



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:44 pm BST

PDB ID : 4LZZ  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

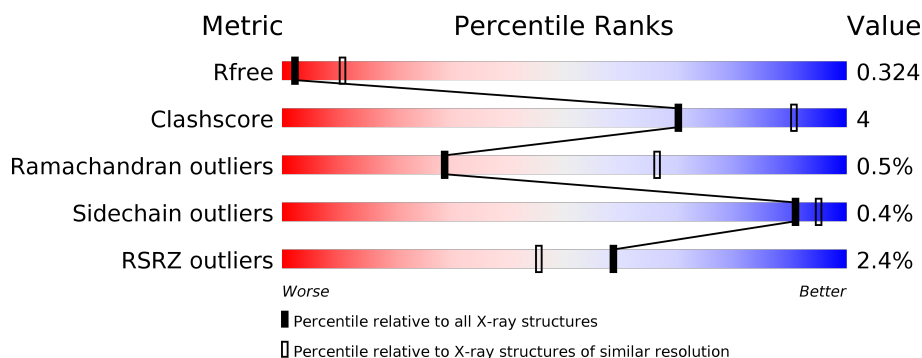
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	268	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	C	268	<div> <div></div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
1	D	268	<div> <div></div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
1	E	268	<div> <div></div> <div> <div></div> <div>85%</div> <div>10%</div> <div>.</div> </div> </div>
1	F	268	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	268	
1	H	268	
1	I	268	
1	J	268	
1	K	268	
1	L	268	
1	M	268	
1	N	268	
1	O	268	
1	P	268	
1	Q	268	
1	R	268	
1	S	268	
1	T	268	
1	U	268	
1	V	268	
1	W	268	
1	X	268	

## 2 Entry composition

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

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

There are 24 discrepancies between the modelled and reference sequences:

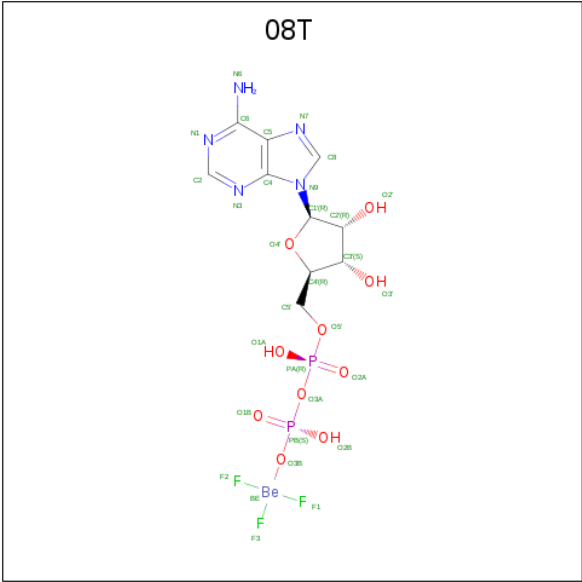
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	INITIATING METHIONINE	UNP O67198
B	120	MET	-	INITIATING METHIONINE	UNP O67198
C	120	MET	-	INITIATING METHIONINE	UNP O67198
D	120	MET	-	INITIATING METHIONINE	UNP O67198
E	120	MET	-	INITIATING METHIONINE	UNP O67198
F	120	MET	-	INITIATING METHIONINE	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-y-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (three-letter code: 08T) (formula: C<sub>10</sub>H<sub>14</sub>BeF<sub>3</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	S	1	Total	Mg	0	0
			1	1		

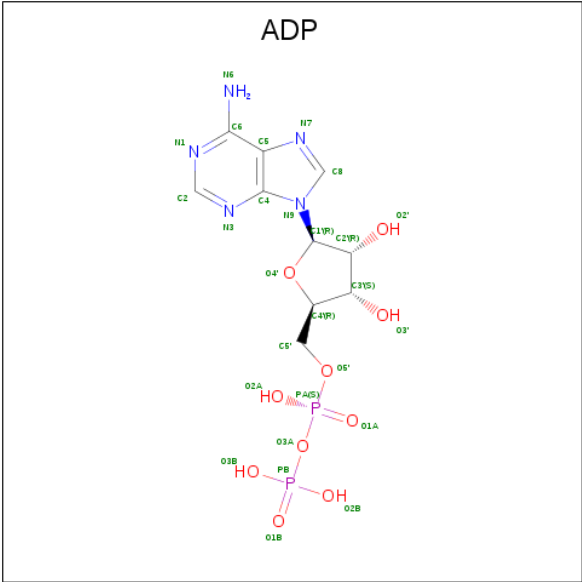
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	V	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	R	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	U	1	Total 1	Mg 1	0	0
3	L	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	Q	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	T	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

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



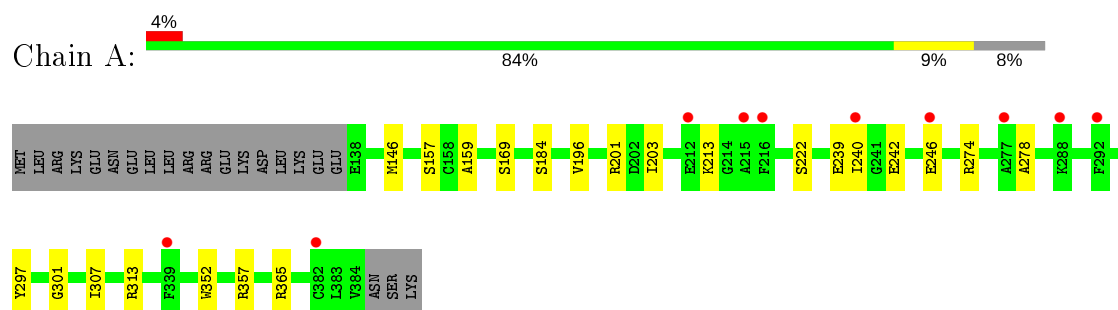


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
4	L	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

