wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:32 AM EDT

PDB ID	:	4LZZ / pdb_00004lzz
Title	:	Nucleotide-induced asymmetry within atpase activator ring drives s54-RNAP interaction and ATP hydrolysis
Authors	:	Sysoeva, T.A.; Chowdhury, S.; Guo, L.; Nixon, B.T.
Deposited on	:	2013-08-01
Resolution	:	3.21 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

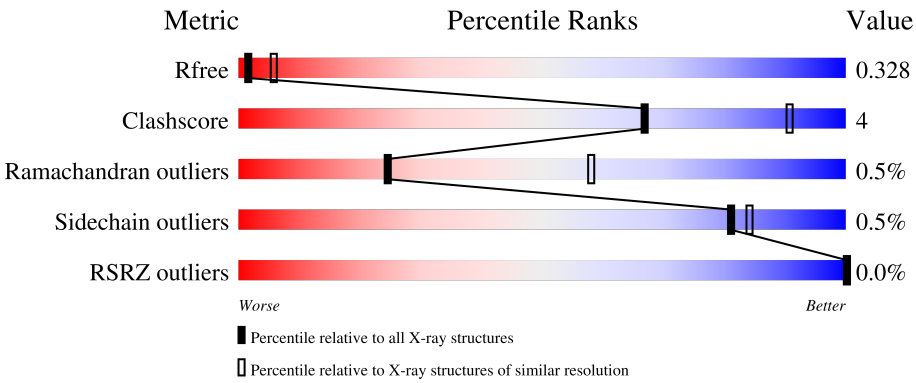
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	268	83% 9% 8%
1	B	268	83% 9% 8%
1	C	268	85% 7% 8%
1	D	268	85% 7% 8%
1	E	268	84% 11% •

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Mol	Chain	Length	Quality of chain
1	F	268	82% 9% 8%
1	G	268	82% 10% 8%
1	H	268	78% 13% 8%
1	I	268	84% 8% • 7%
1	J	268	87% 5% 8%
1	K	268	84% 8% 8%
1	L	268	81% 10% • 8%
1	M	268	81% 10% • 8%
1	N	268	81% 10% 8%
1	O	268	83% 9% • 8%
1	P	268	86% 6% 8%
1	Q	268	84% 7% 8%
1	R	268	75% 15% • 8%
1	S	268	83% 9% 8%
1	T	268	82% 10% 8%
1	U	268	83% 9% 8%
1	V	268	82% 9% • 8%
1	W	268	85% 8% • 7%
1	X	268	79% 10% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 97749 atoms, of which 49378 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 protein called Transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	247	4020	1278	2041	333	364	4	0	0	0
1	B	247	4020	1278	2041	333	364	4	0	0	0
1	C	247	4021	1278	2042	333	364	4	0	0	0
1	D	247	4018	1278	2039	333	364	4	0	0	0
1	E	258	4227	1339	2149	352	383	4	0	0	0
1	F	247	4021	1278	2042	333	364	4	0	0	0
1	G	247	4020	1278	2041	333	364	4	0	0	0
1	H	247	4020	1278	2041	333	364	4	0	0	0
1	I	248	4036	1283	2048	334	367	4	0	0	0
1	J	247	4021	1278	2042	333	364	4	0	0	0
1	K	247	4019	1278	2040	333	364	4	0	0	0
1	L	246	4006	1273	2036	332	361	4	0	0	0
1	M	247	4021	1278	2042	333	364	4	0	0	0
1	N	247	4020	1278	2041	333	364	4	0	0	0
1	O	247	4021	1278	2042	333	364	4	0	0	0
1	P	247	4020	1278	2041	333	364	4	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	Q	247	4020	1278	2041	333	364	4	0	0	0
1	R	247	4021	1278	2042	333	364	4	0	0	0
1	S	247	4020	1278	2041	333	364	4	0	0	0
1	T	247	4021	1278	2042	333	364	4	0	0	0
1	U	247	4021	1278	2042	333	364	4	0	0	0
1	V	247	4021	1278	2042	333	364	4	0	0	0
1	W	250	4065	1292	2060	337	372	4	0	0	0
1	X	246	4006	1273	2036	332	361	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	initiating methionine	UNP O67198
B	120	MET	-	initiating methionine	UNP O67198
C	120	MET	-	initiating methionine	UNP O67198
D	120	MET	-	initiating methionine	UNP O67198
E	120	MET	-	initiating methionine	UNP O67198
F	120	MET	-	initiating methionine	UNP O67198
G	120	MET	-	initiating methionine	UNP O67198
H	120	MET	-	initiating methionine	UNP O67198
I	120	MET	-	initiating methionine	UNP O67198
J	120	MET	-	initiating methionine	UNP O67198
K	120	MET	-	initiating methionine	UNP O67198
L	120	MET	-	initiating methionine	UNP O67198
M	120	MET	-	initiating methionine	UNP O67198
N	120	MET	-	initiating methionine	UNP O67198
O	120	MET	-	initiating methionine	UNP O67198
P	120	MET	-	initiating methionine	UNP O67198
Q	120	MET	-	initiating methionine	UNP O67198
R	120	MET	-	initiating methionine	UNP O67198
S	120	MET	-	initiating methionine	UNP O67198
T	120	MET	-	initiating methionine	UNP O67198
U	120	MET	-	initiating methionine	UNP O67198
V	120	MET	-	initiating methionine	UNP O67198
W	120	MET	-	initiating methionine	UNP O67198

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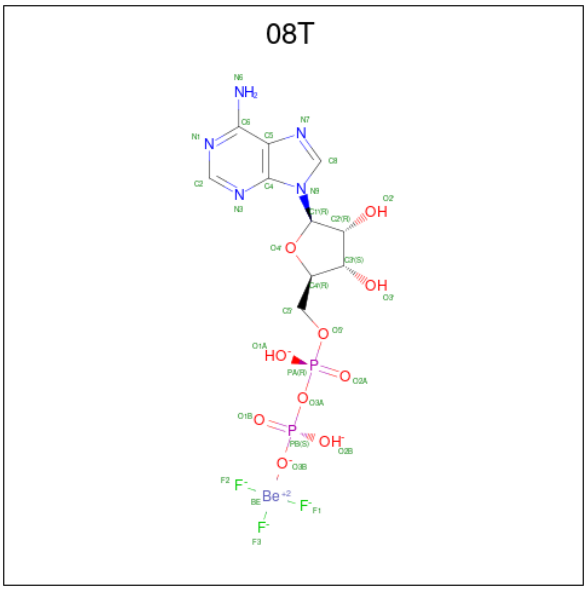
Chain	Residue	Modelled	Actual	Comment	Reference
X	120	MET	-	initiating methionine	UNP O67198

- Molecule 2 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (CCD ID: 08T) (formula: $C_{10}H_{14}BeF_3N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	Be	C	F	H	N	O	P		
2	A	1	42	1	10	3	11	5	10	2	0	0
2	B	1	42	1	10	3	11	5	10	2	0	0
2	C	1	42	1	10	3	11	5	10	2	0	0
2	D	1	42	1	10	3	11	5	10	2	0	0
2	E	1	42	1	10	3	11	5	10	2	0	0
2	G	1	42	1	10	3	11	5	10	2	0	0
2	H	1	42	1	10	3	11	5	10	2	0	0
2	I	1	42	1	10	3	11	5	10	2	0	0
2	J	1	42	1	10	3	11	5	10	2	0	0
2	K	1	42	1	10	3	11	5	10	2	0	0

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Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	Be	C	F	H	N	O	P		
2	M	1	42	1	10	3	11	5	10	2	0	0
2	N	1	42	1	10	3	11	5	10	2	0	0
2	O	1	42	1	10	3	11	5	10	2	0	0
2	P	1	42	1	10	3	11	5	10	2	0	0
2	Q	1	42	1	10	3	11	5	10	2	0	0
2	R	1	42	1	10	3	11	5	10	2	0	0
2	S	1	42	1	10	3	11	5	10	2	0	0
2	T	1	42	1	10	3	11	5	10	2	0	0
2	U	1	42	1	10	3	11	5	10	2	0	0
2	V	1	42	1	10	3	11	5	10	2	0	0
2	W	1	42	1	10	3	11	5	10	2	0	0
2	X	1	42	1	10	3	11	5	10	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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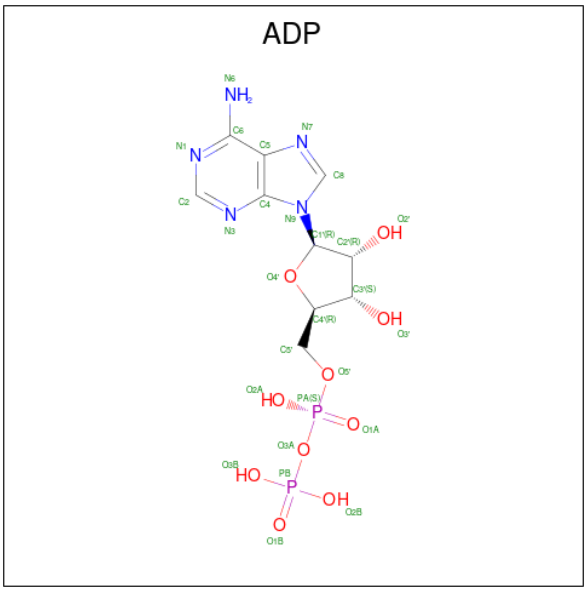
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	H	1	1	1	0	0
3	I	1	1	1	0	0
3	J	1	1	1	0	0
3	K	1	1	1	0	0
3	L	1	1	1	0	0
3	N	1	1	1	0	0
3	O	1	1	1	0	0
3	P	1	1	1	0	0
3	Q	1	1	1	0	0
3	R	1	1	1	0	0
3	S	1	1	1	0	0
3	T	1	1	1	0	0
3	U	1	1	1	0	0
3	V	1	1	1	0	0
3	W	1	1	1	0	0
3	X	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



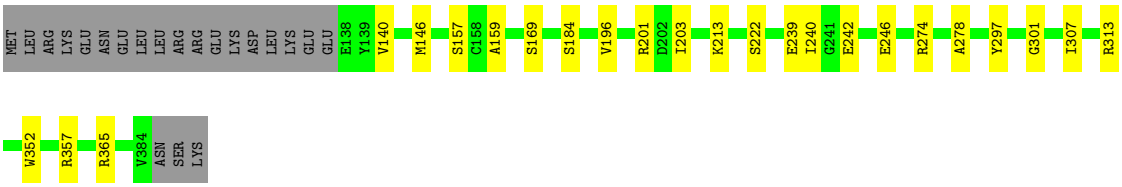
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	F	1	38	10	11	5	10	2	0	0
			Total	C	H	N	O	P		
4	L	1	38	10	11	5	10	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transcriptional regulator (NtrC family)

Chain A:



• Molecule 1: Transcriptional regulator (NtrC family)

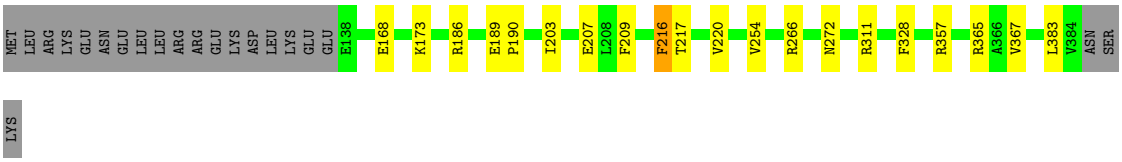
Chain B:

• Molecule 1: Transcriptional regulator (NtrC family)

Chain C:

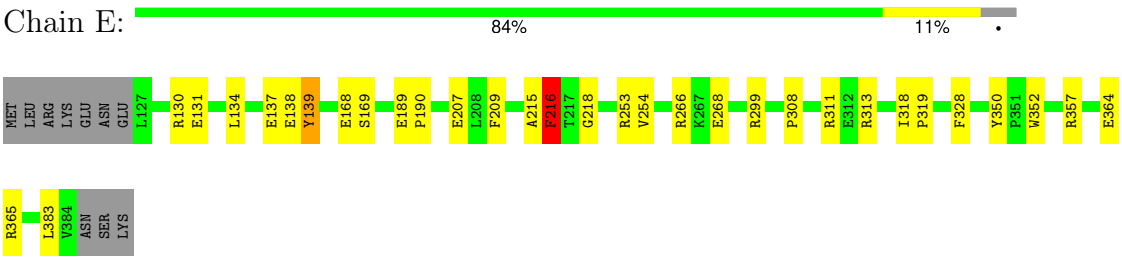
• Molecule 1: Transcriptional regulator (NtrC family)

Chain D:



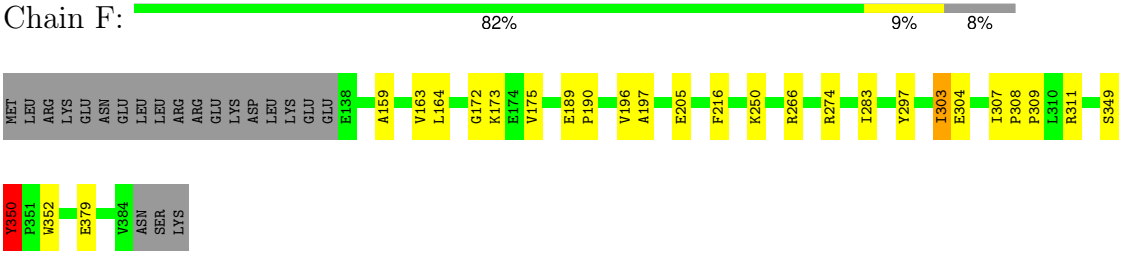
• Molecule 1: Transcriptional regulator (NtrC family)

Chain E:



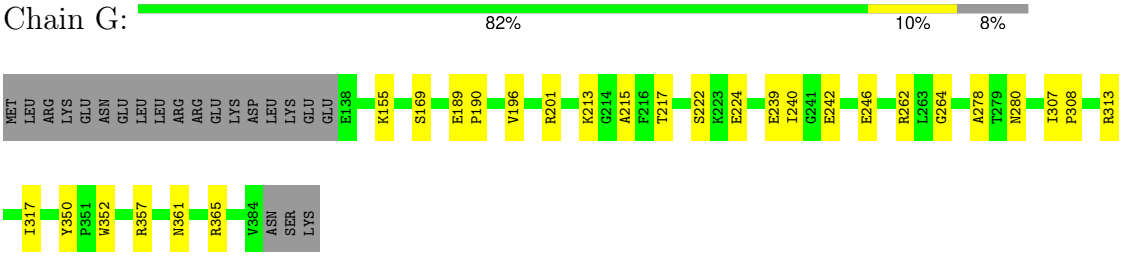
• Molecule 1: Transcriptional regulator (NtrC family)

Chain F:



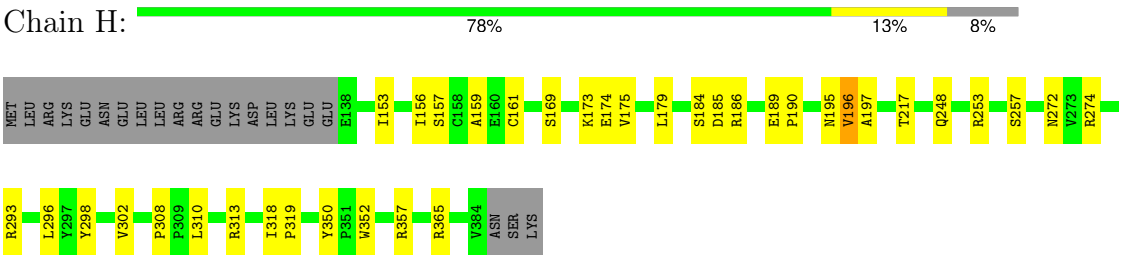
• Molecule 1: Transcriptional regulator (NtrC family)

Chain G:



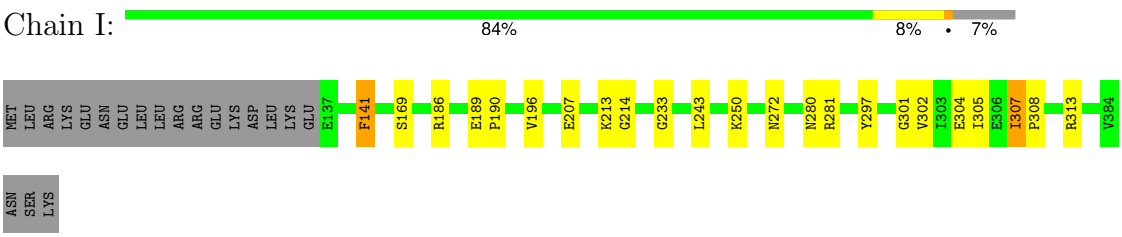
• Molecule 1: Transcriptional regulator (NtrC family)

Chain H:



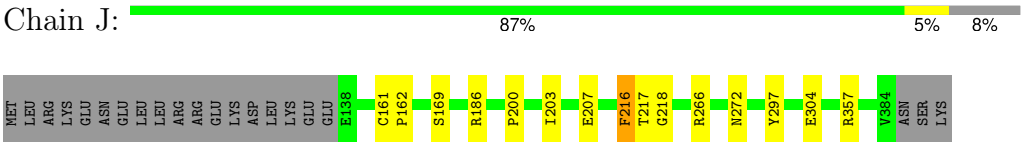
• Molecule 1: Transcriptional regulator (NtrC family)

Chain I:



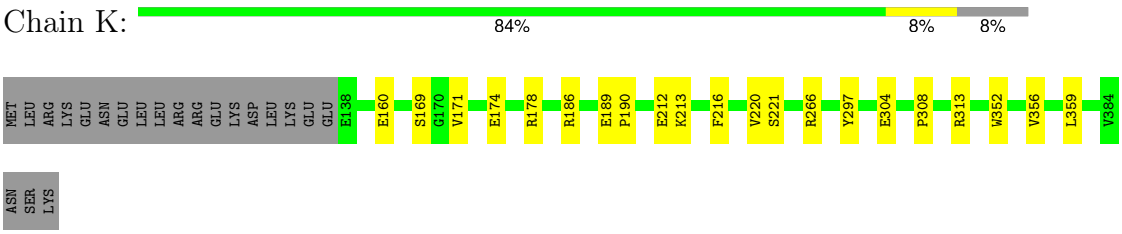
• Molecule 1: Transcriptional regulator (NtrC family)

Chain J:



