.32	0.42
1:E:397:PHE:CE1	1:E:492:GLN:O	2.72	0.42
2:G:82:G:H2'	2:G:83:G:O4'	2.19	0.42
2:H:20:C:H2'	2:H:21:G:C8	2.54	0.42
2:H:133:G:H2'	2:H:134:G:C8	2.54	0.42
2:H:177:U:H2'	2:H:178:U:C5	2.54	0.42
2:I:88:U:H2'	2:I:89:G:C8	2.52	0.42
2:I:145:G:C6	2:I:146:G:C5	3.08	0.42
2:K:26:G:H2'	2:K:27:G:H8	1.84	0.42
1:A:322:LYS:NZ	2:G:127:U:H1'	2.34	0.42
1:C:397:PHE:HE2	2:I:129:C:C2	2.37	0.42
2:J:84:G:C2	2:J:85:G:C8	3.08	0.42
1:F:136:SER:OG	1:F:242:ARG:NH2	2.52	0.42
2:G:49:U:H2'	2:G:50:G:C8	2.55	0.42
2:G:131:U:H4'	2:G:132:G:OP2	2.19	0.42
1:B:410:LEU:HD13	1:B:469:PHE:CE2	2.54	0.42
1:B:411:ASP:HB3	2:H:81:G:N3	2.34	0.42
1:D:137:TYR:CD1	1:D:148:ALA:HB2	2.55	0.42
1:D:390:TYR:HD1	1:D:392:LYS:HG2	1.83	0.42
1:E:486:GLU:HA	1:E:489:MET:CE	2.50	0.42
1:F:170:SER:HA	1:F:276:ASN:HB2	2.00	0.42
1:F:390:TYR:CD1	1:F:392:LYS:HG2	2.54	0.42
2:G:133:G:H2'	2:G:134:G:C8	2.54	0.42
2:I:22:G:N1	2:I:140:A:H2	2.13	0.42
2:I:27:G:N2	2:I:135:U:O2	2.53	0.42
2:K:58:A:H2'	2:K:59:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:G:H2'	2:L:134:G:C8	2.55	0.42
1:B:161:ARG:HG2	1:B:287:THR:HG22	2.01	0.42
1:B:301:LEU:O	1:B:308:LEU:N	2.47	0.42
1:F:149:ILE:HG22	1:F:400:LEU:HD13	2.01	0.42
1:F:472:ILE:HD12	1:F:472:ILE:HA	1.90	0.42
2:H:36:C:C2	2:H:52:G:C2	3.08	0.42
2:H:59:G:H2'	2:H:60:U:C6	2.55	0.42
1:C:144:ASN:OD1	1:C:489:MET:HE1	2.19	0.42
1:C:308:LEU:HD23	1:C:313:VAL:HG22	2.01	0.42
1:D:38:LYS:HE2	1:D:38:LYS:HB3	1.91	0.42
1:C:137:TYR:CD1	1:C:148:ALA:HB2	2.54	0.42
1:D:59:LYS:HB3	1:D:65:TYR:CD2	2.55	0.42
1:D:336:ILE:HD13	1:D:424:LEU:HD23	2.01	0.42
2:G:70:U:H2'	2:G:71:U:H6	1.85	0.42
2:H:176:G:HO2'	2:H:177:U:P	2.39	0.42
2:J:133:G:H2'	2:J:134:G:C8	2.54	0.42
2:L:88:U:H2'	2:L:89:G:C8	2.53	0.42
1:A:59:LYS:HB3	1:A:65:TYR:CD2	2.55	0.42
1:B:149:ILE:HG22	1:B:400:LEU:HD13	2.01	0.42
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.89	0.42
1:B:395:MET:HE3	1:B:476:LEU:HD22	2.02	0.42
1:C:96:VAL:HG22	1:C:97:PRO:HD2	2.01	0.42
1:C:399:PRO:HG3	1:C:489:MET:HG2	2.01	0.42
2:H:22:G:N1	2:H:140:A:H2	2.12	0.42
2:H:174:U:C2	2:H:175:U:C5	3.08	0.42
2:L:58:A:H2'	2:L:59:G:H8	1.85	0.42
1:B:394:ILE:HD12	1:B:394:ILE:HA	1.87	0.42
1:D:139:TYR:HD1	3:P:2:DA:N7	2.18	0.42
2:I:144:U:H2'	2:I:145:G:O4'	2.19	0.42
2:K:58:A:H2'	2:K:59:G:C8	2.55	0.42
1:C:149:ILE:HG22	1:C:400:LEU:HD13	2.00	0.41
2:G:58:A:H2'	2:G:59:G:C8	2.55	0.41
2:G:91:U:H2'	2:G:92:G:H8	1.85	0.41
2:K:109:C:OP2	2:K:110:A:O2'	2.24	0.41
1:A:302:ASP:HB3	1:A:316:LYS:HE3	2.03	0.41
1:C:490:ASN:C	1:C:492:GLN:H	2.28	0.41
1:E:336:ILE:HD13	1:E:424:LEU:HD23	2.02	0.41
1:F:489:MET:H	1:F:489:MET:HG3	1.72	0.41
2:G:31:U:C5	2:G:32:C:H2'	2.54	0.41
2:G:59:G:H2'	2:G:60:U:C6	2.55	0.41
2:G:88:U:H2'	2:G:89:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:59:G:H2'	2:I:60:U:C6	2.55	0.41
2:K:133:G:H2'	2:K:134:G:C8	2.54	0.41
1:A:181:LEU:HA	1:A:181:LEU:HD12	1.85	0.41
1:C:59:LYS:HB3	1:C:65:TYR:CD2	2.56	0.41
1:C:121:PHE:CD2	1:C:216:SER:HB3	2.56	0.41
2:K:19:A:N7	2:K:177:U:H1'	2.35	0.41
2:K:59:G:H2'	2:K:60:U:C6	2.55	0.41
2:L:59:G:H2'	2:L:60:U:C6	2.56	0.41
2:H:4:U:H4'	2:H:20:C:H4'	2.00	0.41
2:K:31:U:C5	2:K:32:C:H2'	2.55	0.41
1:A:176:ILE:H	1:A:210:GLY:HA2	1.85	0.41
1:B:139:TYR:HD1	3:N:2:DA:H62	1.69	0.41
1:E:121:PHE:HD1	1:E:220:PHE:HB2	1.85	0.41
4:E:501:DTP:O2B	4:E:501:DTP:H3'	2.21	0.41
2:H:63:U:H2'	2:H:64:A:C8	2.54	0.41
2:H:145:G:C6	2:H:176:G:C6	3.09	0.41
2:I:63:U:H2'	2:I:64:A:C8	2.54	0.41
2:K:145:G:C6	2:K:146:G:C5	3.09	0.41
2:L:145:G:C6	2:L:146:G:C5	3.09	0.41