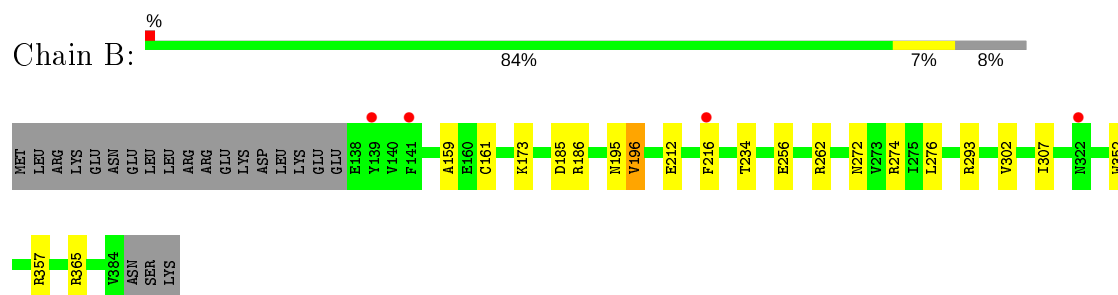
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

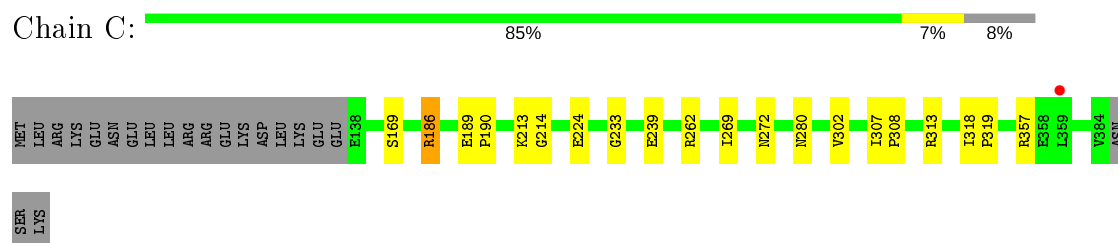
- Molecule 1: Transcriptional regulator (NtrC family)



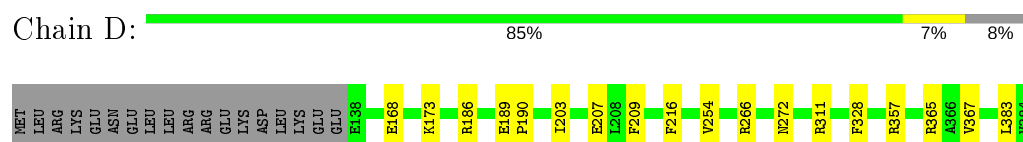
- Molecule 1: Transcriptional regulator (NtrC family)




- Molecule 1: Transcriptional regulator (NtrC family)

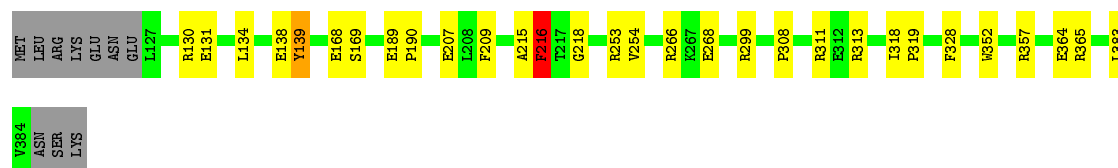


- Molecule 1: Transcriptional regulator (NtrC family)




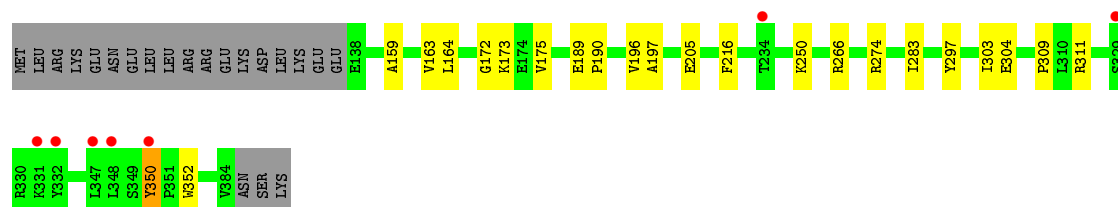
- Molecule 1: Transcriptional regulator (NtrC family)

Chain E: 




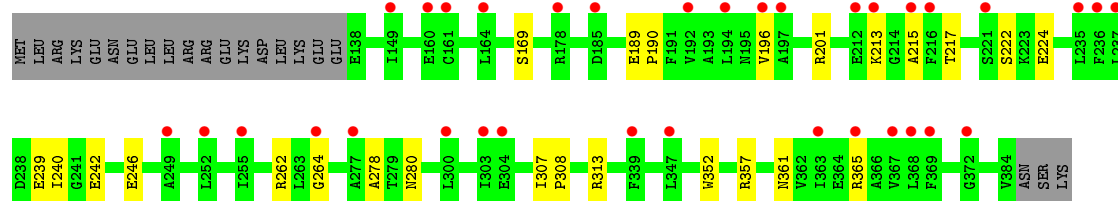
- Molecule 1: Transcriptional regulator (NtrC family)

Chain F: 




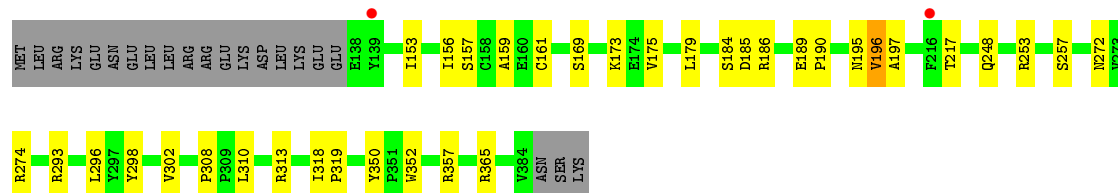
- Molecule 1: Transcriptional regulator (NtrC family)