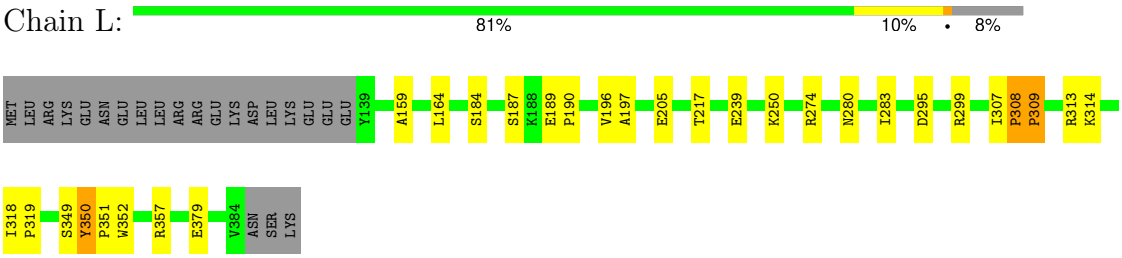
• Molecule 1: Transcriptional regulator (NtrC family)

Chain K:



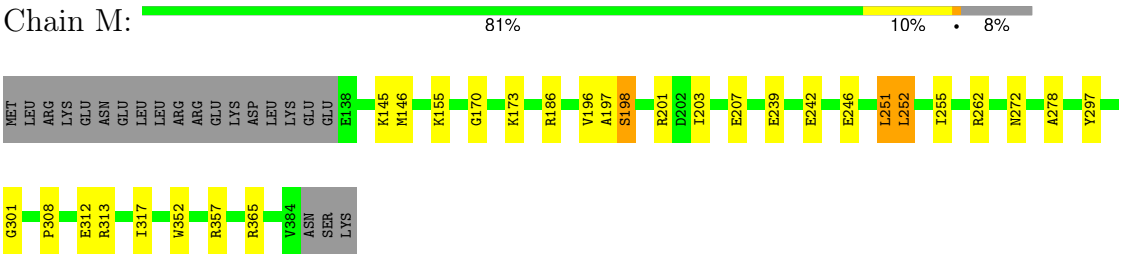
• Molecule 1: Transcriptional regulator (NtrC family)

Chain L:



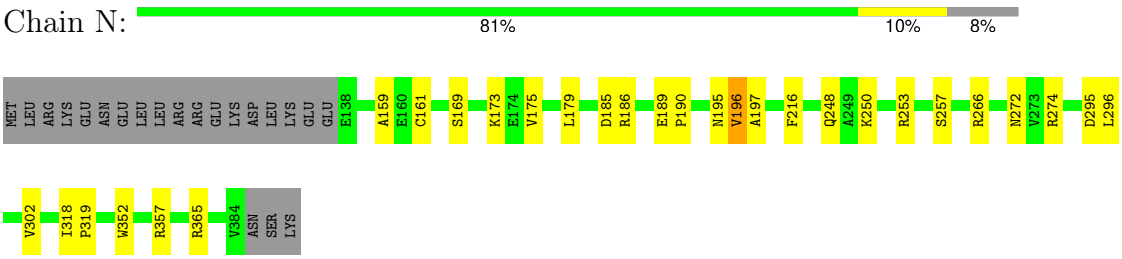
• Molecule 1: Transcriptional regulator (NtrC family)

Chain M:



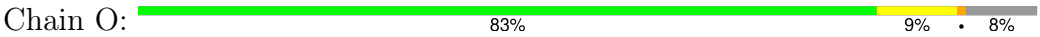
• Molecule 1: Transcriptional regulator (NtrC family)

Chain N:



• Molecule 1: Transcriptional regulator (NtrC family)

Chain O:



MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 S169 E174 R186 E189 P190 S198 I203 E207 E212 K213 G214 A215 F216 A219 V220 E224 F227 K250 V254 N272 R299 V302 I305 E306

I307 V384 ASN SER LYS

- Molecule 1: Transcriptional regulator (NtrC family)

Chain P: 86% 6% 8%

MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 S169 R186 E189 P190 V196 A197 P200 I203 E207 F216 A219 V220 S221 K250 R266 N272 R357 V384 ASN SER LYS

- Molecule 1: Transcriptional regulator (NtrC family)

Chain Q: 84% 7% 8%

MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 A159 S169 K173 E174 R178 S198 G214 A215 F216 A249 L252 R253 R266 K267 E268 R274 Y297 E304 P308 R313 R357 N361 R365

V384 ASN SER LYS

- Molecule 1: Transcriptional regulator (NtrC family)

Chain R: 75% 15% • 8%

MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 M146 I149 K173 E174 V175 L179 E189 P190 I199 P200 R201 D202 I203 E212 K213 G214 A215 F216 T217 G218 S222 F227 L237 I240 K250 S257 G258 K259

R262 G265 R266 A277 I283 F292 D295 L296 V302 I307 P308 P309 R313 I318 P319 S349 Y350 P351 W352 V356 E379 V384 ASN SER LYS

- Molecule 1: Transcriptional regulator (NtrC family)

Chain S: 83% 9% 8%

MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 M146 S169 E174 V192 A193 L194 N195 V196 A197 S198 L208 V220 F226 E239 I240 A278 D295 L296 Y297 G301 I307 P308 R313 Y350 P351 W352

V356 R357 R365 V384 ASN SER LYS

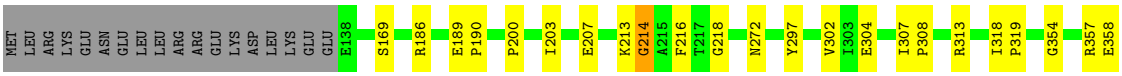
- Molecule 1: Transcriptional regulator (NtrC family)

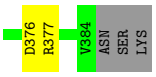
Chain T: 82% 10% 8%

MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 C161 E168 S169 G170 K173 R186 E189 P190 N195 V196 E212 E239 R253 V254 I255 E256 S257 R262 N272 V273 R274 D295 L296 V302 R311 L346

• Molecule 1: Transcriptional regulator (NtrC family)

Chain U:





• Molecule 1: Transcriptional regulator (NtrC family)

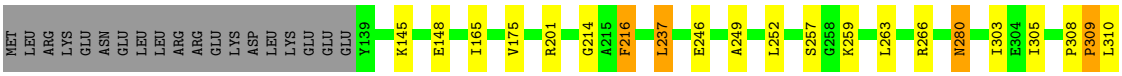
Chain V:

• Molecule 1: Transcriptional regulator (NtrC family)

Chain W:

• Molecule 1: Transcriptional regulator (NtrC family)

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	119.97Å 130.83Å 208.23Å 90.01° 90.01° 89.85°	Depositor
Resolution (Å)	44.27 – 3.21 44.27 – 3.21	Depositor EDS
% Data completeness (in resolution range)	50.5 (44.27-3.21) 50.6 (44.27-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.267 , 0.322 0.270 , 0.328	Depositor DCC
R_{free} test set	1107 reflections (0.53%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.236 for h,-k,-l 0.359 for -h,k,-l 0.229 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	97749	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 08T

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	0.34	0/2013	0.80	1/2700 (0.0%)
1	B	0.37	0/2013	0.80	2/2700 (0.1%)
1	C	0.37	0/2013	0.77	0/2700
1	D	0.41	0/2013	0.79	3/2700 (0.1%)
1	E	0.39	0/2112	0.82	3/2830 (0.1%)
1	F	0.37	0/2013	0.87	6/2700 (0.2%)
1	G	0.36	0/2013	0.80	3/2700 (0.1%)
1	H	0.37	0/2013	0.80	2/2700 (0.1%)
1	I	0.38	0/2022	0.77	0/2712
1	J	0.38	0/2013	0.79	1/2700 (0.0%)
1	K	0.37	0/2013	0.76	0/2700
1	L	0.37	0/2004	0.86	5/2688 (0.2%)
1	M	0.37	0/2013	0.84	4/2700 (0.1%)
1	N	0.36	0/2013	0.76	0/2700
1	O	0.40	0/2013	0.81	0/2700
1	P	0.37	0/2013	0.79	1/2700 (0.0%)
1	Q	0.37	0/2013	0.76	0/2700
1	R	0.43	0/2013	1.09	12/2700 (0.4%)
1	S	0.34	0/2013	0.85	4/2700 (0.1%)
1	T	0.35	0/2013	0.78	1/2700 (0.0%)
1	U	0.36	0/2013	0.77	1/2700 (0.0%)
1	V	0.39	0/2013	0.78	0/2700
1	W	0.38	0/2039	0.77	2/2735 (0.1%)
1	X	0.43	0/2004	1.04	6/2688 (0.2%)
All	All	0.38	0/48428	0.82	57/64953 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	1
1	L	0	1
1	U	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	349	SER	N-CA-C	-9.15	92.55	108.20
1	J	217	THR	N-CA-C	-8.74	103.71	112.97
1	S	220	VAL	N-CA-C	-8.72	104.73	111.62
1	R	350	TYR	N-CA-C	7.68	126.79	109.81
1	W	220	VAL	N-CA-C	-7.64	104.99	111.56

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	216	PHE	Peptide
1	E	216	PHE	Peptide
1	F	350	TYR	Peptide
1	L	350	TYR	Peptide
1	U	213	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1979	2041	2039	15	0
1	B	1979	2041	2039	18	0
1	C	1979	2042	2040	13	0
1	D	1979	2039	2037	13	0
1	E	2078	2149	2147	20	0
1	F	1979	2042	2040	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1979	2041	2039	17	0
1	H	1979	2041	2039	24	0
1	I	1988	2048	2046	15	0
1	J	1979	2042	2040	9	0
1	K	1979	2040	2038	12	0
1	L	1970	2036	2034	14	0
1	M	1979	2042	2040	18	0
1	N	1979	2041	2039	22	0
1	O	1979	2042	2040	21	0
1	P	1979	2041	2039	12	0
1	Q	1979	2041	2039	14	0
1	R	1979	2042	2040	26	0
1	S	1979	2041	2039	14	0
1	T	1979	2042	2040	20	0
1	U	1979	2042	2039	14	0
1	V	1979	2042	2040	17	0
1	W	2005	2060	2058	14	0
1	X	1970	2036	2034	20	0
2	A	31	11	13	1	0
2	B	31	11	13	2	0
2	C	31	11	13	2	0
2	D	31	11	13	5	0
2	E	31	11	13	2	0
2	G	31	11	13	1	0
2	H	31	11	13	2	0
2	I	31	11	13	1	0
2	J	31	11	13	2	0
2	K	31	11	13	3	0
2	M	31	11	13	3	0
2	N	31	11	13	4	0
2	O	31	11	13	2	0
2	P	31	11	13	2	0
2	Q	31	11	12	2	0
2	R	31	11	13	4	0
2	S	31	11	13	3	0
2	T	31	11	13	8	0
2	U	31	11	13	2	0
2	V	31	11	13	3	0
2	W	31	11	13	2	0
2	X	31	11	13	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	F	27	11	12	3	0
4	L	27	11	12	1	0
All	All	48371	49378	49374	357	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 4.

The worst 5 of 357 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:M:146:MET:SD	1:M:313:ARG:NH2	2.51	0.83
1:O:219:ALA:HB1	1:O:220:VAL:HA	1.61	0.82
1:T:186:ARG:NH2	1:T:272:ASN:OD1	2.13	0.82
1:B:186:ARG:NH2	1:B:272:ASN:OD1	2.15	0.79
1:M:357:ARG:NH1	2:M:400:08T:O3'	2.17	0.78

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	
1	A	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	30	61
1	B	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	16	48
1	C	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	30	61
1	D	245/268 (91%)	233 (95%)	12 (5%)	0	100	100
1	E	256/268 (96%)	237 (93%)	16 (6%)	3 (1%)	10	40
1	F	245/268 (91%)	234 (96%)	10 (4%)	1 (0%)	30	61
1	G	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	30	61
1	H	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	16	48
1	I	246/268 (92%)	234 (95%)	11 (4%)	1 (0%)	30	61
1	J	245/268 (91%)	234 (96%)	11 (4%)	0	100	100
1	K	245/268 (91%)	235 (96%)	10 (4%)	0	100	100
1	L	244/268 (91%)	229 (94%)	12 (5%)	3 (1%)	10	40
1	M	245/268 (91%)	228 (93%)	15 (6%)	2 (1%)	16	48
1	N	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	16	48
1	O	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	30	61
1	P	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	30	61
1	Q	245/268 (91%)	236 (96%)	9 (4%)	0	100	100
1	R	245/268 (91%)	233 (95%)	9 (4%)	3 (1%)	10	40
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	30	61
1	T	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	16	48
1	U	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	30	61
1	V	245/268 (91%)	235 (96%)	9 (4%)	1 (0%)	30	61
1	W	248/268 (92%)	238 (96%)	9 (4%)	1 (0%)	30	61
1	X	244/268 (91%)	232 (95%)	10 (4%)	2 (1%)	16	48
All	All	5893/6432 (92%)	5594 (95%)	267 (4%)	32 (0%)	24	58

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	H	196	VAL
1	N	196	VAL
1	R	217	THR
1	R	350	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/233 (91%)	212 (100%)	0	100	100
1	B	212/233 (91%)	212 (100%)	0	100	100
1	C	212/233 (91%)	212 (100%)	0	100	100
1	D	212/233 (91%)	212 (100%)	0	100	100
1	E	223/233 (96%)	222 (100%)	1 (0%)	84	85
1	F	212/233 (91%)	209 (99%)	3 (1%)	59	75
1	G	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	H	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	I	213/233 (91%)	212 (100%)	1 (0%)	81	84
1	J	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	K	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	L	211/233 (91%)	210 (100%)	1 (0%)	81	84
1	M	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	N	212/233 (91%)	212 (100%)	0	100	100
1	O	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	P	212/233 (91%)	212 (100%)	0	100	100
1	Q	212/233 (91%)	210 (99%)	2 (1%)	70	79
1	R	212/233 (91%)	210 (99%)	2 (1%)	70	79
1	S	212/233 (91%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	212/233 (91%)	212 (100%)	0	100	100
1	U	212/233 (91%)	212 (100%)	0	100	100
1	V	212/233 (91%)	211 (100%)	1 (0%)	81	84
1	W	215/233 (92%)	214 (100%)	1 (0%)	81	84
1	X	211/233 (91%)	206 (98%)	5 (2%)	43	68
All	All	5101/5592 (91%)	5078 (100%)	23 (0%)	81	84

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	227	PHE
1	W	216	PHE
1	V	295	ASP
1	X	216	PHE
1	I	141	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	323	HIS
1	W	323	HIS
1	P	280	ASN
1	T	323	HIS
1	O	355	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
2	08T	N	400	1,3	31,33,33	3.23	12 (38%)	41,52,52	2.56	12 (29%)
2	08T	Q	400	1	31,33,33	3.16	13 (41%)	41,52,52	2.77	12 (29%)
2	08T	C	400	3	31,33,33	3.24	14 (45%)	41,52,52	2.47	11 (26%)
4	ADP	F	400	3	28,29,29	1.45	5 (17%)	43,45,45	1.79	11 (25%)
2	08T	T	400	1,3	31,33,33	3.23	13 (41%)	41,52,52	2.53	12 (29%)
2	08T	P	400	1,3	31,33,33	3.19	12 (38%)	41,52,52	2.60	11 (26%)
2	08T	D	400	1,3	31,33,33	3.20	12 (38%)	41,52,52	2.52	10 (24%)
2	08T	B	400	1,3	31,33,33	3.28	13 (41%)	41,52,52	2.52	10 (24%)
2	08T	E	400	3	31,33,33	3.23	12 (38%)	41,52,52	2.49	10 (24%)
2	08T	V	400	3	31,33,33	3.18	12 (38%)	41,52,52	2.55	10 (24%)
2	08T	X	400	-	31,33,33	3.17	11 (35%)	41,52,52	2.58	12 (29%)
2	08T	I	400	3	31,33,33	3.23	13 (41%)	41,52,52	2.40	9 (21%)
2	08T	A	400	1,3	31,33,33	3.19	13 (41%)	41,52,52	2.49	9 (21%)
2	08T	W	400	3	31,33,33	3.26	14 (45%)	41,52,52	2.60	11 (26%)
2	08T	O	400	3	31,33,33	3.18	12 (38%)	41,52,52	2.47	10 (24%)
2	08T	G	400	1,3	31,33,33	3.22	12 (38%)	41,52,52	2.65	11 (26%)
2	08T	K	400	1,3	31,33,33	3.21	12 (38%)	41,52,52	2.60	10 (24%)
2	08T	M	400	1	31,33,33	3.22	12 (38%)	41,52,52	2.55	10 (24%)
2	08T	R	400	3	31,33,33	3.19	12 (38%)	41,52,52	2.52	12 (29%)
2	08T	U	400	1,3	31,33,33	3.20	14 (45%)	41,52,52	2.42	9 (21%)
2	08T	H	400	1,3	31,33,33	3.20	13 (41%)	41,52,52	2.51	10 (24%)
2	08T	S	400	1,3	31,33,33	3.20	11 (35%)	41,52,52	2.53	10 (24%)
4	ADP	L	400	-	28,29,29	1.44	5 (17%)	43,45,45	1.89	10 (23%)
2	08T	J	400	3	31,33,33	3.24	13 (41%)	41,52,52	2.52	11 (26%)

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
2	08T	N	400	1,3	-	4/16/38/38	0/3/3/3
2	08T	Q	400	1	-	4/16/38/38	0/3/3/3
2	08T	C	400	3	-	5/16/38/38	0/3/3/3
4	ADP	F	400	3	-	4/16/32/32	0/3/3/3
2	08T	T	400	1,3	-	5/16/38/38	0/3/3/3
2	08T	P	400	1,3	-	1/16/38/38	0/3/3/3
2	08T	D	400	1,3	-	8/16/38/38	0/3/3/3
2	08T	B	400	1,3	-	3/16/38/38	0/3/3/3
2	08T	E	400	3	-	3/16/38/38	0/3/3/3
2	08T	V	400	3	-	2/16/38/38	0/3/3/3
2	08T	X	400	-	-	4/16/38/38	0/3/3/3
2	08T	I	400	3	-	5/16/38/38	0/3/3/3
2	08T	A	400	1,3	-	2/16/38/38	0/3/3/3
2	08T	W	400	3	-	0/16/38/38	0/3/3/3
2	08T	O	400	3	-	4/16/38/38	0/3/3/3
2	08T	G	400	1,3	-	6/16/38/38	0/3/3/3
2	08T	K	400	1,3	-	6/16/38/38	0/3/3/3
2	08T	M	400	1	-	5/16/38/38	0/3/3/3
2	08T	R	400	3	-	5/16/38/38	0/3/3/3
2	08T	U	400	1,3	-	5/16/38/38	0/3/3/3
2	08T	H	400	1,3	-	1/16/38/38	0/3/3/3
2	08T	S	400	1,3	-	4/16/38/38	0/3/3/3
4	ADP	L	400	-	-	4/16/32/32	0/3/3/3
2	08T	J	400	3	-	3/16/38/38	0/3/3/3

The worst 5 of 285 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	400	08T	F2-BE	-8.40	1.35	1.54
2	C	400	08T	F2-BE	-8.36	1.35	1.54
2	D	400	08T	F2-BE	-8.35	1.35	1.54
2	I	400	08T	F2-BE	-8.30	1.35	1.54
2	J	400	08T	F2-BE	-8.30	1.35	1.54

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	400	08T	C6-C5-N7	-7.02	118.56	132.09
2	P	400	08T	C6-C5-N7	-6.97	118.65	132.09
2	G	400	08T	C6-C5-N7	-6.80	118.98	132.09
2	V	400	08T	C6-C5-N7	-6.78	119.01	132.09
2	M	400	08T	C6-C5-N7	-6.75	119.07	132.09

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	400	08T	C5'-O5'-PA-O1A
2	D	400	08T	C5'-O5'-PA-O2A
2	D	400	08T	C5'-O5'-PA-O3A
2	G	400	08T	C5'-O5'-PA-O1A
2	G	400	08T	C5'-O5'-PA-O2A

There are no ring outliers.