1:A:482:GLU:OE2	1:A:482:GLU:N	2.54	0.41
1:B:137:TYR:CD1	1:B:148:ALA:HB2	2.56	0.41
1:D:257:ILE:HD12	1:D:257:ILE:HA	1.96	0.41
1:D:302:ASP:HB3	1:D:316:LYS:HE3	2.03	0.41
1:E:274:LYS:HA	1:E:274:LYS:HD3	1.87	0.41
1:F:141:ASN:O	3:R:1:DA:C2	2.74	0.41
1:F:146:HIS:CB	1:F:485:ILE:HG21	2.50	0.41
2:G:90:G:H2'	2:G:91:U:C6	2.56	0.41
2:J:59:G:H2'	2:J:60:U:C6	2.55	0.41
1:A:137:TYR:CG	1:A:148:ALA:HB2	2.56	0.41
1:B:96:VAL:HG22	1:B:97:PRO:HD2	2.03	0.41
1:D:103:ILE:HD12	1:D:103:ILE:HA	1.93	0.41
1:D:390:TYR:CD1	1:D:392:LYS:HG2	2.56	0.41
2:H:102:U:H2'	2:H:103:U:C6	2.56	0.41
2:I:133:G:H2'	2:I:134:G:C8	2.55	0.41
1:B:59:LYS:HB3	1:B:65:TYR:CD2	2.56	0.41
1:B:411:ASP:CG	1:B:469:PHE:H	2.29	0.41
1:C:207:ARG:H	1:C:207:ARG:HG2	1.67	0.41
1:D:141:ASN:O	3:P:1:DA:N7	2.53	0.41
1:E:492:GLN:O	1:E:493:SER:C	2.63	0.41
1:F:197:LYS:HE3	1:F:197:LYS:HB2	1.89	0.41
1:F:291:LEU:HD12	1:F:291:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:G:H2'	2:I:28:C:C6	2.56	0.41
1:B:288:LYS:HE3	1:B:288:LYS:HB3	1.95	0.41
1:B:493:SER:O	1:B:495:ASN:N	2.54	0.41
1:C:205:ARG:HB3	2:J:67:U:H3	1.86	0.41
1:E:483:SER:OG	1:E:487:LYS:HG3	2.21	0.41
1:F:38:LYS:HE2	1:F:38:LYS:HB3	1.92	0.41
2:G:55:U:O2'	2:G:56:U:H5'	2.21	0.41
2:G:75:A:H2'	2:G:76:C:C6	2.56	0.41
2:H:145:G:C5	2:H:146:G:C8	3.09	0.41
2:J:50:G:H2'	2:J:51:G:C8	2.56	0.41
2:J:109:C:OP2	2:J:110:A:O2'	2.29	0.41
2:L:47:A:H2'	2:L:48:A:C8	2.56	0.41
1:A:254:TYR:OH	1:E:294:GLU:OE2	2.30	0.41
1:A:411:ASP:HB3	2:G:81:G:N3	2.36	0.41
1:D:48:LYS:HE3	1:D:50:HIS:NE2	2.36	0.41
1:E:390:TYR:CD1	1:E:390:TYR:C	2.98	0.41
1:F:59:LYS:HB3	1:F:65:TYR:CD2	2.56	0.41
1:E:59:LYS:HB3	1:E:65:TYR:CD2	2.56	0.40
1:E:216:SER:HA	1:E:219:LEU:HG	2.02	0.40
1:F:370:TYR:OH	1:F:468:SER:N	2.37	0.40
2:G:104:U:C2	2:G:105:C:C5	3.09	0.40
2:K:132:G:O2'	2:K:133:G:H8	2.05	0.40
2:L:53:U:H2'	2:L:54:C:C6	2.57	0.40
2:L:74:A:H2'	2:L:75:A:H8	1.86	0.40
2:L:84:G:H1	2:L:105:C:H42	1.68	0.40
1:B:87:LEU:HD11	1:B:205:ARG:HD3	2.02	0.40
1:D:152:ILE:HD13	1:D:248:ILE:HD13	2.02	0.40
1:E:181:LEU:HD23	1:E:181:LEU:HA	1.81	0.40
1:F:103:ILE:HD12	1:F:103:ILE:HA	1.89	0.40
1:F:496:TYR:HB2	3:R:4:DA:N6	2.36	0.40
2:G:85:G:O6	2:G:105:C:N4	2.54	0.40
2:J:90:G:H2'	2:J:91:U:C6	2.57	0.40
2:L:141:C:H41	2:L:178:U:H5	1.67	0.40
1:C:302:ASP:HB3	1:C:316:LYS:HE3	2.02	0.40
1:D:137:TYR:HA	1:D:143:ARG:HB3	2.03	0.40
1:E:411:ASP:HB3	2:K:81:G:N3	2.37	0.40
2:I:90:G:H2'	2:I:91:U:C6	2.56	0.40
2:L:29:C:H2'	2:L:30:U:C6	2.57	0.40
2:L:58:A:H2'	2:L:59:G:C8	2.56	0.40
1:A:137:TYR:CD1	1:A:148:ALA:HB2	2.56	0.40
1:E:489:MET:O	1:E:493:SER:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:G:H2'	2:H:79:A:C8	2.56	0.40
2:I:105:C:O2'	2:I:106:A:H5'	2.22	0.40
2:L:55:U:O2'	2:L:56:U:H5'	2.21	0.40
3:O:2:DA:H2''	3:O:3:DA:C5'	2.52	0.40
1:C:93:THR:HB	1:C:105:LYS:HD2	2.02	0.40
1:D:311:GLU:OE1	1:D:311:GLU:N	2.53	0.40
1:E:141:ASN:HB3	3:Q:1:DA:O3'	2.22	0.40
2:I:31:U:C6	2:I:32:C:H2'	2.57	0.40
2:I:104:U:C2	2:I:105:C:C5	3.10	0.40
2:K:55:U:O2'	2:K:56:U:H5'	2.21	0.40
2:K:84:G:C6	2:K:106:A:N6	2.88	0.40
2:K:85:G:O6	2:K:105:C:N4	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	494/499 (99%)	490 (99%)	4 (1%)	0	100	100
1	B	494/499 (99%)	482 (98%)	11 (2%)	1 (0%)	44	76
1	C	494/499 (99%)	485 (98%)	9 (2%)	0	100	100
1	D	494/499 (99%)	483 (98%)	11 (2%)	0	100	100
1	E	494/499 (99%)	486 (98%)	7 (1%)	1 (0%)	44	76
1	F	494/499 (99%)	484 (98%)	10 (2%)	0	100	100
All	All	2964/2994 (99%)	2910 (98%)	52 (2%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	LEU