Chain G: 




- Molecule 1: Transcriptional regulator (NtrC family)

Chain H: 

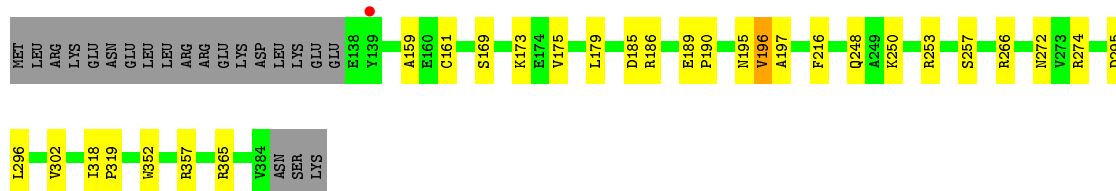


- Molecule 1: Transcriptional regulator (NtrC family)

Chain I: 

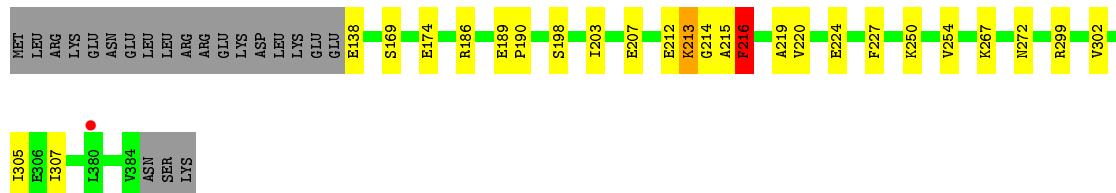






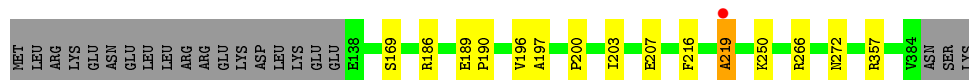
- Molecule 1: Transcriptional regulator (NtrC family)

Chain O: 82% 9% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain P: 87% 5% 8%



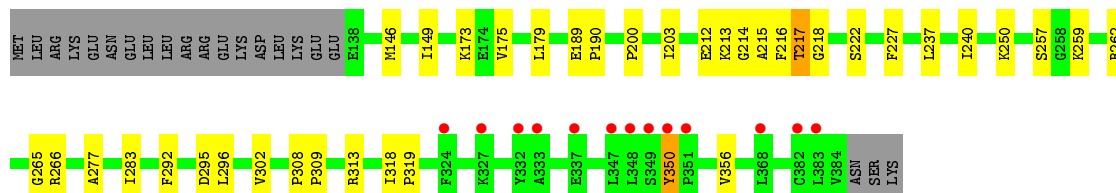
- Molecule 1: Transcriptional regulator (NtrC family)

Chain Q: 85% 6% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

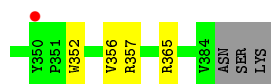
Chain R: 5% 78% 14% 8%



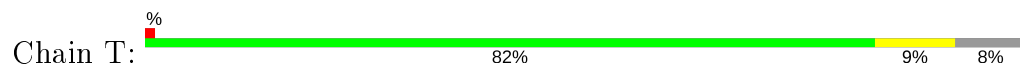
- Molecule 1: Transcriptional regulator (NtrC family)

Chain S: 2% 84% 8% 8%

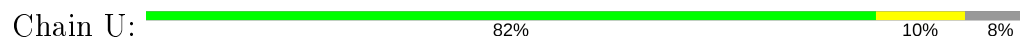




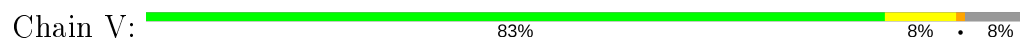
- Molecule 1: Transcriptional regulator (NtrC family)



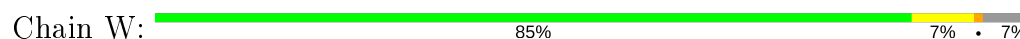
- Molecule 1: Transcriptional regulator (NtrC family)



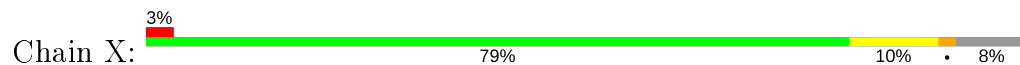
- Molecule 1: Transcriptional regulator (NtrC family)

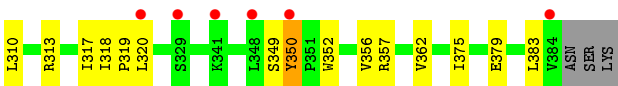


- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 50.5 (44.27-3.21)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.267 , 0.322 0.268 , 0.324	Depositor DCC
$R_{free}$ test set	1107 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 18.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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	0.88	EDS
Total number of atoms	97749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	0.26	0/2013	0.48	0/2700
1	B	0.28	0/2013	0.49	0/2700
1	C	0.28	0/2013	0.49	0/2700
1	D	0.30	0/2013	0.52	0/2700
1	E	0.29	0/2112	0.52	0/2830
1	F	0.28	0/2013	0.54	0/2700
1	G	0.27	0/2013	0.48	0/2700
1	H	0.28	0/2013	0.48	0/2700
1	I	0.29	0/2022	0.51	0/2712
1	J	0.28	0/2013	0.48	0/2700
1	K	0.29	0/2013	0.49	0/2700
1	L	0.27	0/2004	0.52	0/2688
1	M	0.28	0/2013	0.52	0/2700
1	N	0.28	0/2013	0.47	0/2700
1	O	0.30	0/2013	0.55	1/2700 (0.0%)
1	P	0.28	0/2013	0.50	0/2700
1	Q	0.28	0/2013	0.47	0/2700
1	R	0.30	0/2013	0.67	1/2700 (0.0%)
1	S	0.26	0/2013	0.49	0/2700
1	T	0.26	0/2013	0.47	0/2700
1	U	0.28	0/2013	0.49	0/2700
1	V	0.29	0/2013	0.50	0/2700
1	W	0.29	0/2039	0.50	0/2735
1	X	0.30	0/2004	0.65	2/2688 (0.1%)
All	All	0.28	0/48428	0.51	4/64953 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	349	SER	N-CA-C	-6.83	92.55	111.00
1	R	350	TYR	N-CA-C	5.85	126.79	111.00
1	X	350	TYR	N-CA-C	5.62	126.18	111.00
1	O	216	PHE	CB-CG-CD1	5.19	124.43	120.80

There are no chirality outliers.