24 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	400	08T	4	0
2	Q	400	08T	2	0
2	C	400	08T	2	0
4	F	400	ADP	3	0
2	T	400	08T	8	0
2	P	400	08T	2	0
2	D	400	08T	5	0
2	B	400	08T	2	0
2	E	400	08T	2	0
2	V	400	08T	3	0
2	X	400	08T	4	0
2	I	400	08T	1	0
2	A	400	08T	1	0
2	W	400	08T	2	0
2	O	400	08T	2	0
2	G	400	08T	1	0
2	K	400	08T	3	0
2	M	400	08T	3	0
2	R	400	08T	4	0
2	U	400	08T	2	0
2	H	400	08T	2	0
2	S	400	08T	3	0

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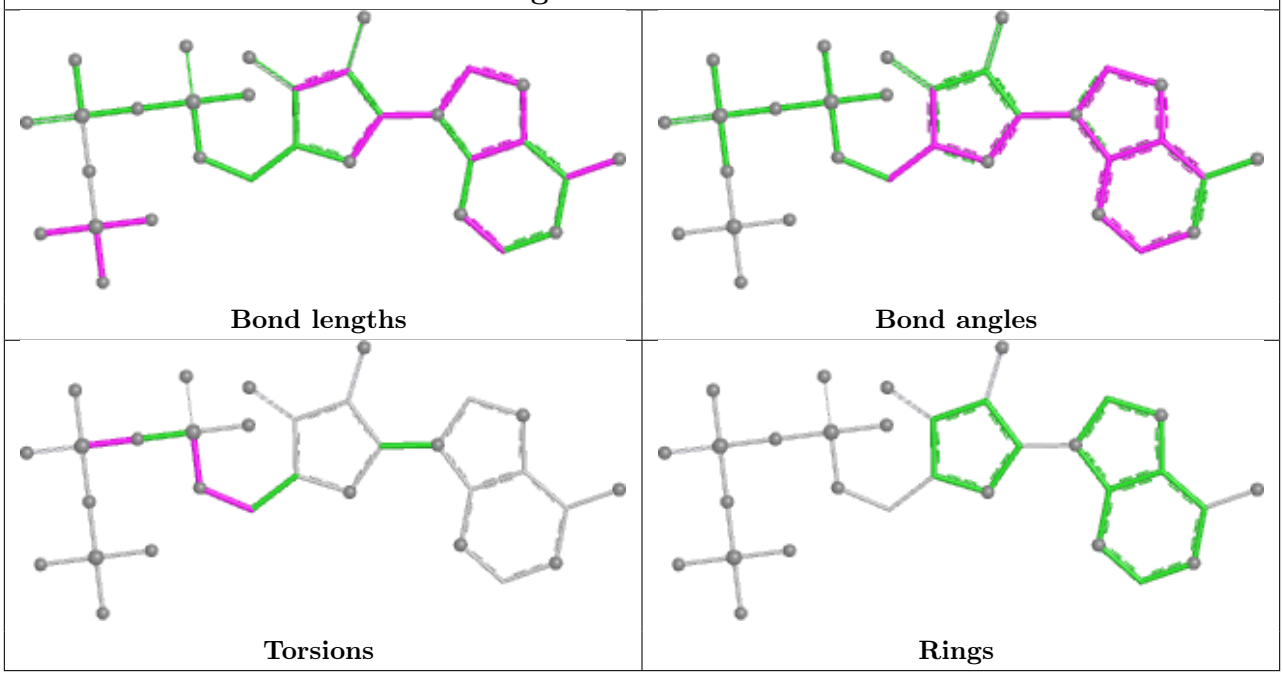
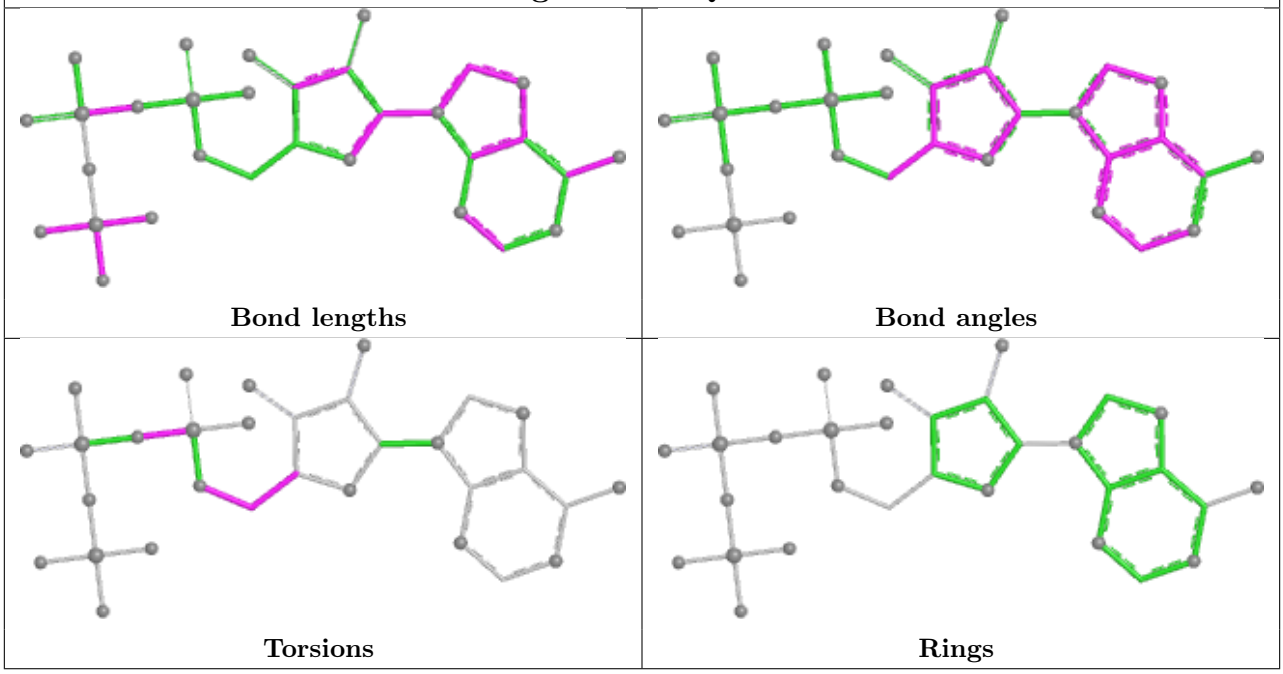
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	400	ADP	1	0
2	J	400	08T	2	0