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Mol	Chain	Res	Type
1	E	495	ASN

### 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 PDB entries followed by that with respect to all EM entries.

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	
1	A	450/456 (99%)	439 (98%)	11 (2%)	44	70
1	B	450/456 (99%)	439 (98%)	11 (2%)	44	70
1	C	450/456 (99%)	436 (97%)	14 (3%)	35	64
1	D	450/456 (99%)	439 (98%)	11 (2%)	44	70
1	E	450/456 (99%)	438 (97%)	12 (3%)	40	67
1	F	450/456 (99%)	440 (98%)	10 (2%)	47	71
All	All	2700/2736 (99%)	2631 (97%)	69 (3%)	42	68

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	145	VAL
1	A	218	SER
1	A	248	ILE
1	A	257	ILE
1	A	265	THR
1	A	273	ILE
1	A	284	SER
1	A	392	LYS
1	A	458	ILE
1	A	489	MET
1	B	106	VAL
1	B	139	TYR
1	B	158	LYS
1	B	211	ILE
1	B	252	GLN
1	B	257	ILE

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Mol	Chain	Res	Type
1	B	265	THR
1	B	273	ILE
1	B	458	ILE
1	B	483	SER
1	B	489	MET
1	C	144	ASN
1	C	158	LYS
1	C	218	SER
1	C	245	ASP
1	C	251	SER
1	C	252	GLN
1	C	257	ILE
1	C	265	THR
1	C	273	ILE
1	C	284	SER
1	C	449	ILE
1	C	458	ILE
1	C	489	MET
1	C	496	TYR
1	D	145	VAL
1	D	218	SER
1	D	248	ILE
1	D	257	ILE
1	D	265	THR
1	D	273	ILE
1	D	284	SER
1	D	458	ILE
1	D	482	GLU
1	D	489	MET
1	D	496	TYR
1	E	96	VAL
1	E	218	SER
1	E	251	SER
1	E	252	GLN
1	E	265	THR
1	E	273	ILE
1	E	284	SER
1	E	291	LEU
1	E	458	ILE
1	E	482	GLU
1	E	489	MET
1	E	495	ASN

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Mol	Chain	Res	Type
1	F	104	ARG
1	F	251	SER
1	F	252	GLN
1	F	265	THR
1	F	273	ILE
1	F	284	SER
1	F	458	ILE
1	F	481	GLN
1	F	489	MET
1	F	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	ASN
1	C	490	ASN
1	D	490	ASN
1	E	495	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	160/188 (85%)	35 (21%)	9 (5%)
2	H	156/188 (82%)	28 (17%)	4 (2%)
2	I	156/188 (82%)	28 (17%)	3 (1%)
2	J	156/188 (82%)	26 (16%)	3 (1%)
2	K	156/188 (82%)	29 (18%)	5 (3%)
2	L	156/188 (82%)	27 (17%)	2 (1%)
All	All	940/1128 (83%)	173 (18%)	26 (2%)

All (173) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2	A
2	G	9	C
2	G	11	U
2	G	12	A
2	G	19	A
2	G	31	U
2	G	32	C

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Mol	Chain	Res	Type
2	G	33	U
2	G	34	A
2	G	39	U
2	G	41	A
2	G	68	C
2	G	69	G
2	G	70	U
2	G	76	C
2	G	111	A
2	G	117	A
2	G	122	A
2	G	125	U
2	G	126	U
2	G	127	U
2	G	128	A
2	G	129	C
2	G	132	G
2	G	133	G
2	G	135	U
2	G	136	U
2	G	137	U
2	G	138	A
2	G	146	G
2	G	149	A
2	G	150	A
2	G	172	U
2	G	177	U
2	G	178	U
2	H	2	A
2	H	9	C
2	H	12	A
2	H	18	A
2	H	19	A
2	H	31	U
2	H	32	C
2	H	39	U
2	H	40	U
2	H	41	A
2	H	68	C
2	H	69	G
2	H	76	C
2	H	111	A