All (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
1	U	214	GLY	Peptide

## 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	1979	2041	2039	15	0
1	B	1979	2041	2039	16	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	23	0
1	I	1988	2048	2046	15	0
1	J	1979	2042	2040	8	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	21	0
1	O	1979	2042	2040	21	0
1	P	1979	2041	2039	12	0
1	Q	1979	2041	2039	12	0
1	R	1979	2042	2040	24	0
1	S	1979	2041	2039	14	0
1	T	1979	2042	2040	19	0
1	U	1979	2042	2039	14	0
1	V	1979	2042	2040	16	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	7	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	347	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.

All (347) 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
1:F:205:GLU:OE1	1:F:250:LYS:NZ	2.16	0.78
1:A:146:MET:SD	1:A:313:ARG:NH2	2.59	0.76
1:T:173:LYS:NZ	2:T:400:08T:O2B	2.18	0.75
1:L:205:GLU:OE1	1:L:250:LYS:NZ	2.21	0.73
1:H:186:ARG:NH2	1:H:272:ASN:OD1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:GLU:OE2	1:H:293:ARG:NH1	2.25	0.68
1:U:169:SER:CB	2:U:400:08T:F3	2.30	0.67
1:D:168:GLU:OE1	1:D:311:ARG:NH2	2.27	0.67
1:N:173:LYS:NZ	2:N:400:08T:O1A	2.23	0.67
1:J:357:ARG:NH2	2:J:400:08T:O3A	2.28	0.67
1:P:186:ARG:NH2	1:P:272:ASN:OD1	2.28	0.67
1:E:168:GLU:OE2	1:E:311:ARG:NH2	2.28	0.67
1:X:350:TYR:O	1:X:352:TRP:N	2.26	0.67
1:U:186:ARG:NH2	1:U:272:ASN:OD1	2.28	0.66
1:O:174:GLU:OE1	2:O:400:08T:O1B	2.14	0.65
1:T:365:ARG:NE	1:U:302:VAL:O	2.27	0.65
1:J:297:TYR:OH	1:J:304:GLU:OE2	2.14	0.65
1:B:357:ARG:NH2	2:B:400:08T:O3A	2.30	0.65
1:K:171:VAL:N	2:K:400:08T:O1B	2.30	0.65
1:I:297:TYR:OH	1:I:304:GLU:OE1	2.15	0.64
1:A:213:LYS:N	1:A:222:SER:OG	2.31	0.64
1:E:130:ARG:HA	1:E:131:GLU:CB	2.27	0.63
1:K:169:SER:OG	2:K:400:08T:F1	2.02	0.63
1:T:170:GLY:N	2:T:400:08T:O1B	2.31	0.63
1:V:295:ASP:OD1	1:V:295:ASP:N	2.26	0.63
1:Q:357:ARG:NH2	2:Q:400:08T:O3A	2.32	0.62
1:G:201:ARG:NH1	1:G:246:GLU:OE1	2.32	0.62
1:G:308:PRO:O	1:G:313:ARG:NH1	2.33	0.62
1:L:309:PRO:O	1:L:313:ARG:NH1	2.33	0.62
1:R:146:MET:SD	1:R:313:ARG:NH2	2.72	0.62
1:R:212:GLU:OE1	1:R:262:ARG:NH1	2.32	0.62
1:H:357:ARG:NH2	2:H:400:08T:O3A	2.32	0.62
1:T:357:ARG:NH2	2:T:400:08T:O3A	2.32	0.62
1:M:242:GLU:N	1:M:242:GLU:OE1	2.32	0.62
1:N:197:ALA:O	1:O:250:LYS:NZ	2.31	0.61
1:D:173:LYS:NZ	2:D:400:08T:O1B	2.26	0.61
1:D:186:ARG:NH2	1:D:272:ASN:OD1	2.34	0.61
1:M:201:ARG:NH1	1:M:246:GLU:OE1	2.33	0.61
1:P:357:ARG:NH2	2:P:400:08T:O3A	2.34	0.61
1:A:201:ARG:NH1	1:A:246:GLU:OE1	2.34	0.61
1:N:357:ARG:NH2	2:N:400:08T:O2A	2.33	0.61
1:U:207:GLU:OE2	1:V:266:ARG:NH1	2.34	0.60
1:C:186:ARG:NH2	1:C:272:ASN:OD1	2.34	0.60
1:N:365:ARG:NE	1:O:302:VAL:O	2.32	0.60
1:L:159:ALA:O	1:L:274:ARG:NH1	2.35	0.60
1:F:159:ALA:O	1:F:274:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:357:ARG:NH2	2:W:400:08T:O3A	2.34	0.60
1:X:320:LEU:HD21	2:X:400:08T:H13	1.67	0.60
1:W:137:GLU:OE1	1:W:182:LYS:NZ	2.29	0.59
1:V:207:GLU:OE2	1:W:266:ARG:NH1	2.35	0.59
1:E:169:SER:OG	2:E:400:08T:F1	2.10	0.59