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

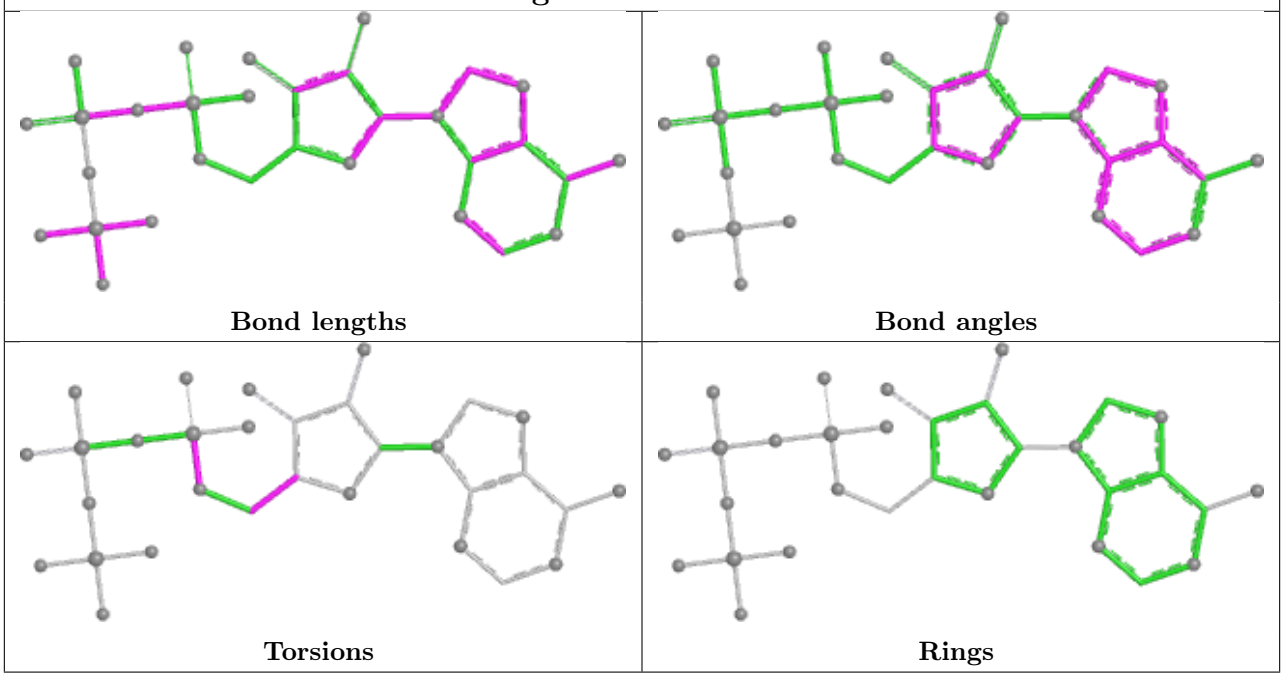
Ligand 08T N 400



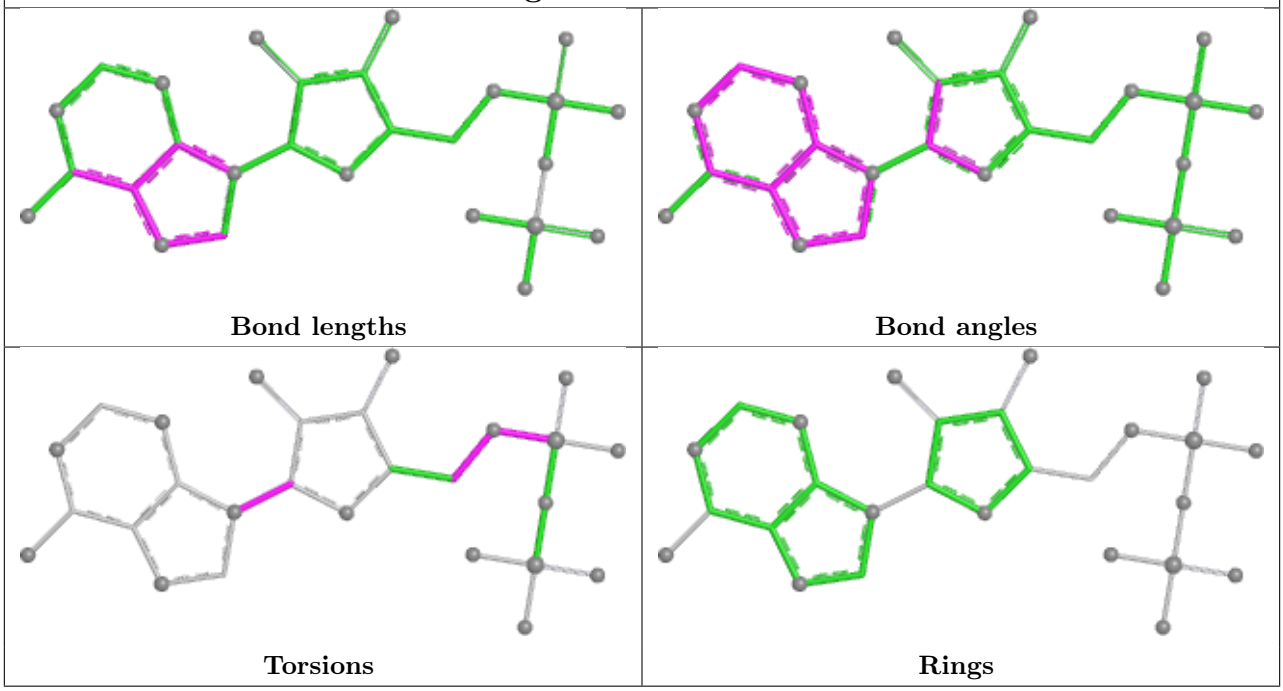
Ligand 08T Q 400



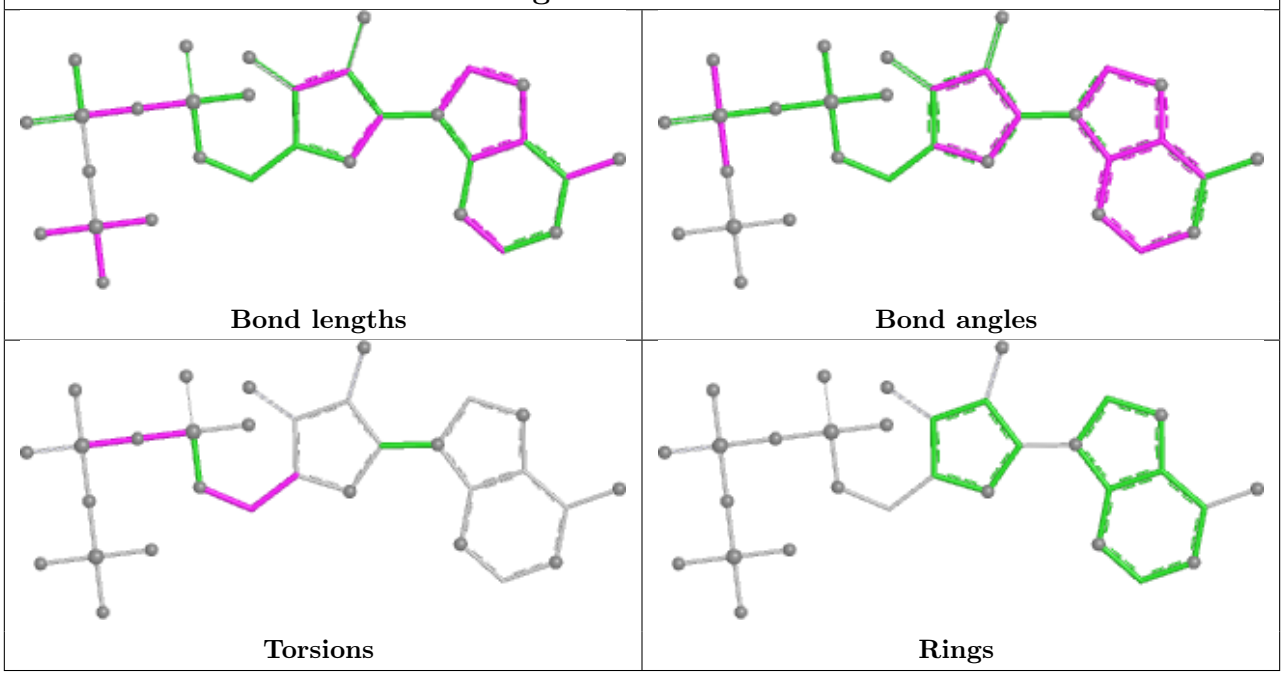
Ligand 08T C 400



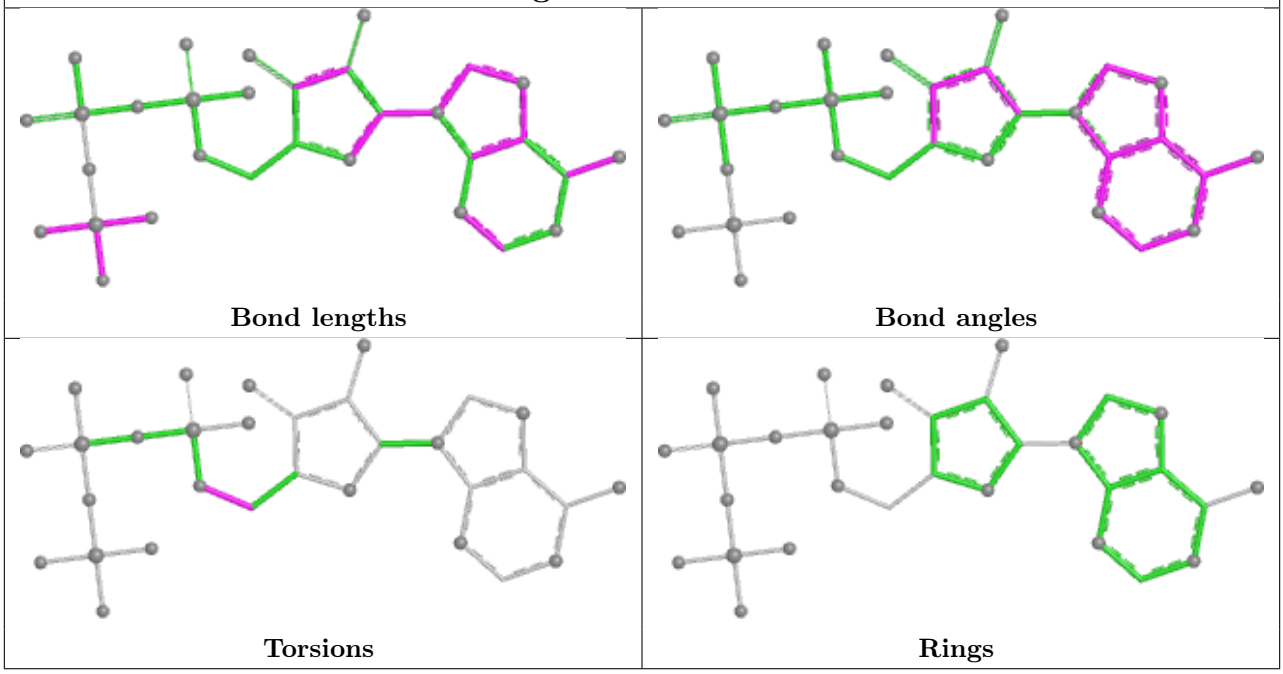
Ligand ADP F 400



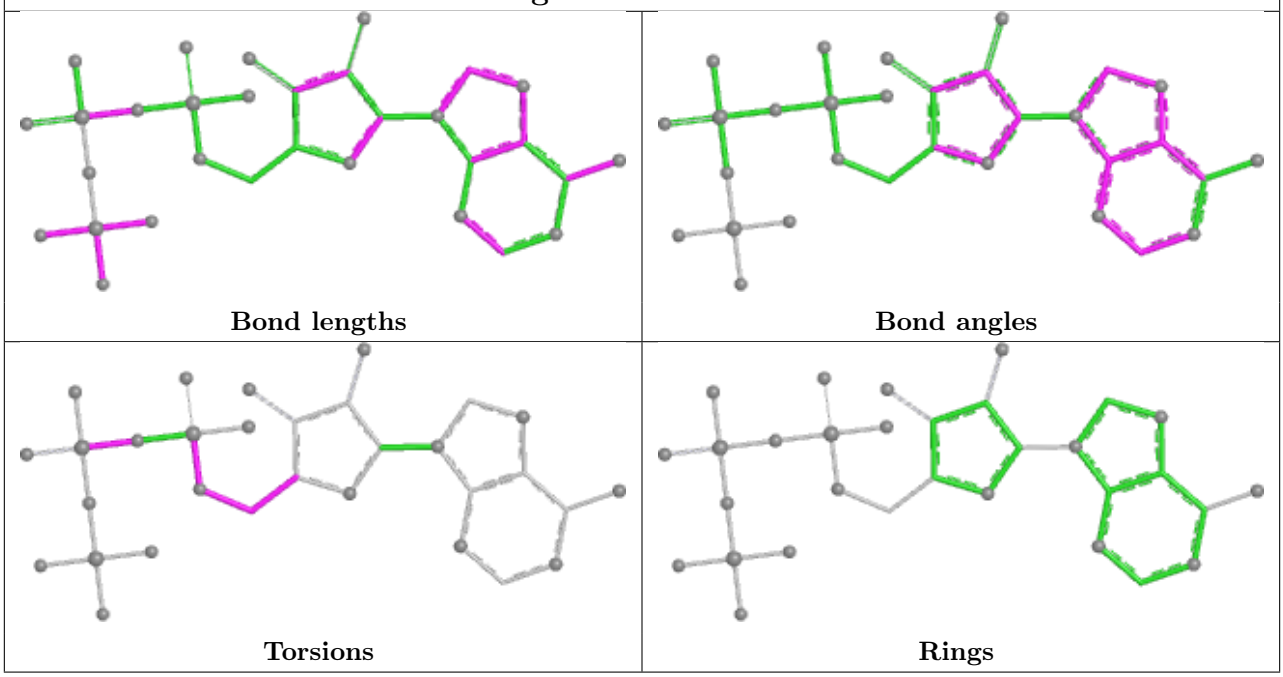
Ligand 08T T 400



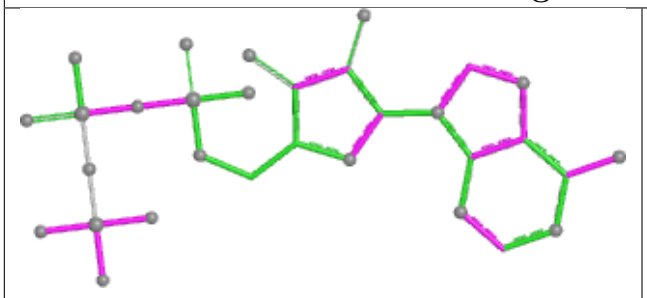
Ligand 08T P 400



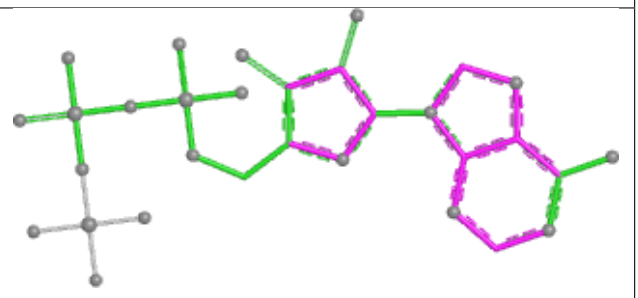
Ligand 08T D 400



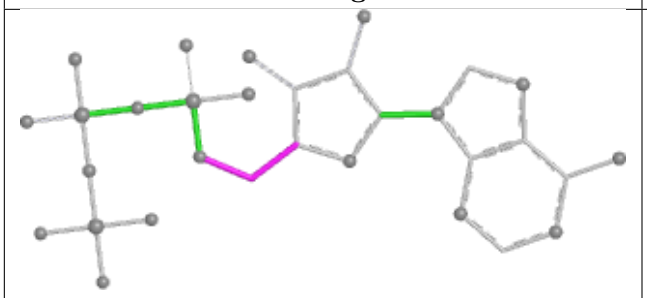
Ligand 08T B 400



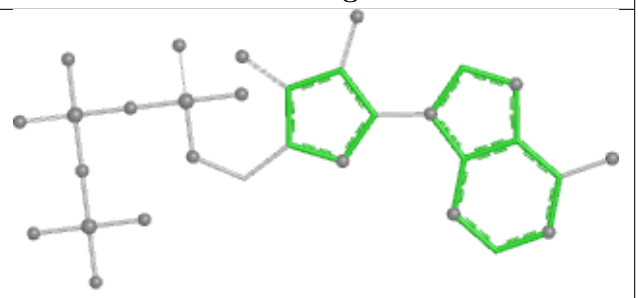
Bond lengths



Bond angles

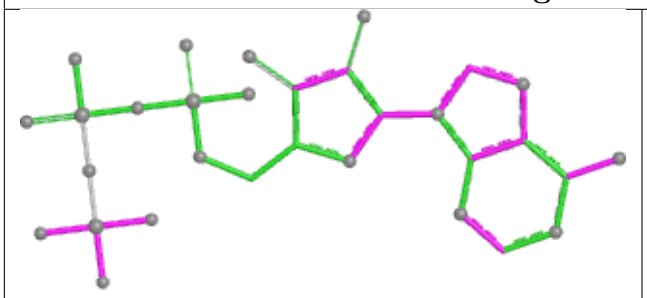


Torsions

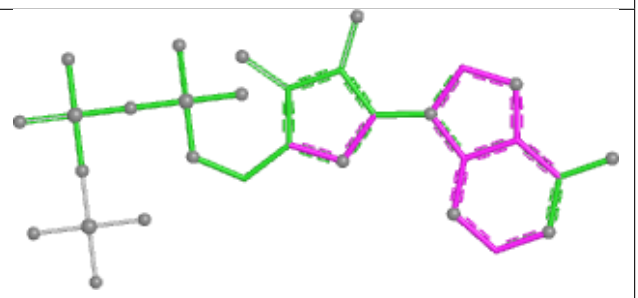


Rings

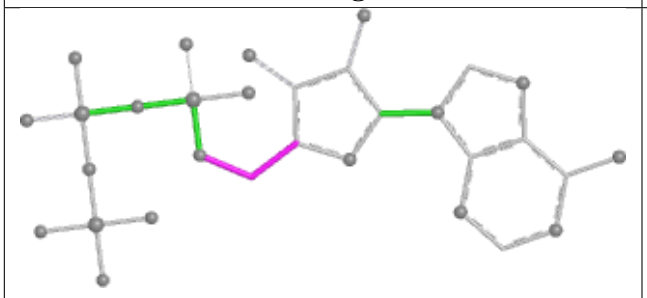
Ligand 08T E 400



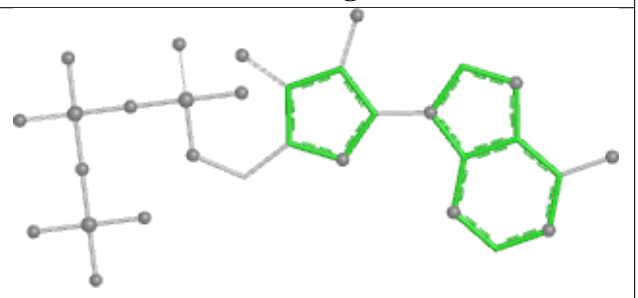
Bond lengths



Bond angles

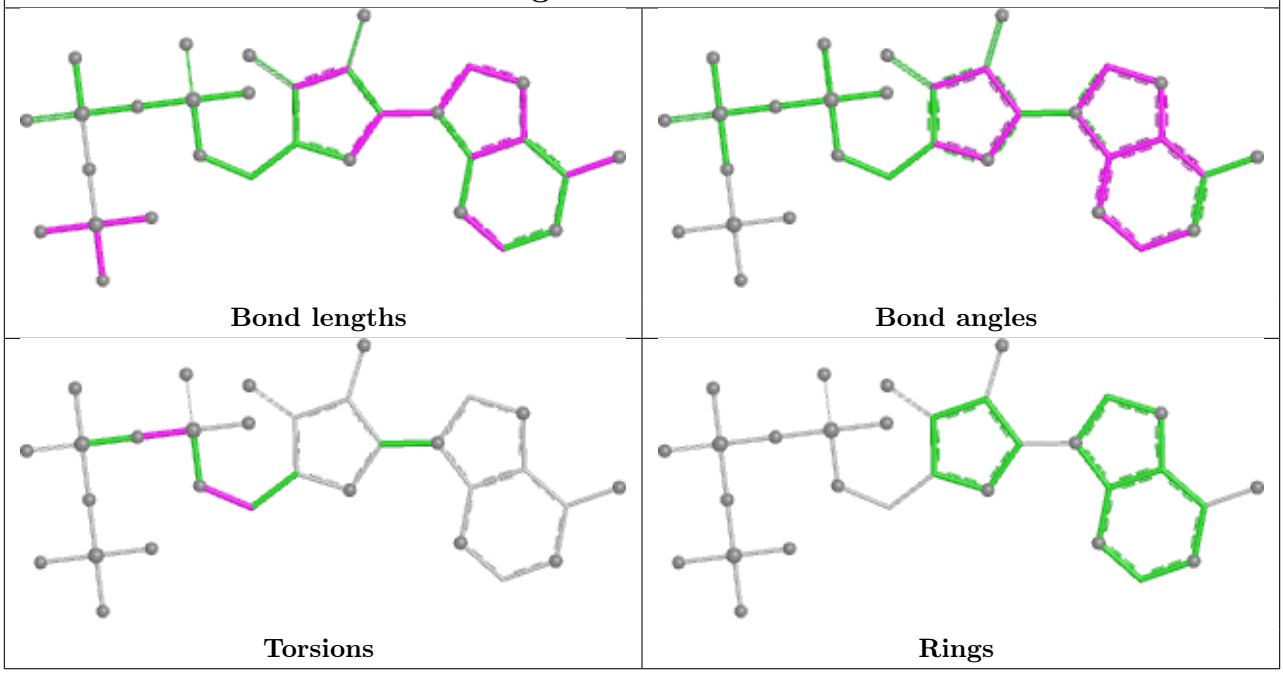


Torsions

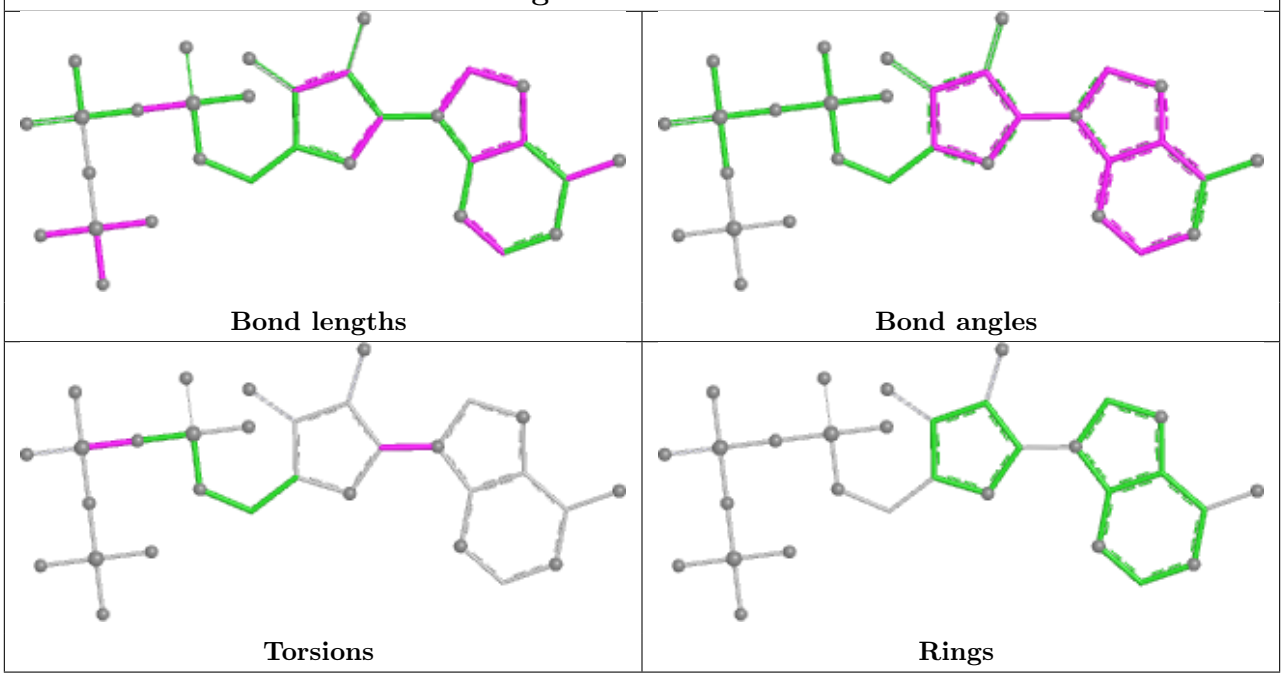


Rings

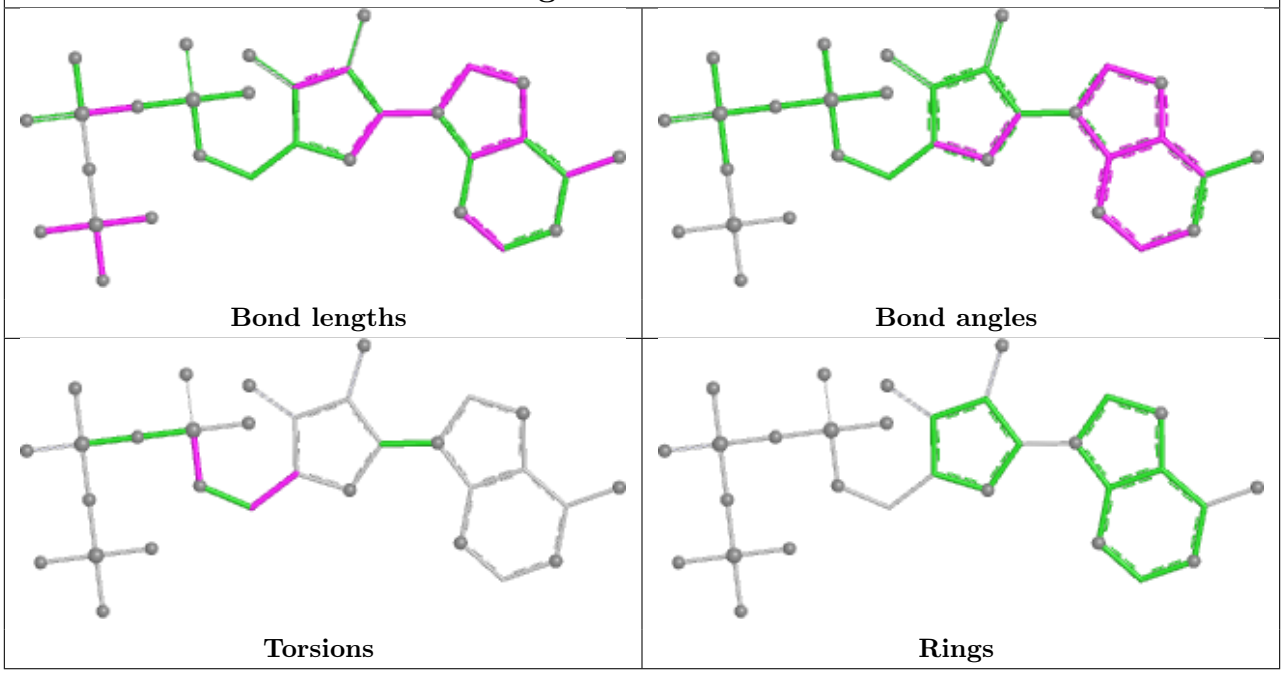
Ligand 08T V 400



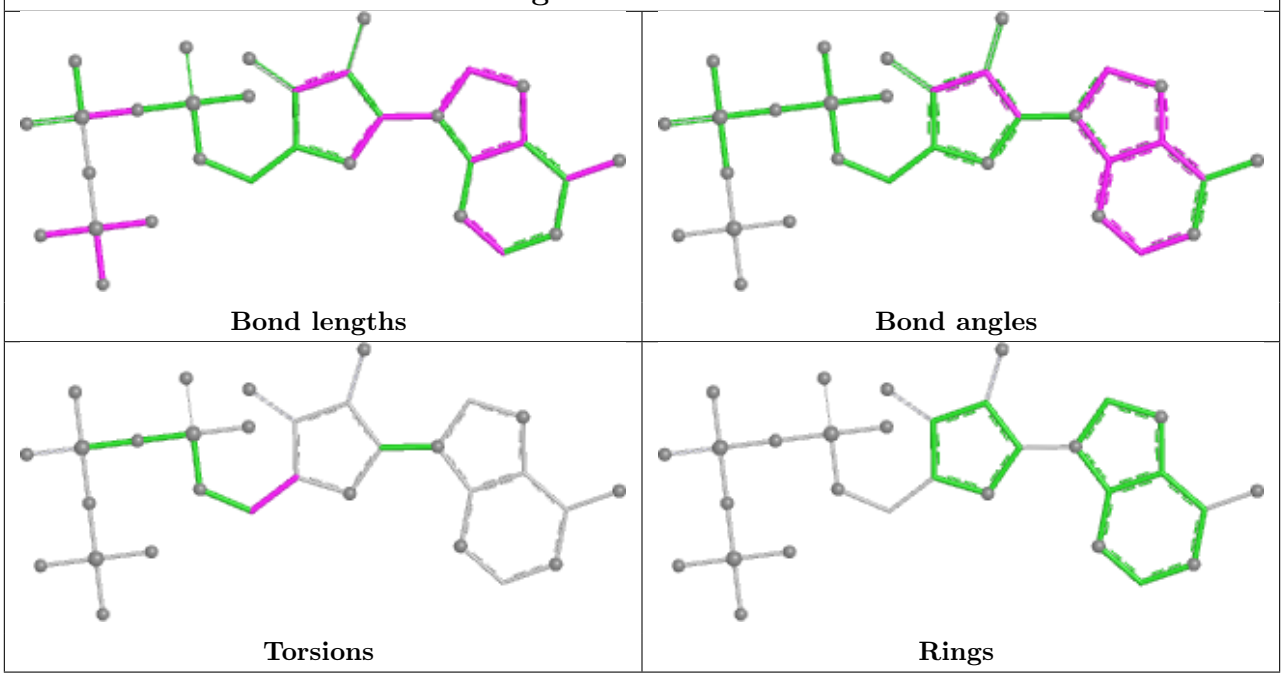
Ligand 08T X 400



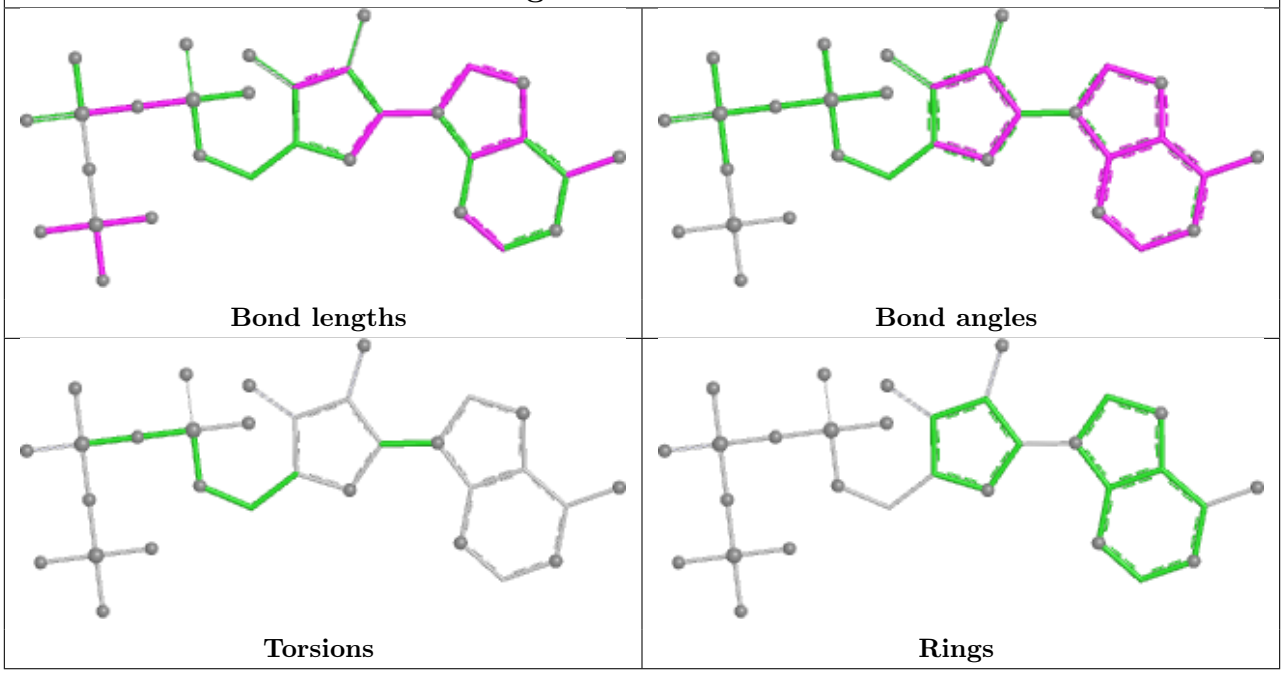
Ligand 08T I 400



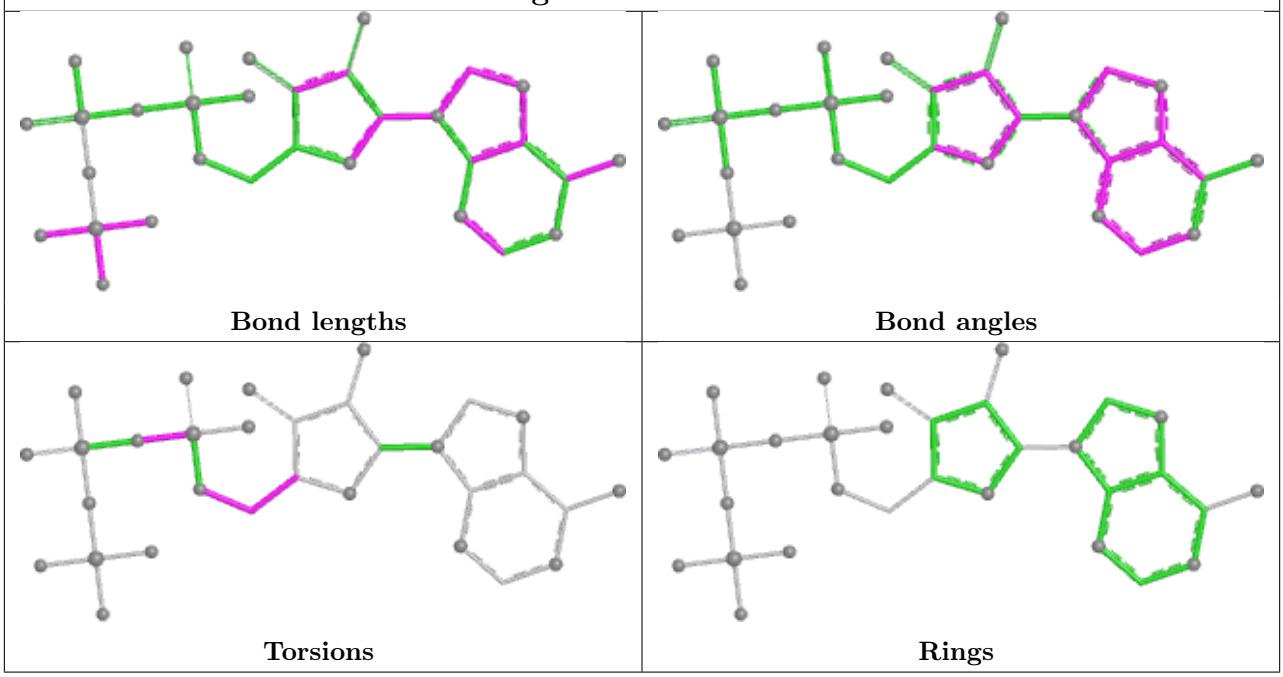
Ligand 08T A 400



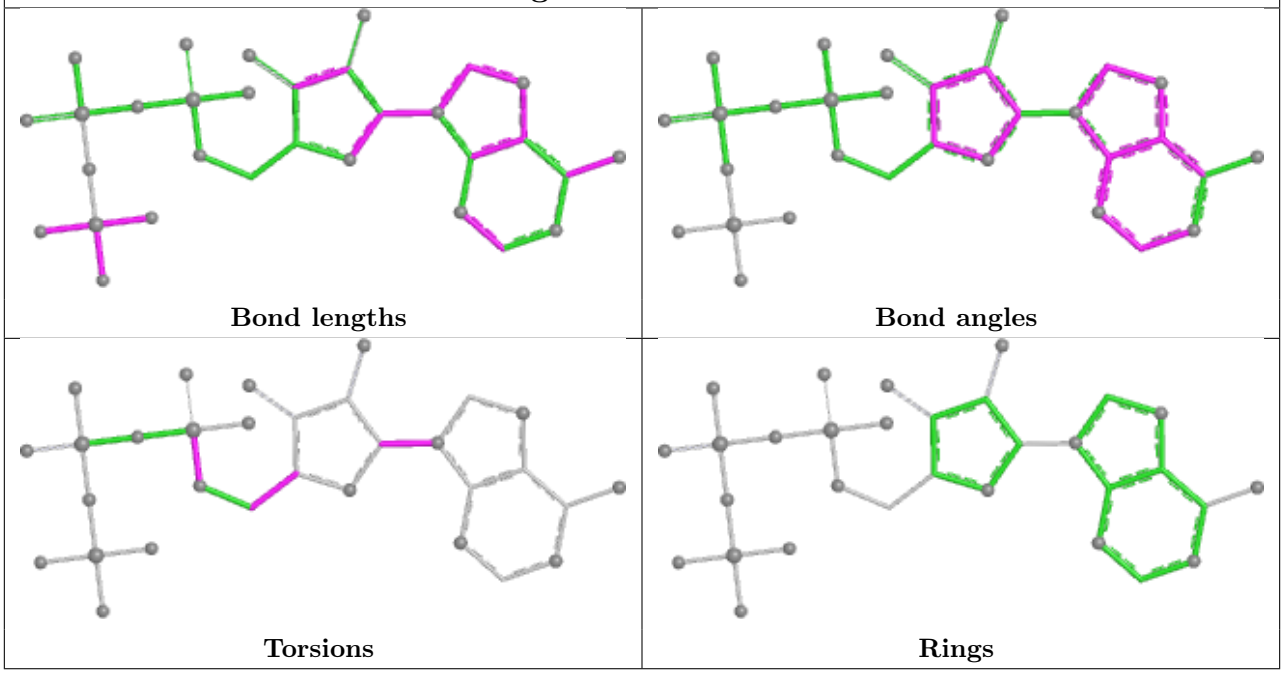
Ligand 08T W 400



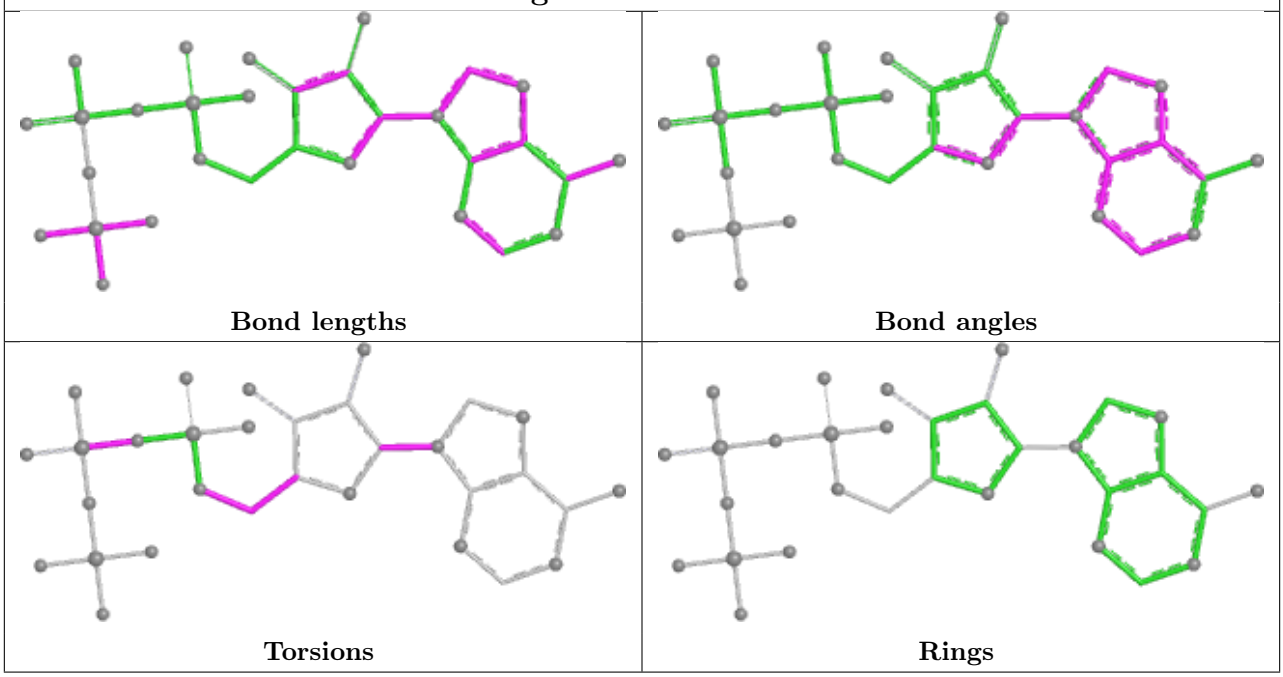
Ligand 08T O 400



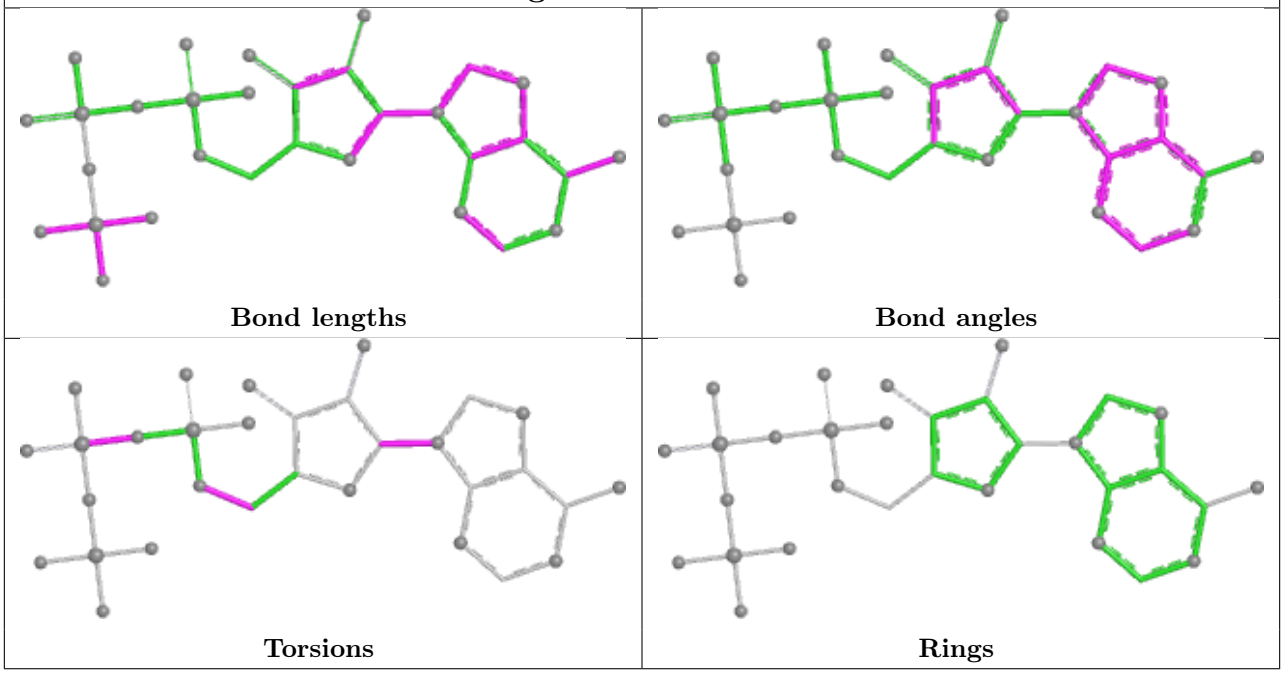
Ligand 08T G 400



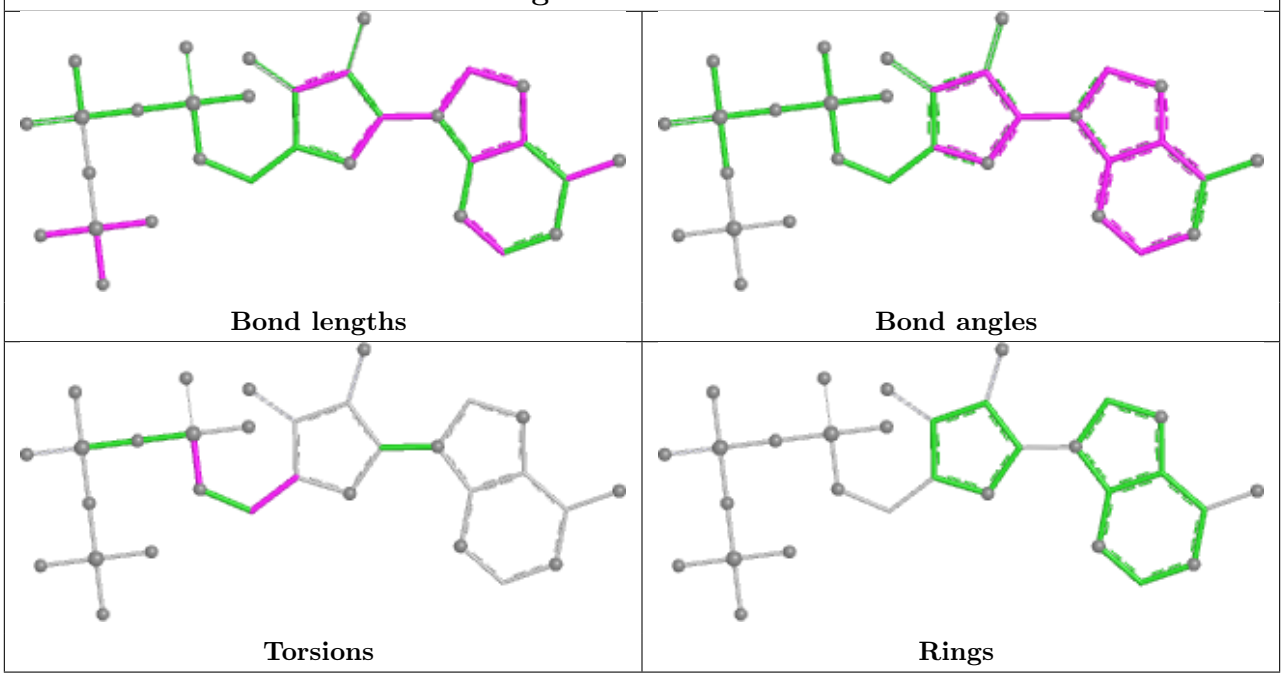
Ligand 08T K 400