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Mol	Chain	Res	Type
2	H	117	A
2	H	122	A
2	H	132	G
2	H	133	G
2	H	135	U
2	H	136	U
2	H	137	U
2	H	138	A
2	H	146	G
2	H	149	A
2	H	150	A
2	H	172	U
2	H	177	U
2	H	178	U
2	I	2	A
2	I	9	C
2	I	12	A
2	I	19	A
2	I	32	C
2	I	33	U
2	I	34	A
2	I	39	U
2	I	40	U
2	I	41	A
2	I	68	C
2	I	69	G
2	I	76	C
2	I	111	A
2	I	117	A
2	I	122	A
2	I	132	G
2	I	133	G
2	I	135	U
2	I	136	U
2	I	137	U
2	I	138	A
2	I	146	G
2	I	149	A
2	I	150	A
2	I	172	U
2	I	177	U
2	I	178	U

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Mol	Chain	Res	Type
2	J	2	A
2	J	9	C
2	J	11	U
2	J	12	A
2	J	19	A
2	J	32	C
2	J	33	U
2	J	41	A
2	J	68	C
2	J	69	G
2	J	76	C
2	J	111	A
2	J	117	A
2	J	122	A
2	J	132	G
2	J	133	G
2	J	135	U
2	J	136	U
2	J	137	U
2	J	138	A
2	J	146	G
2	J	149	A
2	J	150	A
2	J	172	U
2	J	177	U
2	J	178	U
2	K	2	A
2	K	9	C
2	K	12	A
2	K	19	A
2	K	31	U
2	K	32	C
2	K	33	U
2	K	34	A
2	K	39	U
2	K	40	U
2	K	41	A
2	K	68	C
2	K	69	G
2	K	76	C
2	K	111	A
2	K	117	A

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Mol	Chain	Res	Type
2	K	122	A
2	K	132	G
2	K	133	G
2	K	135	U
2	K	136	U
2	K	137	U
2	K	138	A
2	K	146	G
2	K	149	A
2	K	150	A
2	K	172	U
2	K	177	U
2	K	178	U
2	L	2	A
2	L	9	C
2	L	12	A
2	L	19	A
2	L	31	U
2	L	32	C
2	L	34	A
2	L	39	U
2	L	41	A
2	L	68	C
2	L	69	G
2	L	76	C
2	L	111	A
2	L	117	A
2	L	122	A
2	L	129	C
2	L	132	G
2	L	133	G
2	L	135	U
2	L	136	U
2	L	137	U
2	L	138	A
2	L	146	G
2	L	149	A
2	L	150	A
2	L	177	U
2	L	178	U

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	32	C
2	G	38	G
2	G	67	U
2	G	125	U
2	G	126	U
2	G	127	U
2	G	128	A
2	G	131	U
2	G	176	G
2	H	38	G
2	H	67	U
2	H	131	U
2	H	176	G
2	I	38	G
2	I	67	U
2	I	131	U
2	J	32	C
2	J	67	U
2	J	131	U
2	K	32	C
2	K	33	U
2	K	67	U
2	K	131	U
2	K	176	G
2	L	67	U
2	L	131	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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	$\# Z  > 2$
4	DTP	A	501	-	26,32,32	0.70	0	30,50,50	0.81	1 (3%)
4	DTP	E	501	-	26,32,32	0.71	0	30,50,50	0.84	1 (3%)
4	DTP	B	501	-	26,32,32	0.70	0	30,50,50	0.80	1 (3%)
4	DTP	F	501	-	26,32,32	0.70	0	30,50,50	0.79	1 (3%)
4	DTP	D	501	5	26,32,32	0.68	0	30,50,50	0.75	1 (3%)
4	DTP	C	501	5	26,32,32	0.71	0	30,50,50	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	501	-	-	3/18/34/34	0/3/3/3
4	DTP	E	501	-	-	4/18/34/34	0/3/3/3
4	DTP	B	501	-	-	5/18/34/34	0/3/3/3
4	DTP	F	501	-	-	3/18/34/34	0/3/3/3
4	DTP	D	501	5	-	6/18/34/34	0/3/3/3
4	DTP	C	501	5	-	4/18/34/34	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	DTP	C5-C6-N6	2.38	123.97	120.35
4	B	501	DTP	C5-C6-N6	2.36	123.94	120.35
4	D	501	DTP	C5-C6-N6	2.31	123.86	120.35
4	A	501	DTP	C5-C6-N6	2.29	123.83	120.35
4	F	501	DTP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	DTP	PB-O3A-PA-O5'
4	B	501	DTP	O4'-C4'-C5'-O5'
4	C	501	DTP	C5'-O5'-PA-O1A
4	C	501	DTP	C3'-C4'-C5'-O5'
4	D	501	DTP	C5'-O5'-PA-O1A
4	E	501	DTP	PB-O3A-PA-O5'
4	E	501	DTP	C5'-O5'-PA-O2A
4	E	501	DTP	C5'-O5'-PA-O3A
4	A	501	DTP	O4'-C4'-C5'-O5'
4	F	501	DTP	O4'-C4'-C5'-O5'
4	C	501	DTP	O4'-C4'-C5'-O5'
4	A	501	DTP	C3'-C4'-C5'-O5'
4	A	501	DTP	PB-O3A-PA-O5'
4	D	501	DTP	PB-O3A-PA-O5'
4	F	501	DTP	PB-O3A-PA-O5'
4	B	501	DTP	C5'-O5'-PA-O3A
4	B	501	DTP	PG-O3B-PB-O1B
4	D	501	DTP	PA-O3A-PB-O1B
4	B	501	DTP	C5'-O5'-PA-O2A
4	F	501	DTP	C3'-C4'-C5'-O5'
4	C	501	DTP	C5'-O5'-PA-O3A
4	D	501	DTP	O4'-C4'-C5'-O5'
4	D	501	DTP	PG-O3B-PB-O1B
4	D	501	DTP	PA-O3A-PB-O2B
4	E	501	DTP	O4'-C4'-C5'-O5'