1:I:186:ARG:NH2	1:I:272:ASN:OD1	2.34	0.59
1:E:357:ARG:NH2	2:E:400:08T:O3A	2.35	0.59
1:N:186:ARG:NH2	1:N:272:ASN:OD1	2.33	0.59
1:O:186:ARG:NH2	1:O:272:ASN:OD1	2.36	0.59
1:R:308:PRO:O	1:R:313:ARG:NH1	2.36	0.58
1:O:219:ALA:CB	1:O:220:VAL:HA	2.33	0.58
1:R:257:SER:OG	1:R:259:LYS:NZ	2.22	0.58
1:F:311:ARG:N	1:F:350:TYR:OH	2.37	0.58
1:J:169:SER:OG	2:J:400:08T:F1	2.12	0.58
1:R:200:PRO:HD2	1:R:203:ILE:HD11	1.85	0.57
1:R:173:LYS:N	2:R:400:08T:O2B	2.37	0.57
1:L:189:GLU:HB3	1:L:190:PRO:HD2	1.87	0.57
1:O:215:ALA:O	1:O:216:PHE:CD1	2.58	0.57
1:P:207:GLU:OE2	1:Q:266:ARG:NH1	2.38	0.56
1:S:146:MET:SD	1:S:313:ARG:NH2	2.79	0.56
1:Q:253:ARG:NH2	1:Q:268:GLU:OE2	2.38	0.56
1:A:357:ARG:NH2	1:B:256:GLU:OE1	2.38	0.56
1:I:169:SER:OG	2:I:400:08T:F1	2.14	0.56
1:J:207:GLU:OE2	1:K:266:ARG:NH1	2.38	0.56
1:B:365:ARG:NE	1:C:302:VAL:O	2.39	0.56
1:E:253:ARG:NH2	1:E:268:GLU:OE2	2.39	0.55
1:M:145:LYS:NZ	1:M:312:GLU:OE1	2.40	0.55
1:F:175:VAL:HG21	4:F:400:ADP:C8	2.41	0.55
1:K:297:TYR:OH	1:K:304:GLU:OE1	2.18	0.55
1:E:216:PHE:HB3	1:E:218:GLY:N	2.21	0.55
1:C:169:SER:OG	2:C:400:08T:F1	2.14	0.55
1:M:365:ARG:NE	1:N:302:VAL:O	2.39	0.54
1:E:138:GLU:O	1:E:139:TYR:CG	2.60	0.54
1:B:173:LYS:NZ	2:B:400:08T:O1B	2.29	0.54
1:M:173:LYS:NZ	2:M:400:08T:O2B	2.39	0.54
1:V:170:GLY:N	2:V:400:08T:O1B	2.37	0.54
1:E:130:ARG:HA	1:E:131:GLU:HB3	1.89	0.54
1:B:161:CYS:O	1:B:274:ARG:NE	2.41	0.53
1:F:311:ARG:HB3	1:F:350:TYR:CE2	2.43	0.53
1:V:357:ARG:NH2	2:V:400:08T:O1B	2.41	0.53
1:X:280:ASN:N	1:X:280:ASN:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:TYR:O	1:L:352:TRP:N	2.42	0.53
1:K:212:GLU:HG3	1:K:213:LYS:H	1.73	0.53
1:R:173:LYS:NZ	2:R:400:08T:F3	2.30	0.53
1:G:361:ASN:ND2	1:H:298:TYR:O	2.41	0.53
1:T:195:ASN:O	1:T:196:VAL:HG12	2.09	0.53
1:D:357:ARG:NH2	2:D:400:08T:O1A	2.42	0.53
1:O:169:SER:OG	2:O:400:08T:F3	2.17	0.53
1:Q:174:GLU:OE2	1:Q:178:ARG:NH1	2.42	0.52
1:G:215:ALA:HB1	1:G:264:GLY:HA3	1.91	0.52
1:H:365:ARG:NE	1:I:302:VAL:O	2.37	0.52
1:L:357:ARG:NH2	4:L:400:ADP:O3A	2.43	0.52
1:O:207:GLU:OE2	1:P:266:ARG:NH1	2.43	0.52
1:Q:365:ARG:NH2	1:R:302:VAL:O	2.41	0.52
1:W:203:ILE:HD11	1:X:263:LEU:HD11	1.91	0.52
1:F:173:LYS:NZ	4:F:400:ADP:O2B	2.38	0.51
1:T:253:ARG:O	1:T:257:SER:OG	2.25	0.51
1:G:239:GLU:OE1	1:G:280:ASN:ND2	2.42	0.51
1:R:217:THR:O	1:R:217:THR:HG22	2.10	0.51
1:N:175:VAL:O	1:N:179:LEU:N	2.44	0.51
1:D:207:GLU:OE2	1:E:266:ARG:NH1	2.44	0.51
1:R:265:GLY:O	1:R:266:ARG:HD3	2.11	0.51
1:V:215:ALA:O	1:V:216:PHE:CB	2.59	0.51
1:F:163:VAL:HG13	1:F:303:ILE:HD11	1.93	0.51
1:G:365:ARG:NE	1:H:302:VAL:O	2.43	0.51
1:U:297:TYR:OH	1:U:304:GLU:OE1	2.24	0.50
1:N:169:SER:CB	2:N:400:08T:F2	2.45	0.50
1:A:242:GLU:OE2	1:B:293:ARG:NH2	2.43	0.50
1:T:168:GLU:OE2	1:T:311:ARG:NH2	2.44	0.50
1:C:213:LYS:HG3	1:C:214:GLY:H	1.76	0.50
1:A:159:ALA:O	1:A:274:ARG:NH1	2.44	0.50
1:B:195:ASN:O	1:B:196:VAL:HG12	2.11	0.50
1:V:166:THR:OG1	1:V:306:GLU:OE2	2.28	0.50
1:F:172:GLY:HA2	4:F:400:ADP:O4'	2.12	0.50
1:H:159:ALA:O	1:H:274:ARG:NH1	2.45	0.50
1:A:169:SER:CB	2:A:400:08T:F3	2.37	0.49