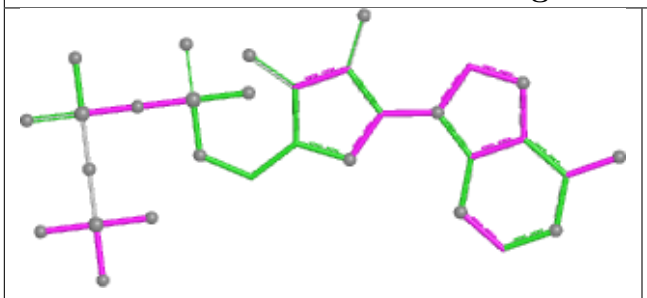
Ligand 08T M 400



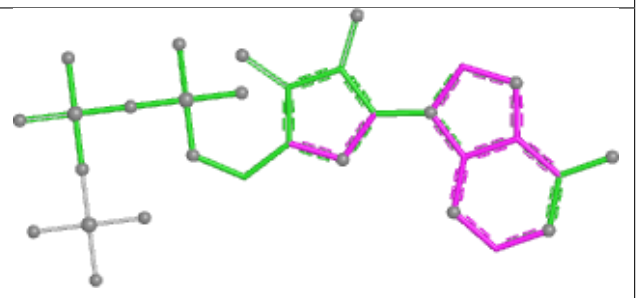
Ligand 08T R 400



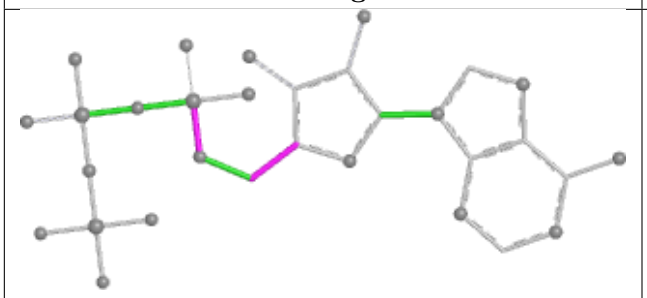
Ligand 08T U 400



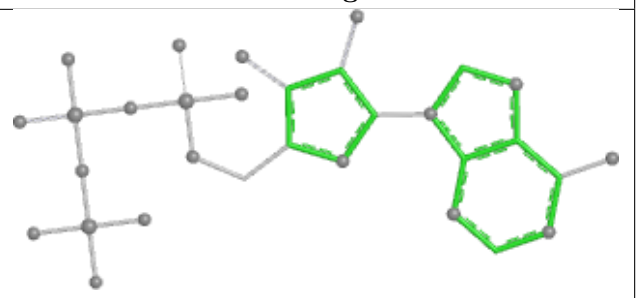
Bond lengths



Bond angles

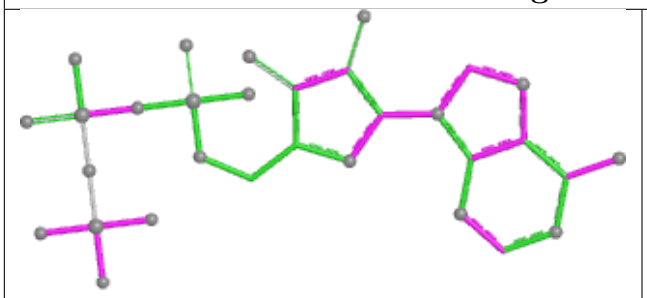


Torsions

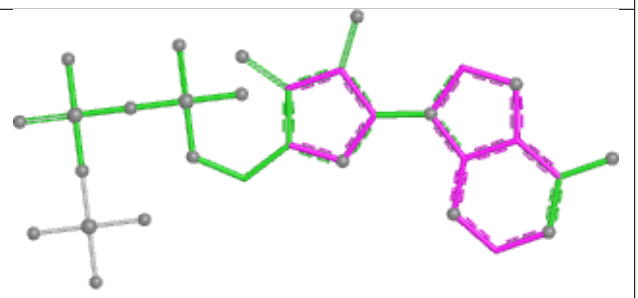


Rings

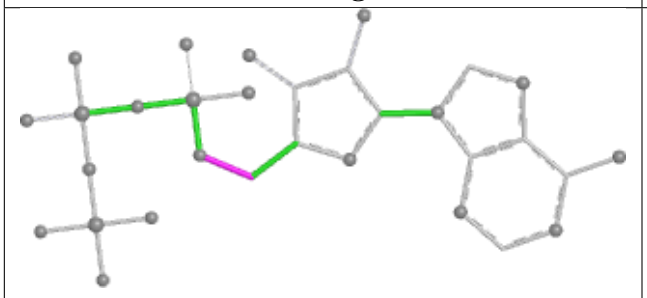
Ligand 08T H 400



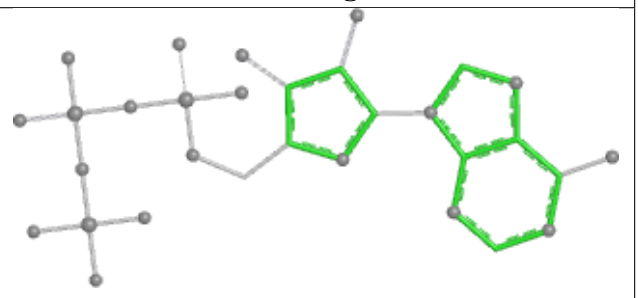
Bond lengths



Bond angles

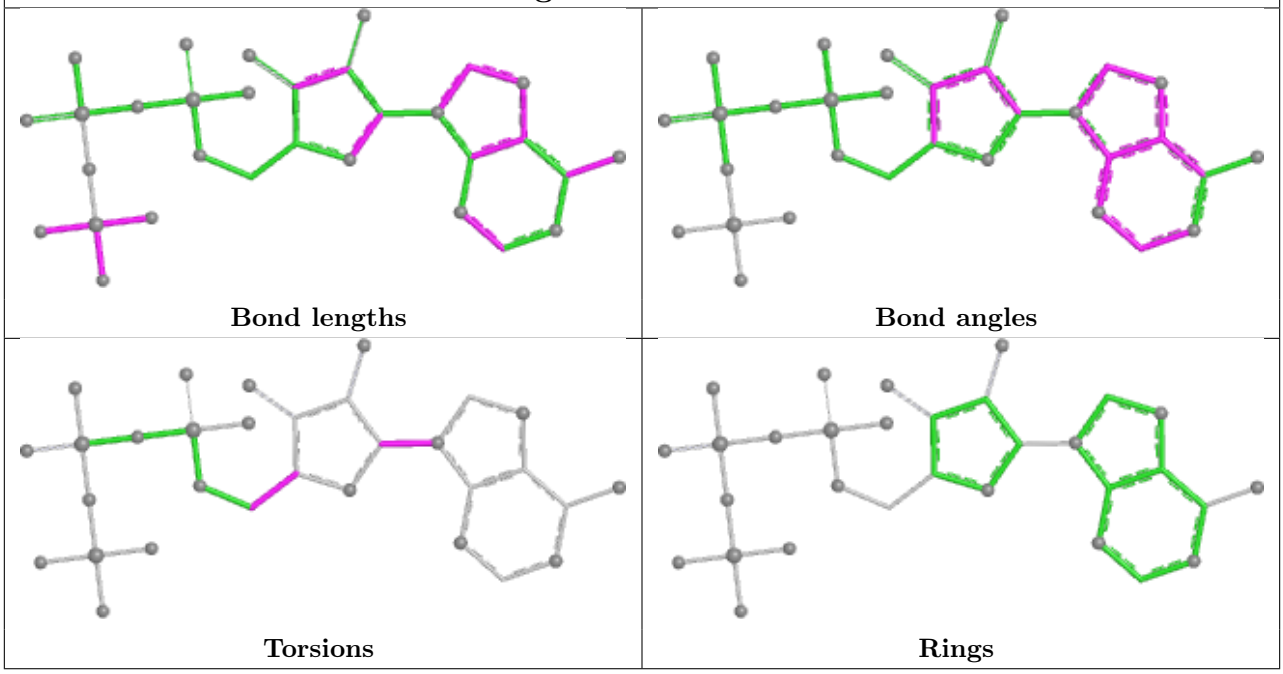


Torsions

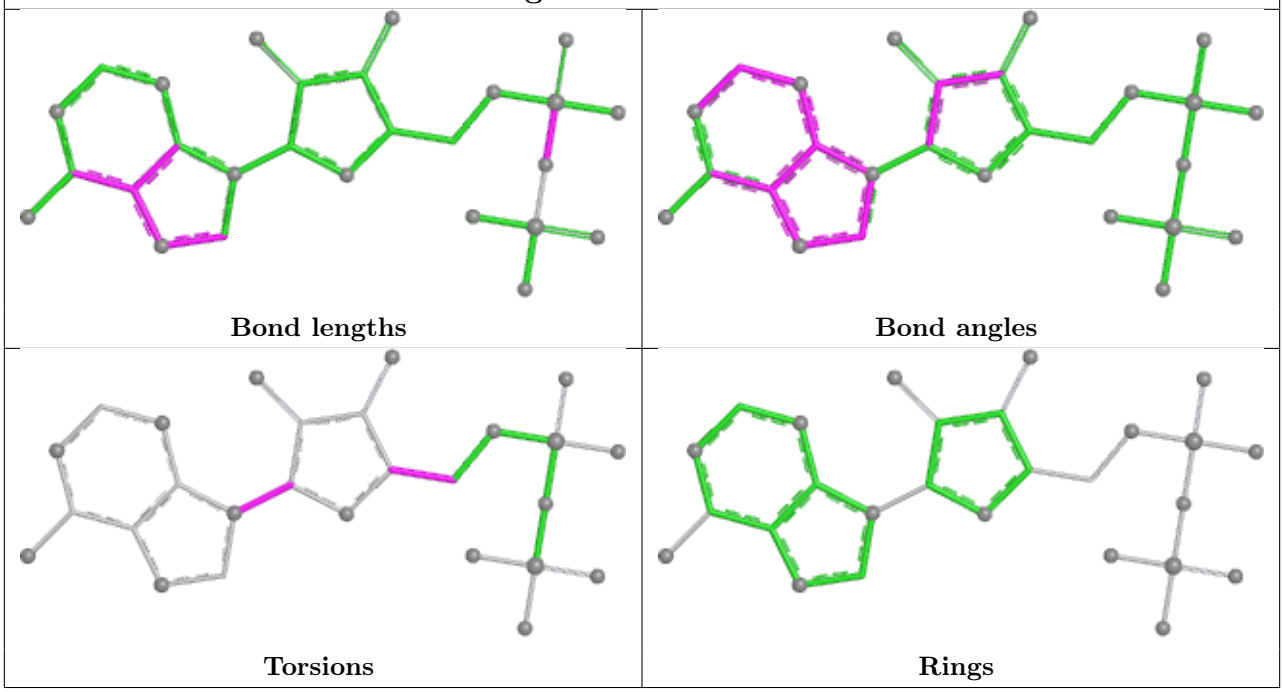


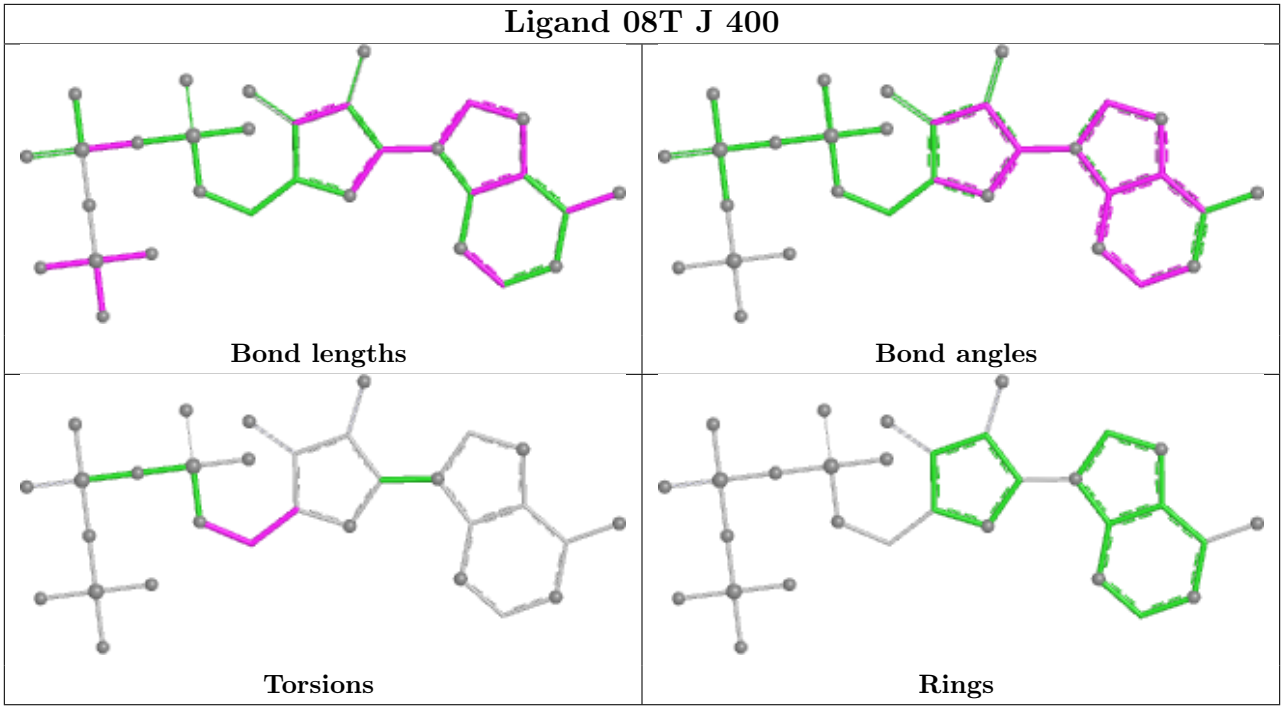
Rings

Ligand 08T S 400



Ligand ADP L 400





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	247/268 (92%)	-1.32	0	100	100	90, 130, 156, 173	0
1	B	247/268 (92%)	-1.39	0	100	100	44, 98, 128, 144	0
1	C	247/268 (92%)	-1.48	0	100	100	40, 80, 128, 155	0
1	D	247/268 (92%)	-1.47	0	100	100	33, 67, 98, 125	0
1	E	258/268 (96%)	-1.45	0	100	100	35, 69, 102, 148	8 (3%)
1	F	247/268 (92%)	-1.33	0	100	100	44, 91, 155, 198	0
1	G	247/268 (92%)	-1.15	0	100	100	103, 148, 175, 194	0
1	H	247/268 (92%)	-1.31	0	100	100	53, 96, 129, 148	0
1	I	248/268 (92%)	-1.41	0	100	100	35, 83, 122, 139	0
1	J	247/268 (92%)	-1.49	0	100	100	44, 75, 106, 125	0
1	K	247/268 (92%)	-1.45	0	100	100	40, 71, 100, 134	0
1	L	246/268 (91%)	-1.27	0	100	100	46, 96, 181, 216	0
1	M	247/268 (92%)	-1.21	0	100	100	109, 146, 171, 201	0
1	N	247/268 (92%)	-1.31	0	100	100	52, 96, 132, 150	0