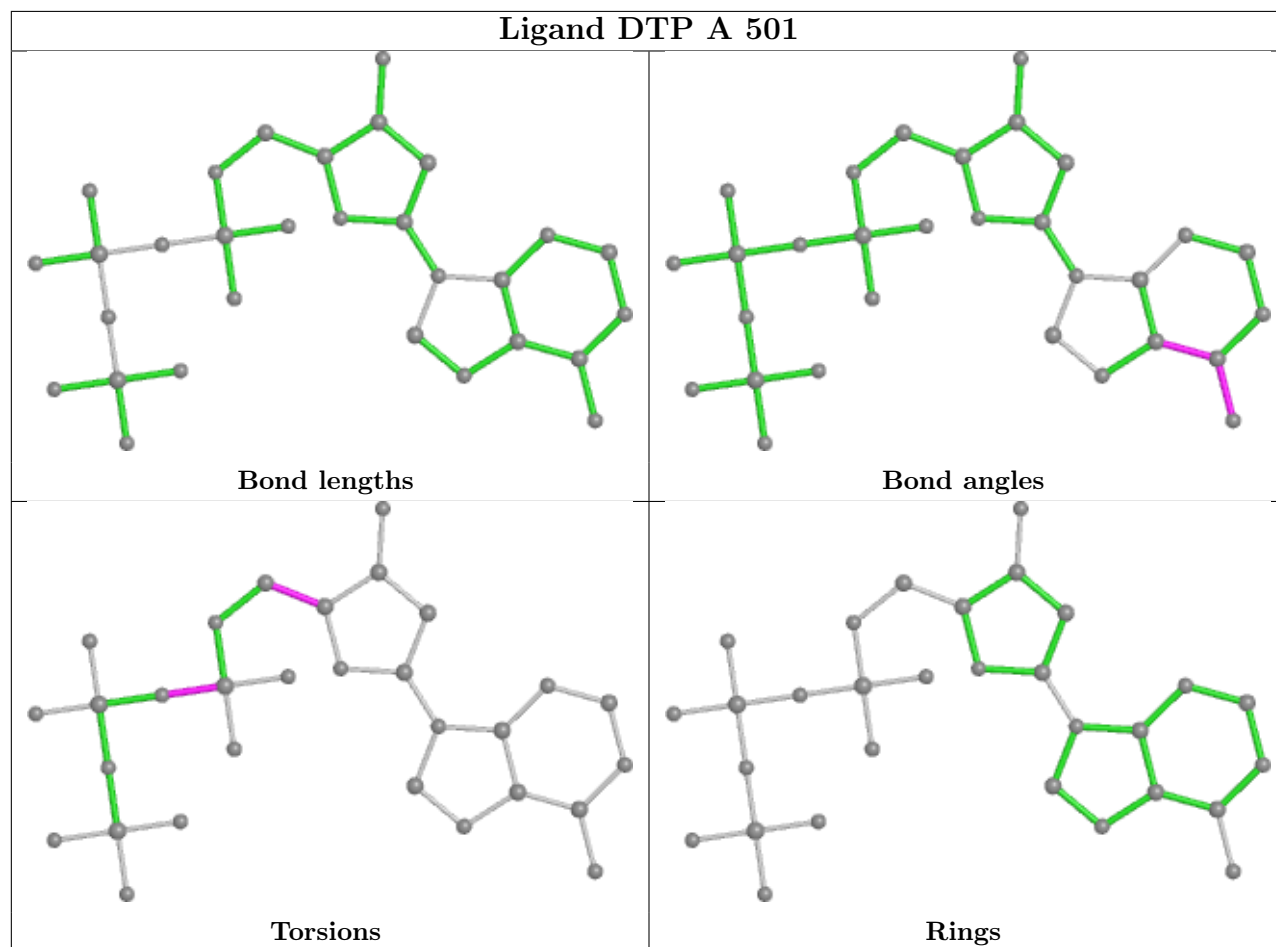
There are no ring outliers.

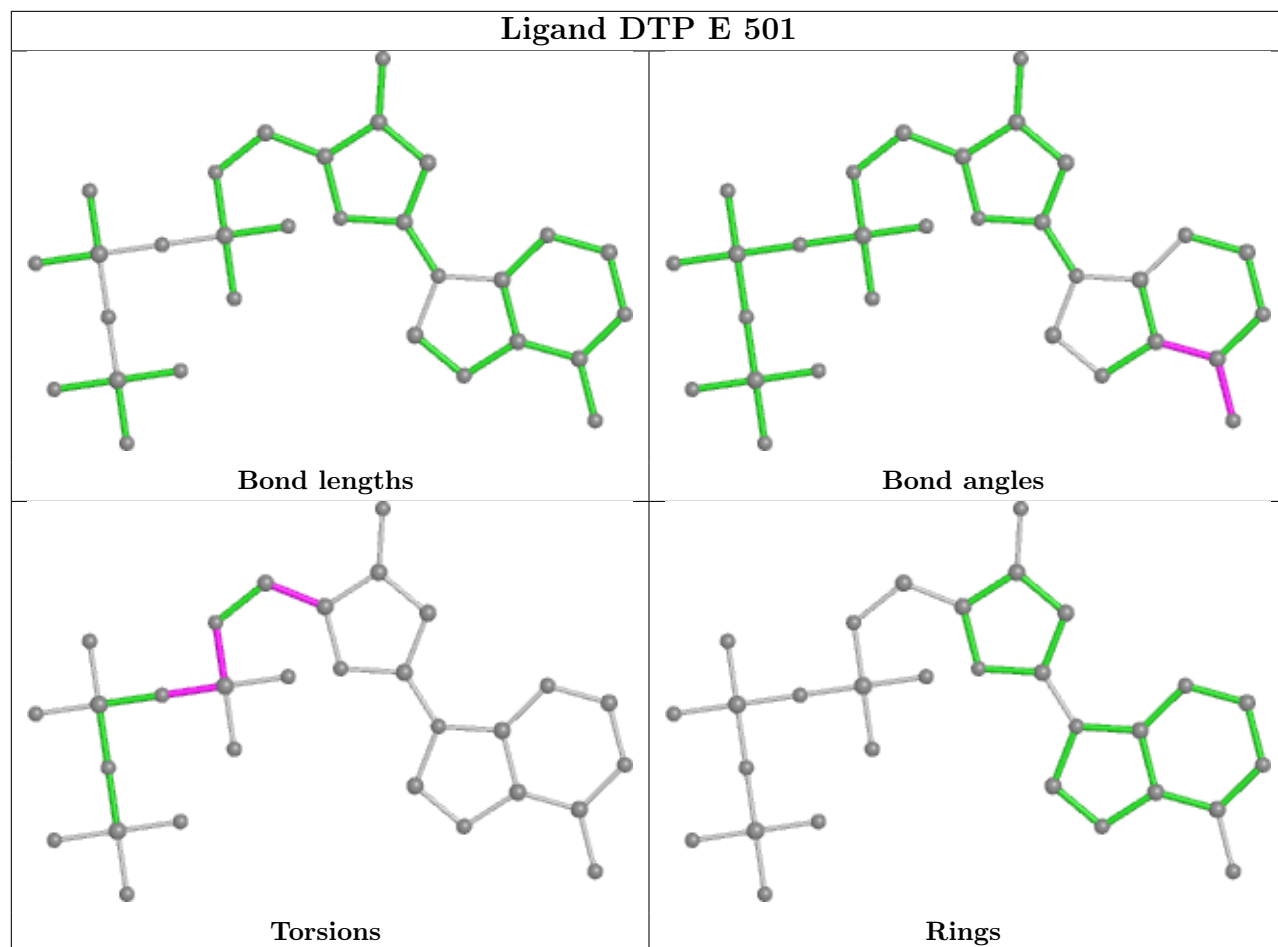
3 monomers are involved in 9 short contacts:

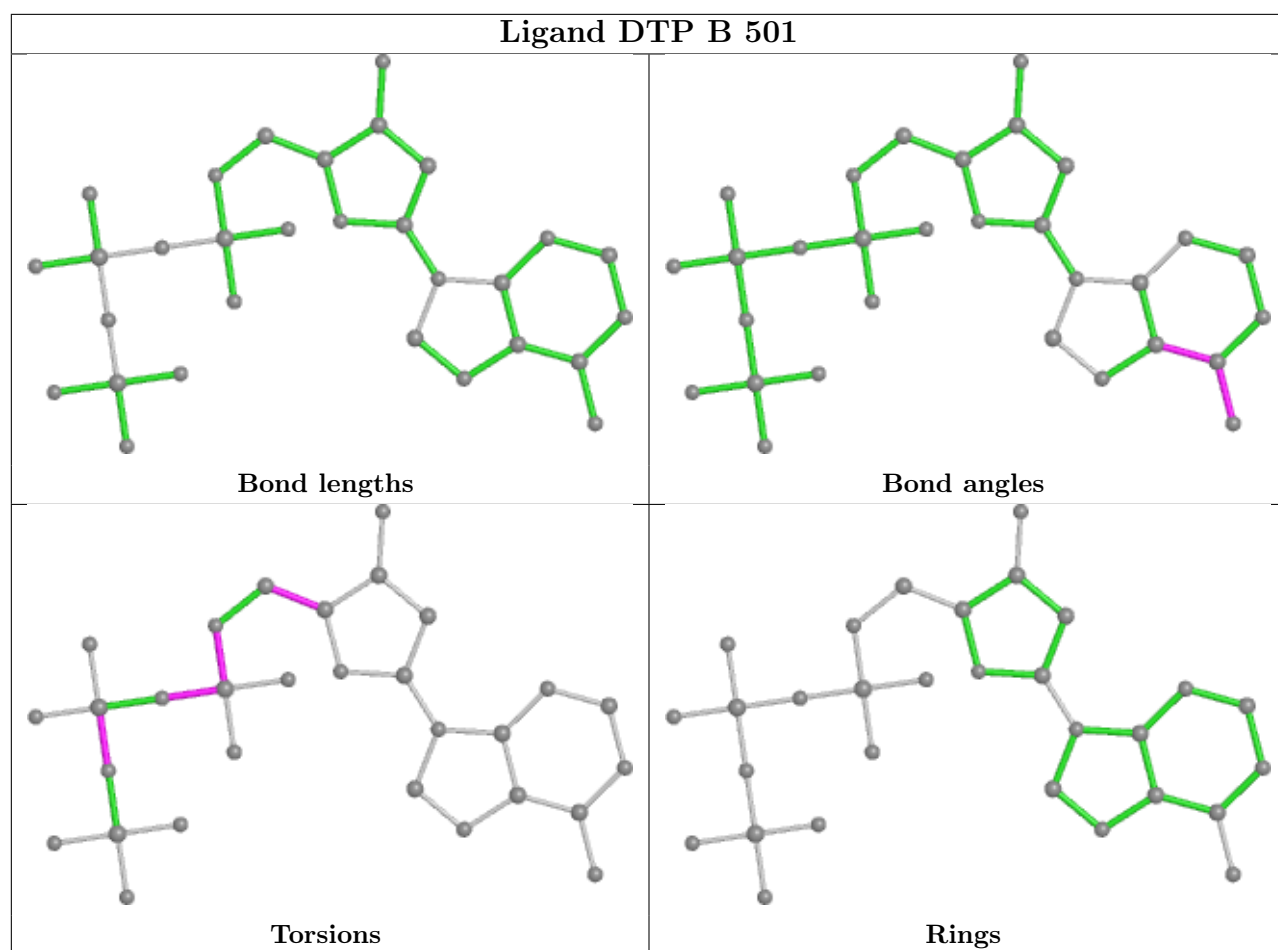
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	DTP	3	0
4	E	501	DTP	5	0
4	C	501	DTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