1:O:305:ILE:HG22	1:O:307:ILE:HG13	1.93	0.49
1:R:356:VAL:HG12	2:R:400:08T:H8	1.93	0.49
1:B:212:GLU:OE1	1:B:262:ARG:NH1	2.46	0.49
1:E:138:GLU:HG2	1:E:139:TYR:H	1.78	0.49
1:N:159:ALA:O	1:N:274:ARG:NH1	2.45	0.49
1:P:219:ALA:HB2	1:Q:214:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:318:ILE:HB	1:R:319:PRO:HD3	1.94	0.49
1:F:196:VAL:HG13	1:F:197:ALA:N	2.28	0.49
1:F:297:TYR:OH	1:F:304:GLU:OE2	2.30	0.49
1:W:219:ALA:HB2	1:X:214:GLY:HA3	1.94	0.49
1:N:253:ARG:O	1:N:257:SER:OG	2.27	0.49
1:O:138:GLU:N	1:O:138:GLU:OE1	2.46	0.49
1:S:169:SER:CB	2:S:400:08T:F3	2.42	0.48
2:V:400:08T:O1A	2:V:400:08T:H4	2.12	0.48
1:R:189:GLU:HB3	1:R:190:PRO:HD2	1.95	0.48
1:U:189:GLU:HB3	1:U:190:PRO:CD	2.43	0.48
1:A:157:SER:HB3	1:A:184:SER:HA	1.94	0.48
1:H:253:ARG:O	1:H:257:SER:OG	2.26	0.48
1:N:161:CYS:O	1:N:274:ARG:NE	2.41	0.48
1:C:357:ARG:NH2	2:C:400:08T:O3A	2.47	0.48
1:S:365:ARG:NE	1:T:302:VAL:O	2.45	0.48
1:V:220:VAL:HB	1:W:213:LYS:HE2	1.95	0.48
1:X:309:PRO:O	1:X:313:ARG:NH1	2.46	0.48
1:G:357:ARG:NH1	2:G:400:08T:O3A	2.47	0.48
1:L:295:ASP:O	1:L:299:ARG:NH1	2.47	0.48
1:F:350:TYR:O	1:F:352:TRP:N	2.46	0.48
1:I:305:ILE:HG22	1:I:307:ILE:HG13	1.95	0.48
1:R:356:VAL:CG1	2:R:400:08T:H8	2.44	0.48
1:B:159:ALA:O	1:B:274:ARG:NH1	2.47	0.47
1:J:186:ARG:NH2	1:J:272:ASN:OD1	2.47	0.47
1:P:169:SER:CB	2:P:400:08T:F3	2.44	0.47
1:X:310:LEU:HD21	1:X:317:ILE:HG12	1.95	0.47
1:O:189:GLU:HB3	1:O:190:PRO:CD	2.45	0.47
1:H:185:ASP:N	1:H:185:ASP:OD1	2.48	0.47
1:V:168:GLU:OE1	1:V:311:ARG:NH2	2.46	0.47
1:H:161:CYS:O	1:H:274:ARG:NE	2.45	0.47
1:S:196:VAL:HG11	1:S:240:ILE:HA	1.97	0.47
1:A:365:ARG:NE	1:B:302:VAL:O	2.46	0.47
1:C:189:GLU:HB3	1:C:190:PRO:CD	2.44	0.47
1:S:239:GLU:N	1:S:278:ALA:O	2.46	0.47
1:K:174:GLU:OE2	1:K:178:ARG:NH1	2.44	0.47
1:R:295:ASP:OD1	1:R:296:LEU:N	2.48	0.47
1:X:257:SER:OG	1:X:259:LYS:NZ	2.33	0.47
1:X:237:LEU:N	1:X:237:LEU:HD12	2.29	0.47
1:N:248:GLN:HB3	1:N:296:LEU:HD22	1.97	0.46
1:U:357:ARG:NH2	2:U:400:08T:O3A	2.48	0.46
1:S:208:LEU:O	1:S:226:PHE:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:357:ARG:NH2	1:T:256:GLU:OE1	2.48	0.46
1:T:169:SER:OG	2:T:400:08T:O1B	2.24	0.46
1:A:196:VAL:HG11	1:A:240:ILE:HA	1.96	0.46
2:D:400:08T:F2	1:E:299:ARG:NH1	2.36	0.46
2:N:400:08T:F1	1:O:299:ARG:NH1	2.38	0.46
1:O:214:GLY:CA	1:O:219:ALA:HB2	2.46	0.46
1:O:216:PHE:CD1	1:O:216:PHE:C	2.89	0.46
1:D:357:ARG:HH22	2:D:400:08T:PB	2.39	0.46
1:W:207:GLU:OE2	1:X:266:ARG:NH1	2.49	0.46
1:I:297:TYR:O	1:I:301:GLY:N	2.49	0.46
1:O:224:GLU:O	1:P:266:ARG:NH2	2.49	0.46
1:L:350:TYR:N	1:L:351:PRO:HD3	2.31	0.46
1:R:216:PHE:O	1:R:218:GLY:N	2.48	0.46
1:G:224:GLU:OE1	1:G:262:ARG:NH2	2.49	0.46
1:M:239:GLU:N	1:M:278:ALA:O	2.49	0.46
1:I:207:GLU:OE2	1:J:266:ARG:NH1	2.49	0.45
1:U:216:PHE:CB	1:U:218:GLY:H	2.29	0.45
1:G:239:GLU:N	1:G:278:ALA:O	2.50	0.45
1:H:195:ASN:O	1:H:196:VAL:HG12	2.16	0.45
1:Q:169:SER:HA	1:Q:173:LYS:NZ	2.32	0.45
1:E:209:PHE:CE1	1:E:254:VAL:HG21	2.52	0.45
1:E:189:GLU:HB3	1:E:190:PRO:CD	2.47	0.45
1:X:357:ARG:NH1	2:X:400:08T:F1	2.39	0.45