1	O	247/268 (92%)	-1.43	0	100	100	40, 78, 123, 147	0
1	P	247/268 (92%)	-1.49	0	100	100	41, 76, 111, 132	0
1	Q	247/268 (92%)	-1.38	0	100	100	42, 74, 101, 131	0
1	R	247/268 (92%)	-1.35	0	100	100	52, 99, 178, 204	0
1	S	247/268 (92%)	-1.37	0	100	100	94, 126, 152, 165	0
1	T	247/268 (92%)	-1.38	0	100	100	47, 98, 134, 156	0
1	U	247/268 (92%)	-1.42	0	100	100	43, 84, 128, 147	0
1	V	247/268 (92%)	-1.46	0	100	100	39, 68, 104, 135	0
1	W	250/268 (93%)	-1.43	0	100	100	34, 70, 101, 125	1 (0%)
1	X	246/268 (91%)	-1.34	1 (0%)	88	79	42, 93, 159, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5941/6432 (92%)	-1.38	1 (0%)	100	100	33, 89, 156, 216	9 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	348	LEU	2.2

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	R	401	1/1	0.97	0.07	100,100,100,100	1
3	MG	D	401	1/1	0.98	0.07	57,57,57,57	1
3	MG	U	401	1/1	0.98	0.06	70,70,70,70	1
2	08T	I	400	31/31	0.99	0.03	50,63,78,85	42
2	08T	M	400	31/31	0.99	0.03	88,102,120,128	42
2	08T	N	400	31/31	0.99	0.03	51,76,92,99	42
2	08T	O	400	31/31	0.99	0.05	46,61,78,82	42
2	08T	Q	400	31/31	0.99	0.03	36,65,79,83	0
2	08T	S	400	31/31	0.99	0.04	72,95,115,119	42
2	08T	T	400	31/31	0.99	0.04	45,81,97,100	42
2	08T	U	400	31/31	0.99	0.04	48,68,82,83	42
2	08T	X	400	31/31	0.99	0.03	74,98,116,126	0
2	08T	A	400	31/31	0.99	0.03	77,92,110,125	42
3	MG	J	401	1/1	0.99	0.03	57,57,57,57	0
3	MG	L	401	1/1	0.99	0.04	63,63,63,63	0
3	MG	Q	401	1/1	0.99	0.03	57,57,57,57	1