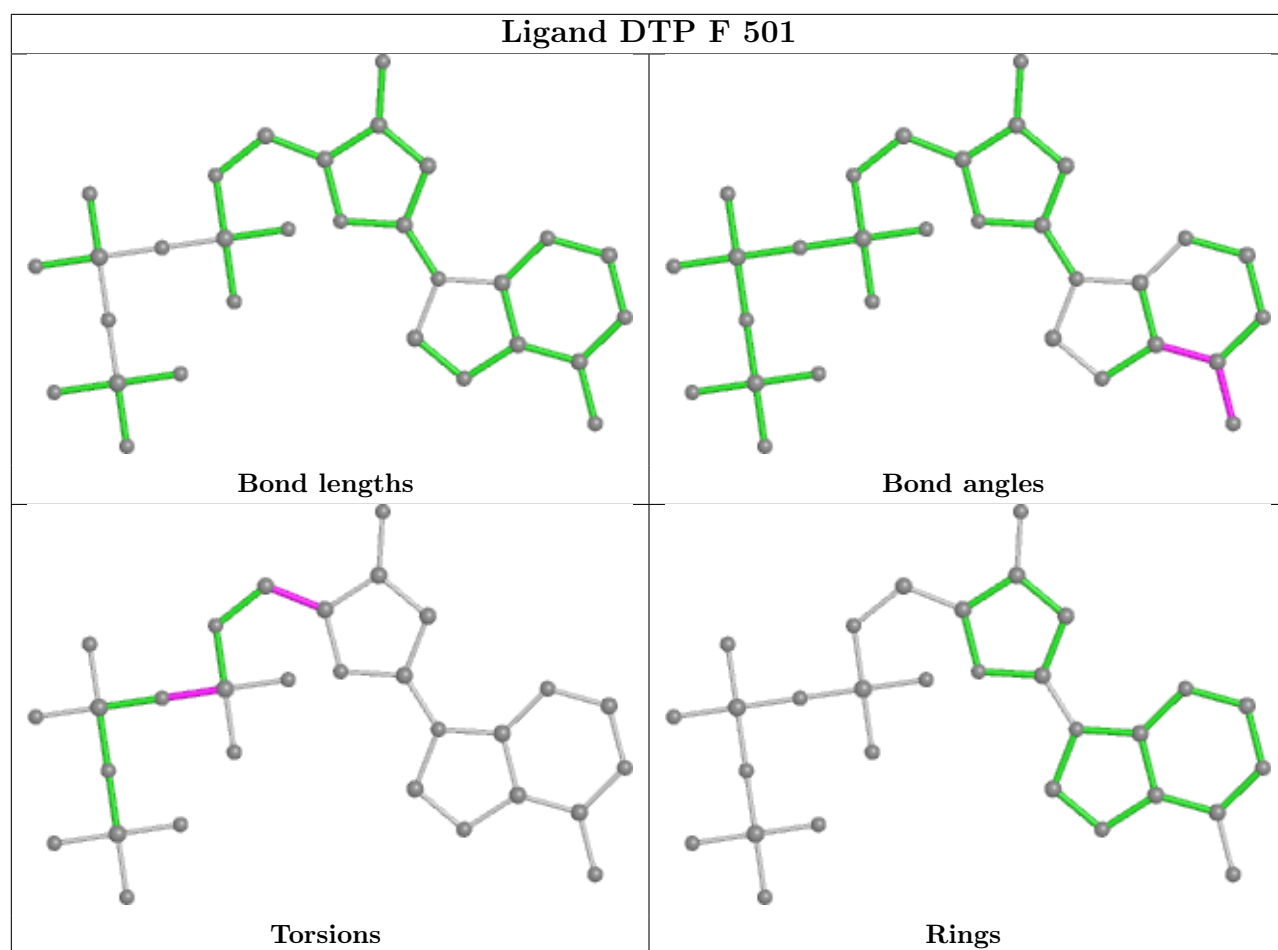
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