1:C:224:GLU:O	1:D:266:ARG:NH2	2.49	0.45
1:S:308:PRO:O	1:S:313:ARG:NH1	2.50	0.45
1:G:213:LYS:N	1:G:222:SER:OG	2.50	0.44
1:J:200:PRO:HG2	1:J:203:ILE:CG1	2.47	0.44
1:L:196:VAL:HG13	1:L:197:ALA:N	2.32	0.44
1:Q:159:ALA:O	1:Q:274:ARG:NH1	2.51	0.44
1:N:195:ASN:O	1:N:196:VAL:HG12	2.16	0.44
1:R:146:MET:HA	1:R:149:ILE:HG22	1.99	0.44
1:F:164:LEU:HD21	1:F:283:ILE:HG21	1.98	0.44
1:X:356:VAL:CG1	2:X:400:08T:H14	2.47	0.44
1:D:357:ARG:CZ	2:D:400:08T:F2	2.32	0.44
1:X:249:ALA:HA	1:X:252:LEU:HD13	1.98	0.44
1:O:198:SER:HA	1:P:250:LYS:HD3	1.99	0.44
1:S:307:ILE:N	1:S:307:ILE:HD12	2.33	0.44
1:G:169:SER:HB2	1:G:280:ASN:CB	2.48	0.44
1:L:318:ILE:HB	1:L:319:PRO:HD3	2.00	0.44
1:M:198:SER:HA	1:N:250:LYS:HD3	2.00	0.44
1:R:213:LYS:N	1:R:222:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:346:LEU:HD21	1:T:384:VAL:HG11	2.00	0.44
1:K:220:VAL:HG23	1:K:221:SER:N	2.32	0.44
1:Q:169:SER:CB	2:Q:400:08T:F3	2.44	0.44
1:R:237:LEU:N	1:R:237:LEU:HD12	2.33	0.44
1:B:173:LYS:HG2	1:B:307:ILE:HD12	1.99	0.44
1:B:185:ASP:N	1:B:185:ASP:OD1	2.49	0.44
1:I:141:PHE:CD1	1:I:141:PHE:N	2.85	0.44
1:M:308:PRO:O	1:M:313:ARG:NH1	2.51	0.44
1:Q:308:PRO:HG2	1:Q:313:ARG:HD2	2.00	0.44
1:S:174:GLU:HB3	2:S:400:08T:O1A	2.18	0.44
1:T:212:GLU:OE1	1:T:262:ARG:NH1	2.51	0.43
1:T:357:ARG:HH22	2:T:400:08T:PB	2.41	0.43
1:W:308:PRO:HG2	1:W:313:ARG:HD2	1.99	0.43
1:I:213:LYS:HG3	1:I:214:GLY:H	1.83	0.43
1:X:145:LYS:O	1:X:148:GLU:HG2	2.18	0.43
1:A:239:GLU:N	1:A:278:ALA:O	2.51	0.43
1:F:189:GLU:HB3	1:F:190:PRO:CD	2.48	0.43
1:S:297:TYR:O	1:S:301:GLY:N	2.50	0.43
1:K:308:PRO:HG2	1:K:313:ARG:HD2	2.00	0.43
1:R:214:GLY:O	1:R:215:ALA:HB3	2.19	0.43
1:V:215:ALA:O	1:V:216:PHE:HB3	2.18	0.43
1:D:365:ARG:HD2	1:D:383:LEU:HD23	2.01	0.43
1:H:157:SER:HB2	1:H:184:SER:HA	2.00	0.43
1:N:185:ASP:OD1	1:N:185:ASP:N	2.46	0.43
1:T:357:ARG:NH1	2:T:400:08T:O1B	2.48	0.43
1:X:165:ILE:HG12	1:X:305:ILE:HD11	2.01	0.43
1:A:307:ILE:HD12	1:A:307:ILE:N	2.33	0.43
1:U:308:PRO:HG2	1:U:313:ARG:HD2	2.01	0.43
1:V:141:PHE:HD1	1:V:146:MET:HB3	1.82	0.43
1:M:297:TYR:O	1:M:301:GLY:N	2.45	0.43
1:B:234:THR:CG2	1:B:276:LEU:HD13	2.49	0.43
1:H:310:LEU:O	1:H:313:ARG:N	2.47	0.43
1:M:203:ILE:HG22	1:N:216:PHE:CE2	2.53	0.43
1:W:168:GLU:OE2	1:W:311:ARG:NH2	2.51	0.43
1:W:209:PHE:CE1	1:W:254:VAL:HG21	2.54	0.43
1:C:308:PRO:HG2	1:C:313:ARG:HD2	2.01	0.42
1:E:207:GLU:OE2	1:F:266:ARG:NH1	2.51	0.42
1:P:196:VAL:HG13	1:P:197:ALA:N	2.33	0.42
1:P:200:PRO:HG2	1:P:203:ILE:CG1	2.49	0.42
1:D:203:ILE:HG21	1:E:215:ALA:O	2.19	0.42
1:H:197:ALA:O	1:I:250:LYS:NZ	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:308:PRO:O	1:L:313:ARG:NH1	2.41	0.42
1:V:186:ARG:NH2	1:V:272:ASN:OD1	2.52	0.42
1:D:328:PHE:HB2	1:D:367:VAL:HG21	2.02	0.42
1:K:356:VAL:CG1	2:K:400:08T:H8	2.49	0.42
1:M:207:GLU:HG2	1:N:266:ARG:HH12	1.84	0.42
1:O:227:PHE:CZ	1:O:254:VAL:HG11	2.55	0.42
1:E:365:ARG:NH1	1:E:383:LEU:HG	2.33	0.42
1:M:186:ARG:NH2	1:M:272:ASN:OD1	2.53	0.42
1:P:189:GLU:HB3	1:P:190:PRO:CD	2.50	0.42
1:X:362:VAL:HG13	1:X:383:LEU:HD22	2.02	0.42
1:H:308:PRO:O	1:H:313:ARG:NH1	2.52	0.42