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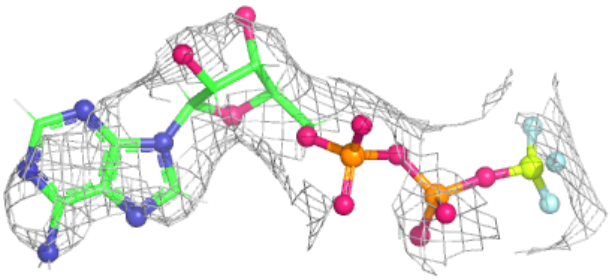
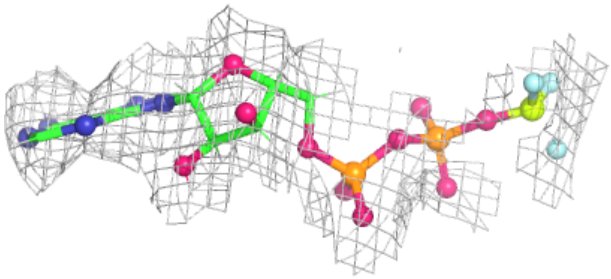
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	08T	B	400	31/31	0.99	0.03	50,70,87,94	42
3	MG	T	401	1/1	0.99	0.04	68,68,68,68	1
2	08T	G	400	31/31	0.99	0.04	93,105,129,132	42
4	ADP	L	400	27/27	0.99	0.04	76,95,114,139	0
2	08T	W	400	31/31	1.00	0.03	40,55,70,74	42
2	08T	C	400	31/31	1.00	0.02	39,63,75,88	42
3	MG	A	401	1/1	1.00	0.01	54,54,54,54	0
3	MG	B	401	1/1	1.00	0.03	62,62,62,62	1
3	MG	C	401	1/1	1.00	0.02	51,51,51,51	1
2	08T	H	400	31/31	1.00	0.03	62,73,87,90	42
3	MG	E	401	1/1	1.00	0.04	55,55,55,55	0
3	MG	F	401	1/1	1.00	0.03	79,79,79,79	1
3	MG	G	401	1/1	1.00	0.02	98,98,98,98	1
3	MG	H	401	1/1	1.00	0.01	51,51,51,51	0
3	MG	I	401	1/1	1.00	0.02	61,61,61,61	1
2	08T	P	400	31/31	1.00	0.02	47,59,75,81	0
3	MG	K	401	1/1	1.00	0.02	46,46,46,46	0
2	08T	D	400	31/31	1.00	0.03	42,63,82,85	0
3	MG	N	401	1/1	1.00	0.03	62,62,62,62	1
3	MG	O	401	1/1	1.00	0.05	71,71,71,71	1
3	MG	P	401	1/1	1.00	0.02	56,56,56,56	1
2	08T	R	400	31/31	1.00	0.03	93,110,133,149	0
2	08T	J	400	31/31	1.00	0.02	51,64,77,87	0
3	MG	S	401	1/1	1.00	0.02	64,64,64,64	0
2	08T	K	400	31/31	1.00	0.03	42,59,74,81	42
2	08T	E	400	31/31	1.00	0.03	44,57,69,80	42
3	MG	V	401	1/1	1.00	0.04	53,53,53,53	1
3	MG	W	401	1/1	1.00	0.02	51,51,51,51	1
3	MG	X	401	1/1	1.00	0.02	77,77,77,77	1
4	ADP	F	400	27/27	1.00	0.03	71,91,118,119	38
2	08T	V	400	31/31	1.00	0.02	34,56,71,75	0

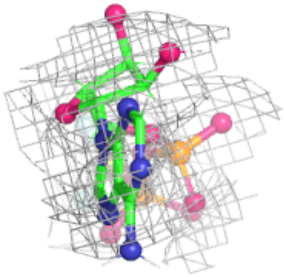
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 08T I 400:

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

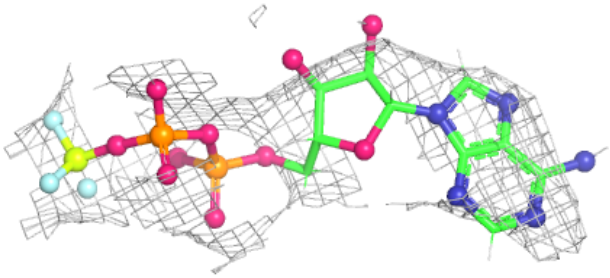


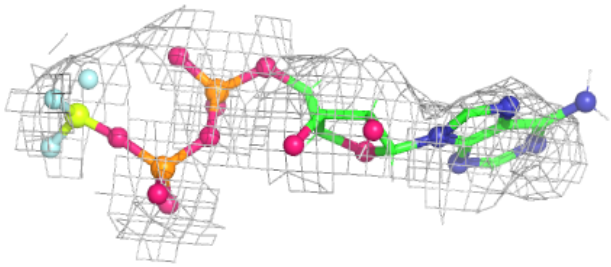


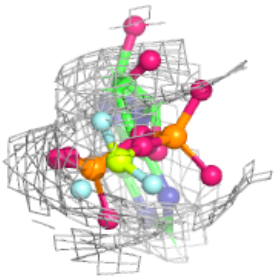


Electron density around 08T M 400:

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

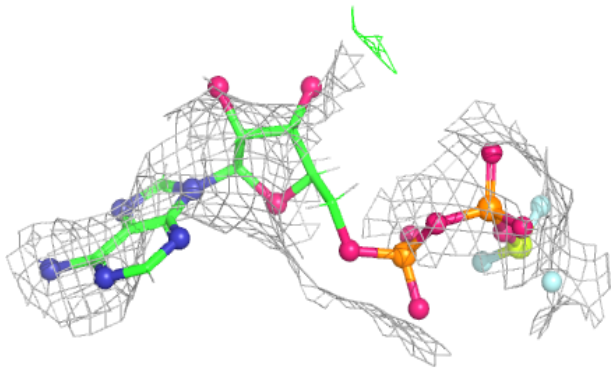


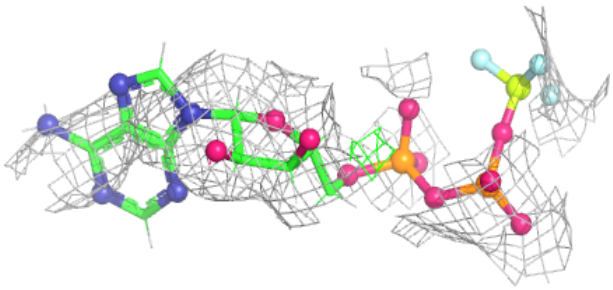


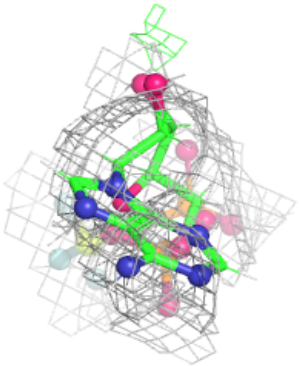


Electron density around 08T N 400:

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

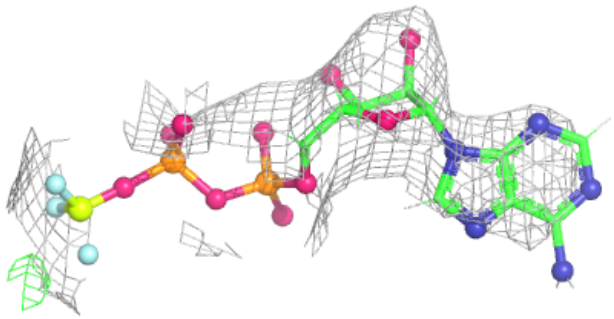


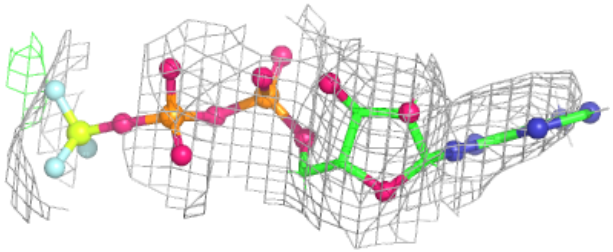


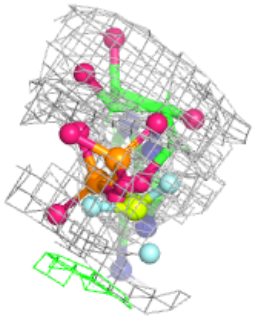


Electron density around 08T O 400:

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

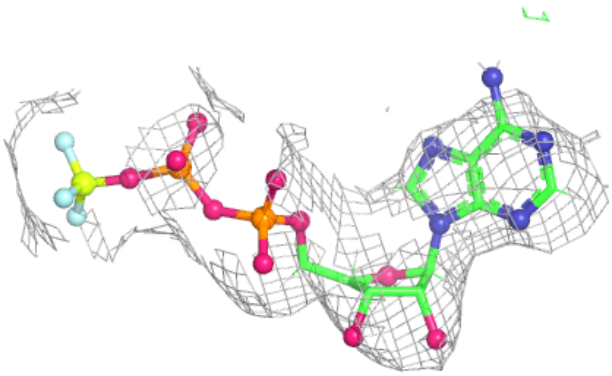


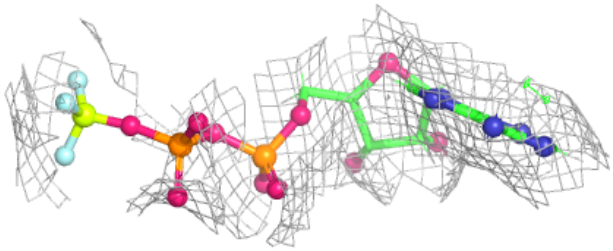


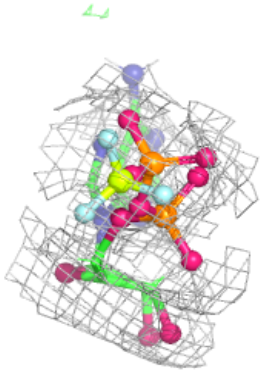


Electron density around 08T Q 400:

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

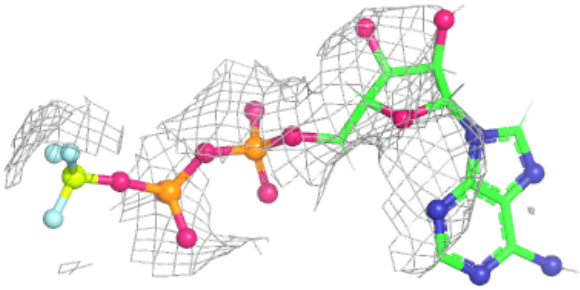


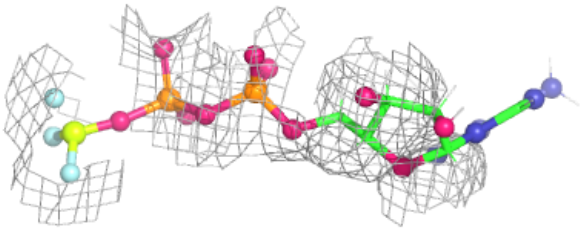


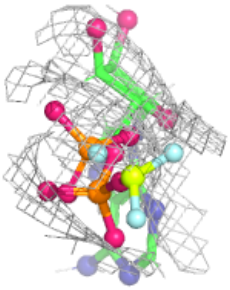


Electron density around 08T S 400:

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

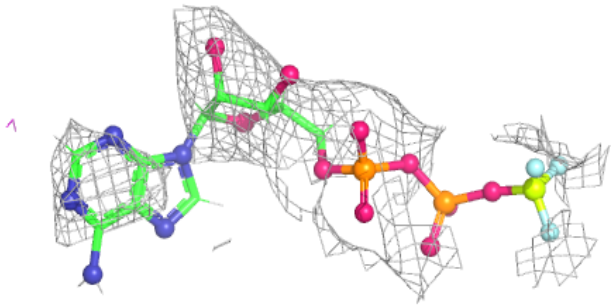


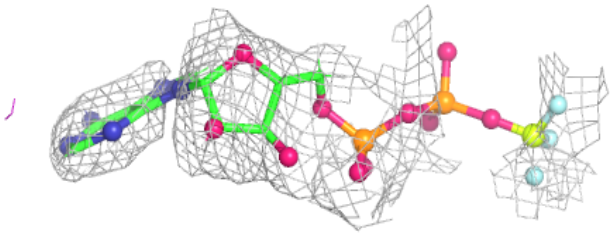


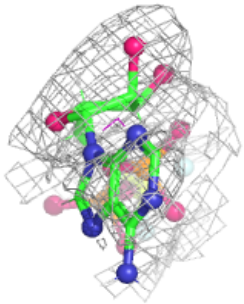


Electron density around 08T T 400:

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

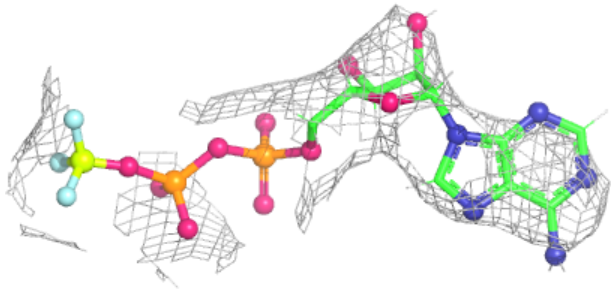


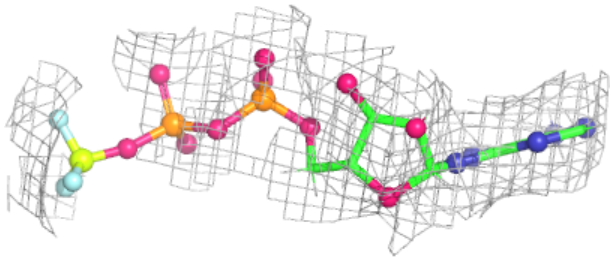


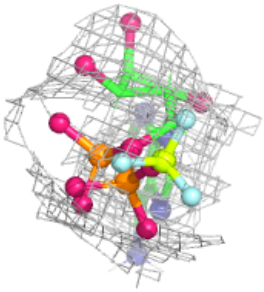


Electron density around 08T U 400:

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

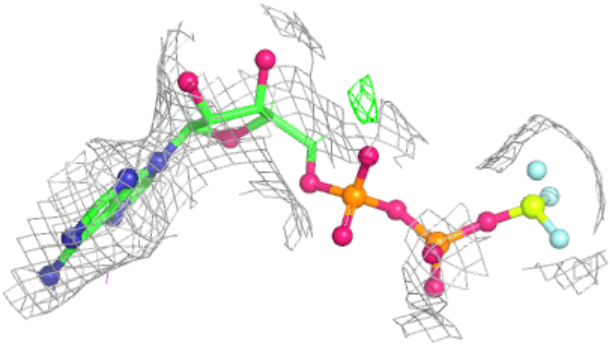


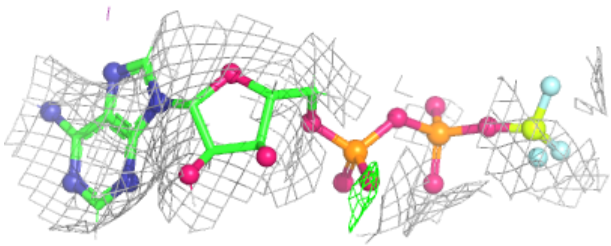


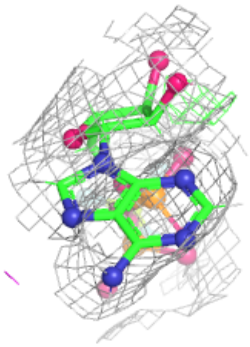


Electron density around 08T X 400:

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

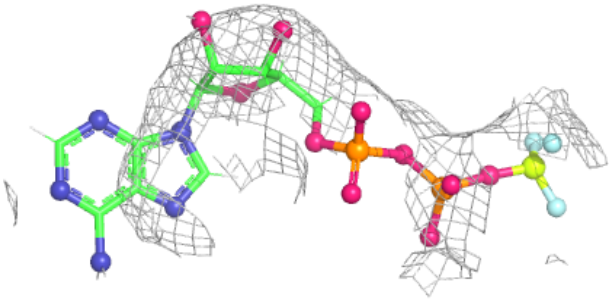


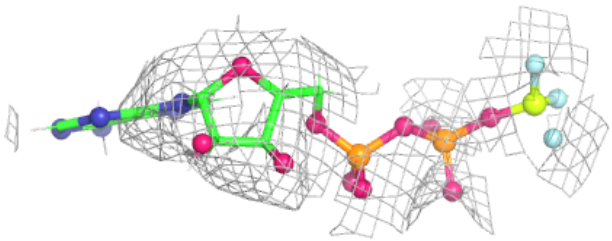


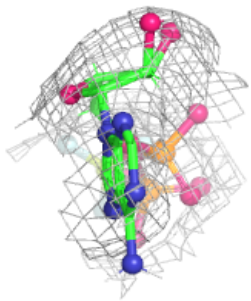


Electron density around 08T A 400:

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

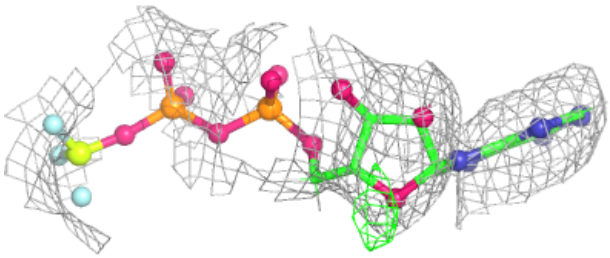


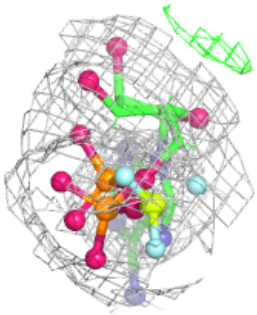




Electron density around 08T B 400:

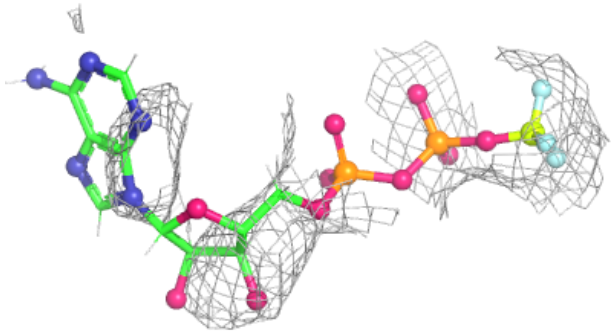
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

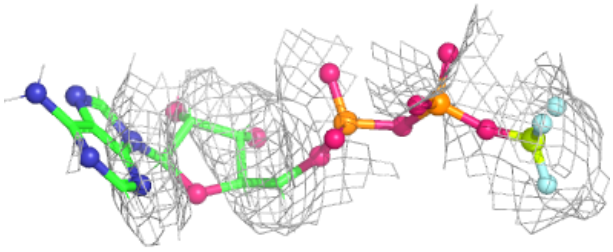


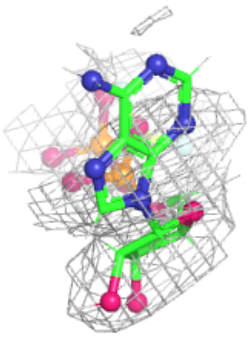


Electron density around 08T G 400:

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

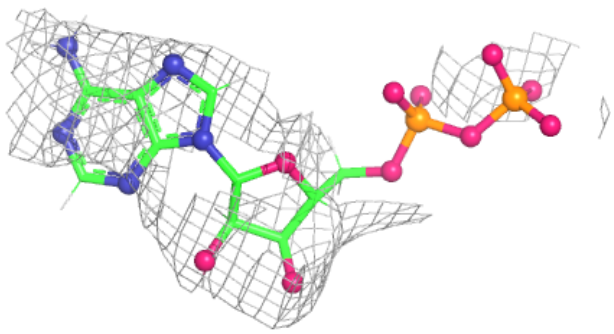


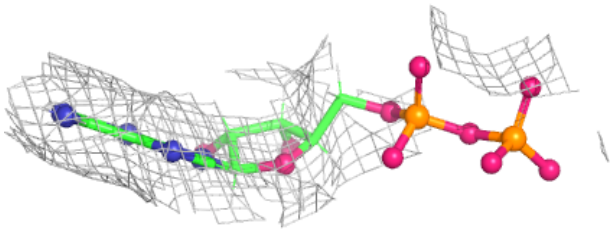


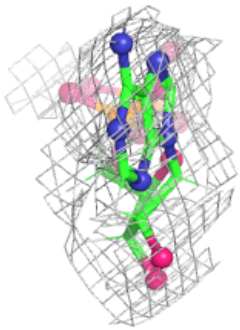


Electron density around ADP L 400:

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

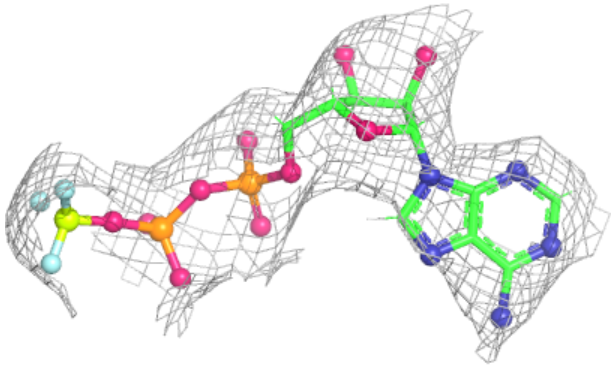


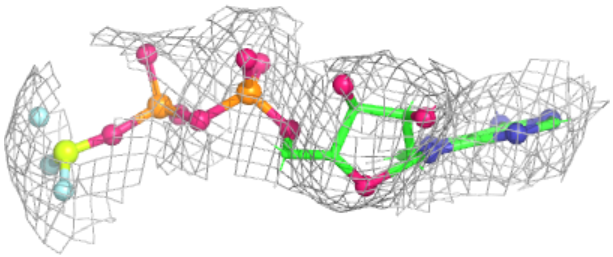


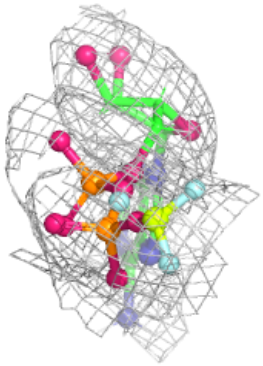


Electron density around 08T W 400:

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

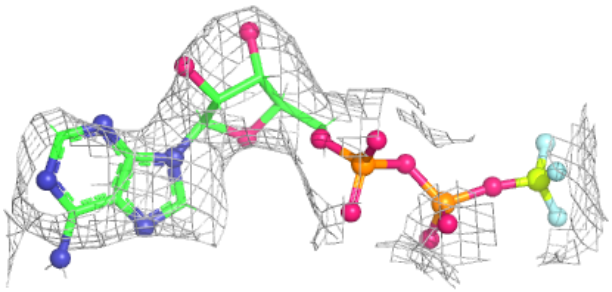


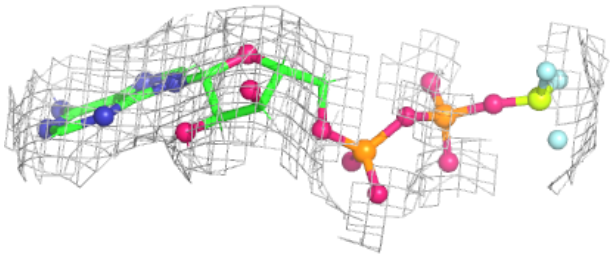


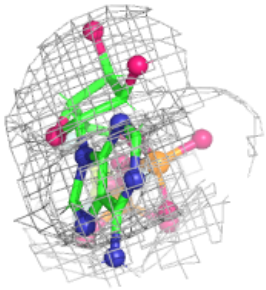


Electron density around 08T C 400:

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

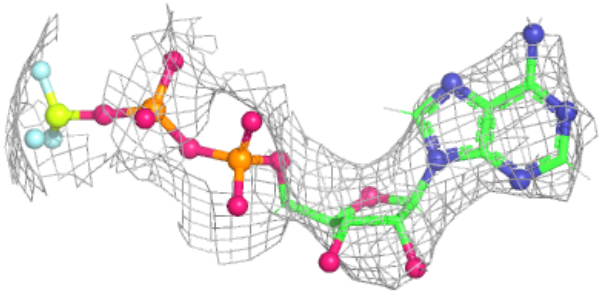


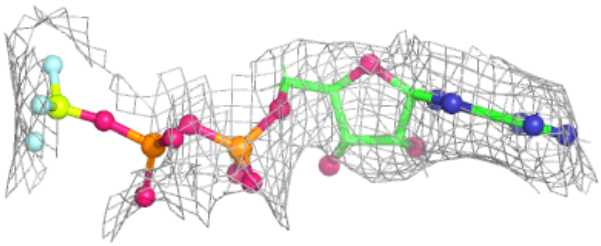


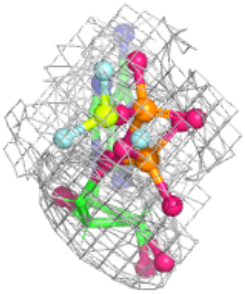


Electron density around 08T H 400:

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

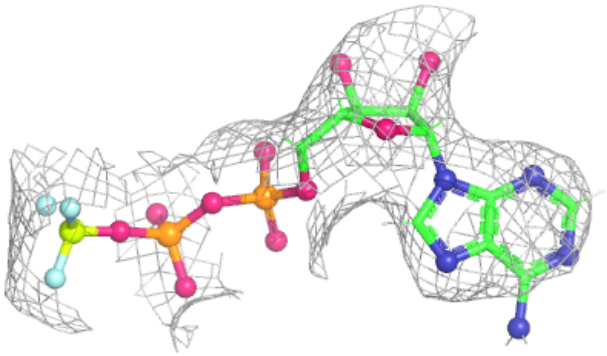


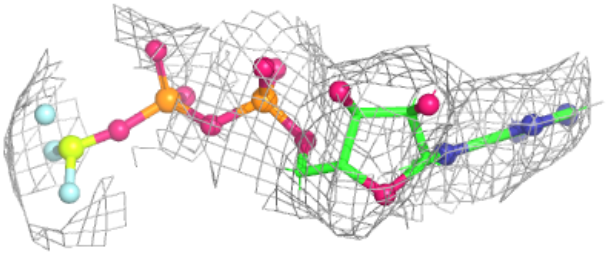


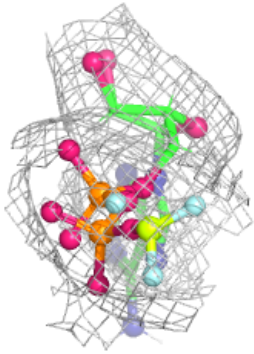


Electron density around 08T P 400:

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

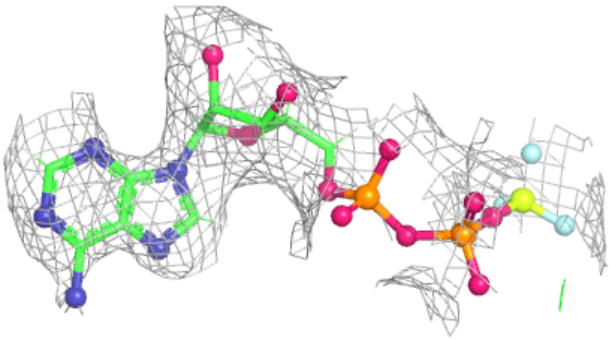


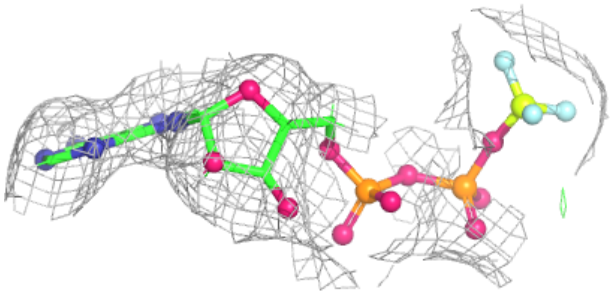


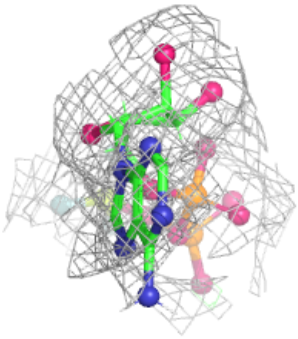


Electron density around 08T D 400:

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

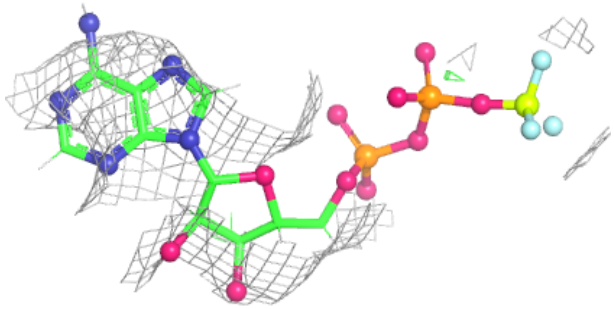


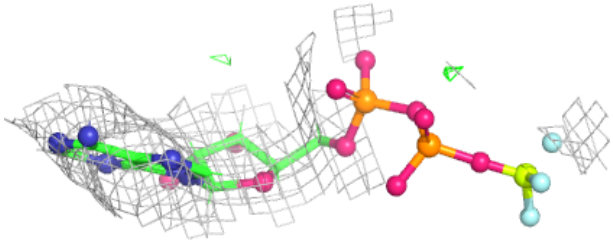


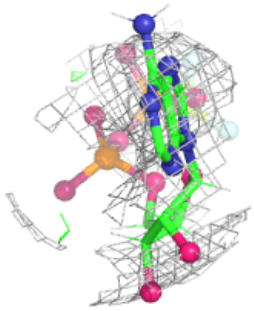


Electron density around 08T R 400:

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

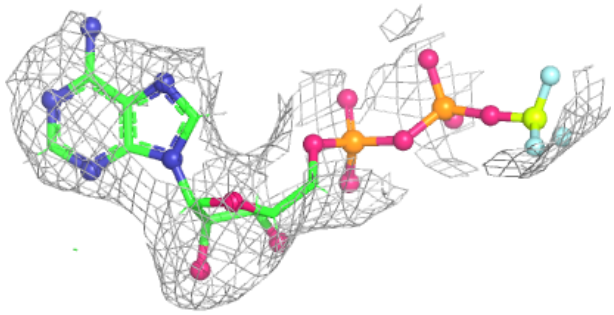


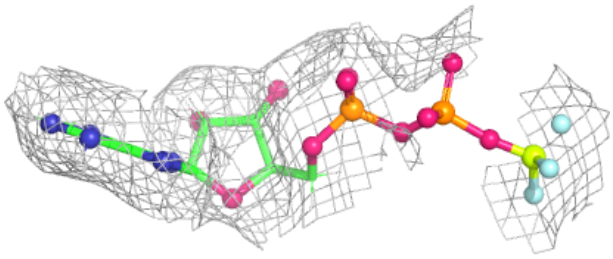


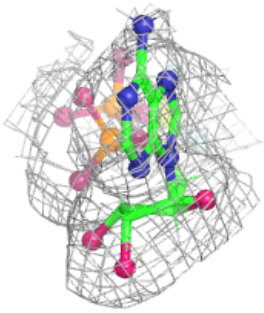


Electron density around 08T J 400:

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

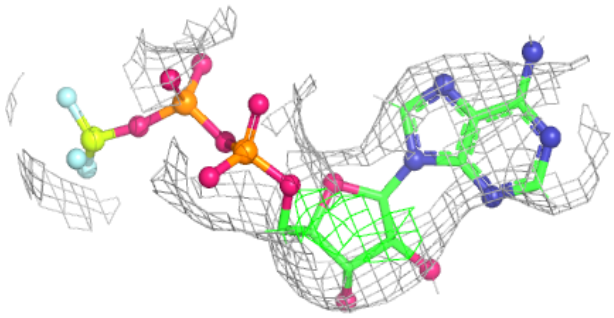


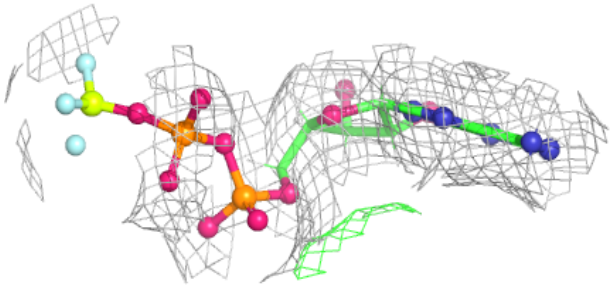


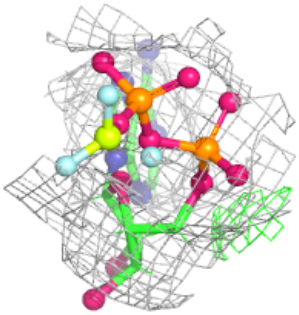


Electron density around 08T K 400:

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

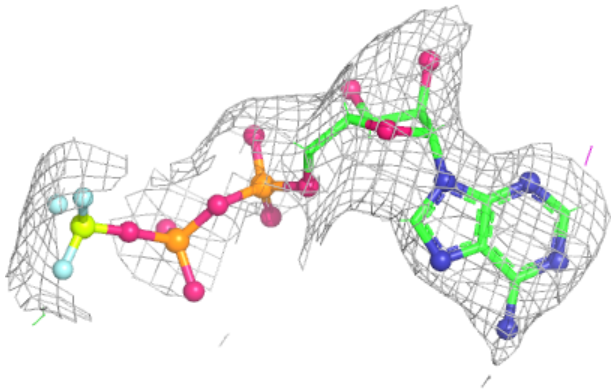


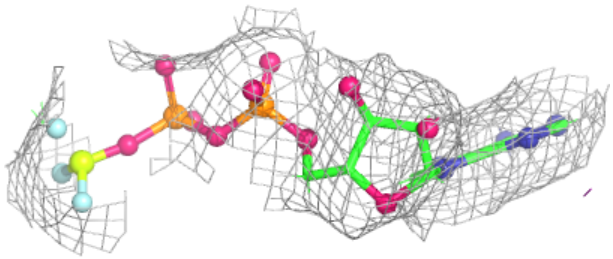


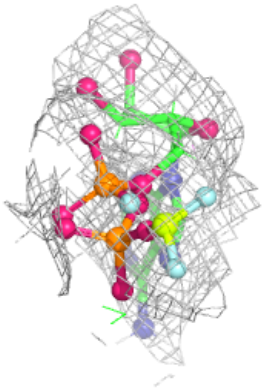


Electron density around 08T E 400:

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

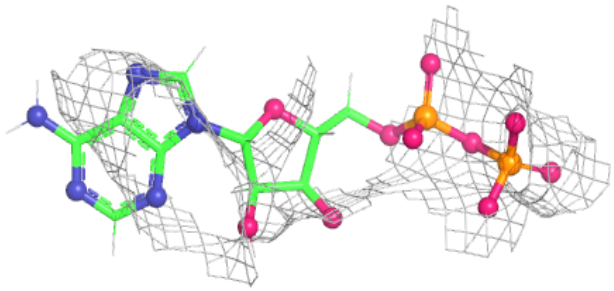


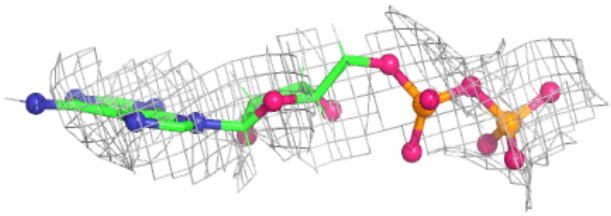


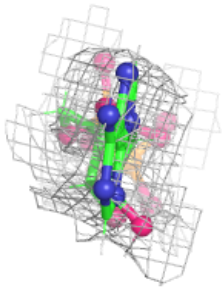


Electron density around ADP F 400:

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

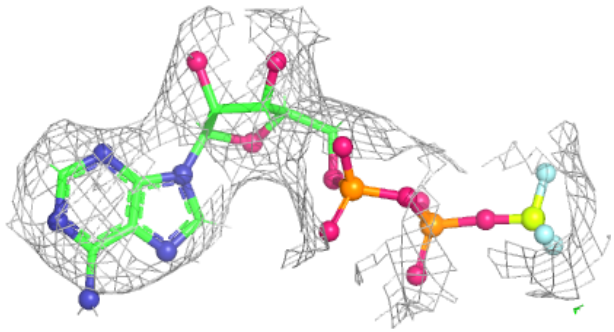


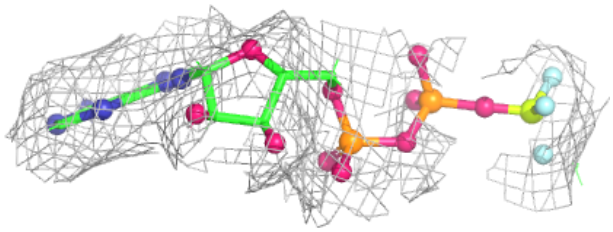


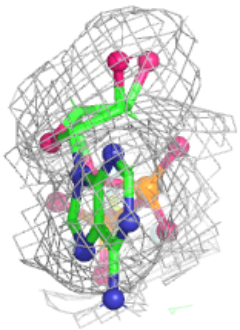


Electron density around 08T V 400:

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







6.5 Other polymers (i)

There are no such residues in this entry.