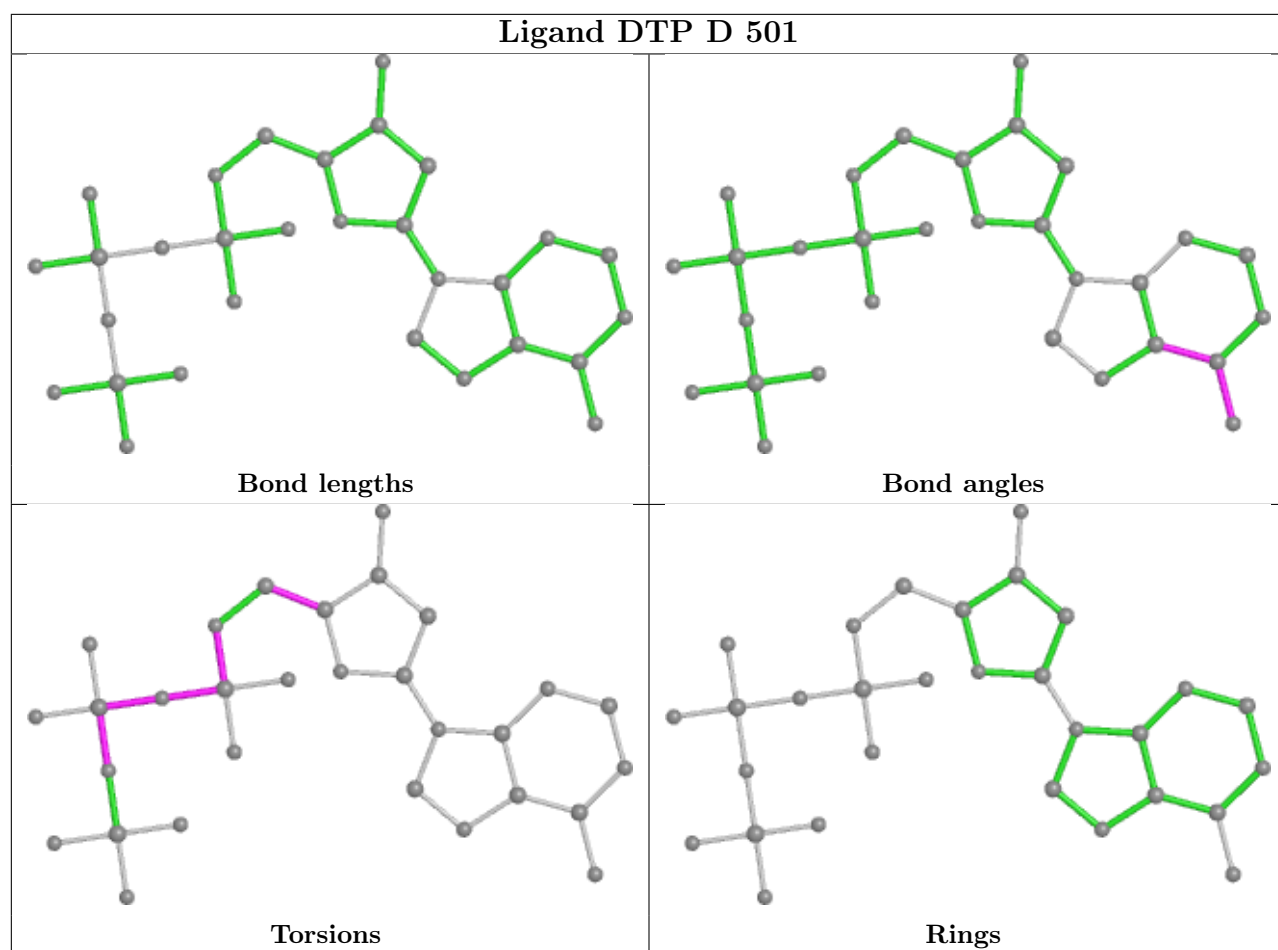


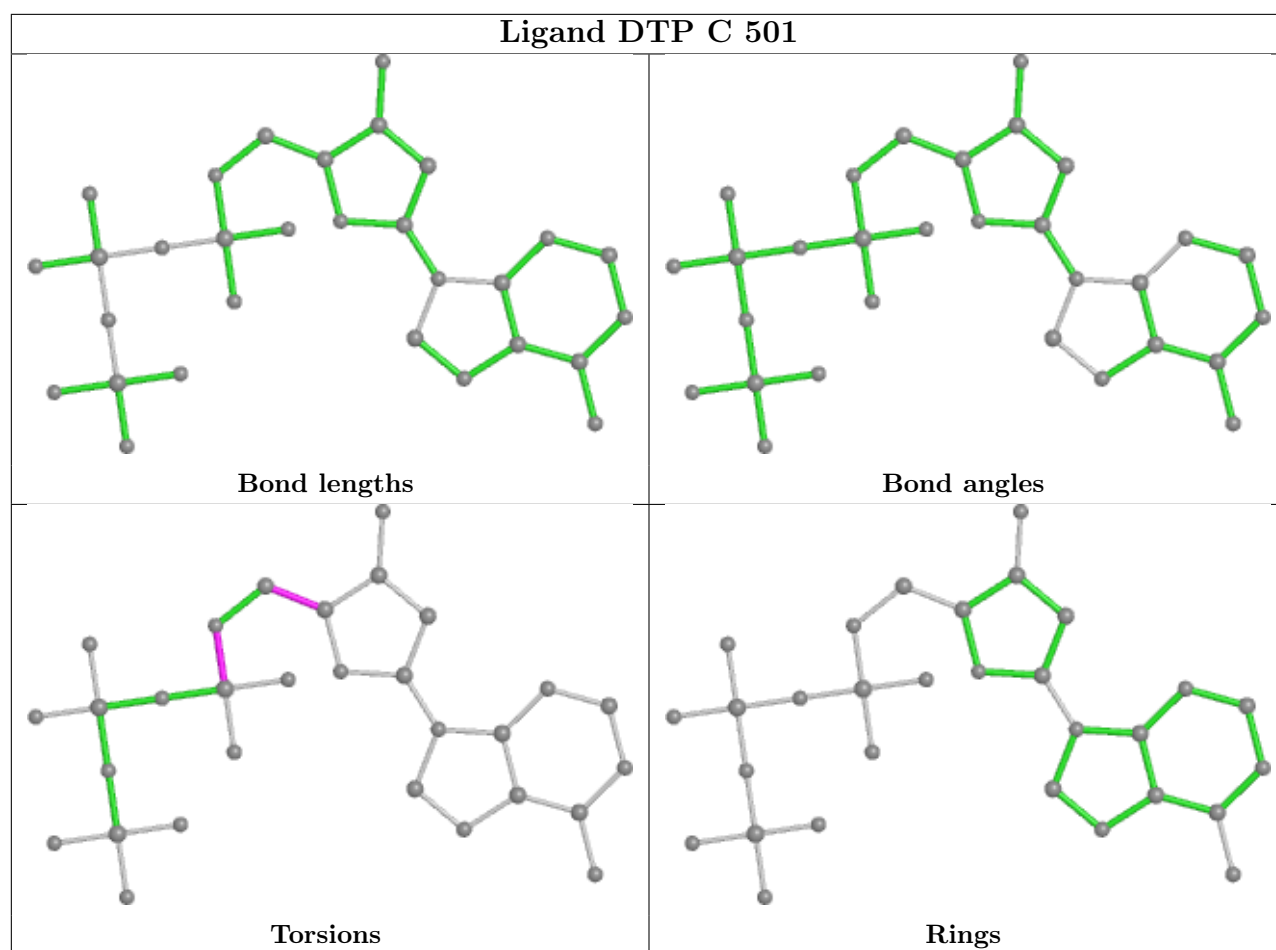












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.