1:T:173:LYS:N	2:T:400:08T:O2A	2.53	0.42
1:U:189:GLU:HB3	1:U:190:PRO:HD2	2.01	0.42
1:V:350:TYR:O	1:V:352:TRP:N	2.52	0.42
1:K:352:TRP:CZ3	1:K:359:LEU:HA	2.55	0.42
1:O:203:ILE:CG2	1:P:216:PHE:HB2	2.50	0.42
1:W:169:SER:OG	2:W:400:08T:F1	2.20	0.42
1:X:318:ILE:HB	1:X:319:PRO:HD3	2.01	0.42
1:D:189:GLU:HB3	1:D:190:PRO:CD	2.49	0.42
1:H:169:SER:CB	2:H:400:08T:F3	2.54	0.42
1:M:251:LEU:O	1:M:252:LEU:HB3	2.20	0.42
1:E:308:PRO:HG2	1:E:313:ARG:HD2	2.01	0.42
1:F:189:GLU:HB3	1:F:190:PRO:HD2	2.02	0.42
1:G:307:ILE:HD12	1:G:307:ILE:N	2.35	0.42
1:K:160:GLU:OE2	1:K:186:ARG:NH2	2.52	0.42
1:X:375:ILE:HG23	1:X:379:GLU:CG	2.50	0.42
1:R:175:VAL:O	1:R:179:LEU:HD13	2.20	0.42
1:S:356:VAL:HG11	2:S:400:08T:N3	2.35	0.42
1:T:295:ASP:OD1	1:T:296:LEU:N	2.53	0.42
1:I:280:ASN:OD1	1:I:281:ARG:NH1	2.53	0.41
1:T:161:CYS:O	1:T:274:ARG:NE	2.51	0.41
1:V:328:PHE:HB2	1:V:367:VAL:HG21	2.02	0.41
1:W:365:ARG:HD2	1:W:383:LEU:HG	2.02	0.41
1:C:186:ARG:NH1	1:C:233:GLY:O	2.53	0.41
1:E:318:ILE:HB	1:E:319:PRO:HD3	2.03	0.41
1:W:216:PHE:O	1:W:217:THR:CB	2.68	0.41
1:C:318:ILE:HB	1:C:319:PRO:HD3	2.02	0.41
1:F:311:ARG:HB3	1:F:350:TYR:CZ	2.56	0.41
1:I:196:VAL:HG13	1:I:243:LEU:CD1	2.49	0.41
1:N:318:ILE:HB	1:N:319:PRO:HD3	2.02	0.41
1:O:212:GLU:HG3	1:O:213:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:249:ALA:HA	1:Q:252:LEU:HD13	2.02	0.41
1:O:189:GLU:HB3	1:O:190:PRO:HD2	2.02	0.41
1:G:189:GLU:HB3	1:G:190:PRO:CD	2.49	0.41
1:X:201:ARG:NH2	1:X:246:GLU:OE2	2.54	0.41
1:C:239:GLU:OE1	1:C:280:ASN:ND2	2.52	0.41
1:J:161:CYS:HB2	1:J:162:PRO:HD2	2.02	0.41
1:C:262:ARG:HG3	1:C:269:ILE:HD12	2.02	0.41
1:L:164:LEU:HD21	1:L:283:ILE:HG21	2.02	0.41
1:N:189:GLU:HB3	1:N:190:PRO:CD	2.50	0.41
1:U:200:PRO:HG2	1:U:203:ILE:CG1	2.50	0.41
1:X:175:VAL:HG22	2:X:400:08T:N3	2.36	0.41
1:E:216:PHE:HA	1:E:216:PHE:HD1	1.75	0.41
1:E:328:PHE:CE2	1:E:364:GLU:HB2	2.55	0.41
1:G:196:VAL:HG11	1:G:240:ILE:HA	2.02	0.41
1:M:252:LEU:O	1:M:255:ILE:N	2.48	0.41
1:R:240:ILE:HD12	1:R:277:ALA:HB1	2.02	0.41
1:S:192:VAL:HG12	1:S:194:LEU:CD1	2.50	0.41
1:A:297:TYR:O	1:A:301:GLY:N	2.48	0.41
1:D:209:PHE:CE1	1:D:254:VAL:HG21	2.56	0.41
1:N:295:ASP:OD1	1:N:296:LEU:N	2.54	0.41
1:Q:198:SER:HA	1:R:250:LYS:HD3	2.02	0.41
1:G:217:THR:O	1:H:217:THR:OG1	2.38	0.41
1:H:175:VAL:O	1:H:179:LEU:N	2.53	0.41
1:I:186:ARG:NH1	1:I:233:GLY:O	2.53	0.41
1:L:239:GLU:OE1	1:L:280:ASN:ND2	2.52	0.41
1:R:283:ILE:HD11	1:R:292:PHE:CD2	2.55	0.41
1:U:354:GLY:HA3	1:U:358:GLU:HB2	2.02	0.41
1:A:203:ILE:HG22	1:B:216:PHE:CE2	2.56	0.41
1:H:169:SER:HA	1:H:173:LYS:NZ	2.36	0.41
1:H:248:GLN:HB3	1:H:296:LEU:HD22	2.03	0.41
1:L:184:SER:O	1:L:187:SER:OG	2.39	0.41
1:W:189:GLU:HB3	1:W:190:PRO:CD	2.50	0.41
1:A:242:GLU:OE2	1:B:293:ARG:NH1	2.54	0.40
1:M:196:VAL:O	1:M:197:ALA:HB3	2.21	0.40
1:T:189:GLU:HB3	1:T:190:PRO:CD	2.51	0.40
1:U:318:ILE:HB	1:U:319:PRO:HD3	2.02	0.40
1:H:189:GLU:HB3	1:H:190:PRO:CD	2.51	0.40
1:S:295:ASP:OD1	1:S:296:LEU:N	2.55	0.40
1:V:200:PRO:HG2	1:V:203:ILE:CG1	2.51	0.40
1:C:189:GLU:HB3	1:C:190:PRO:HD2	2.03	0.40
1:H:153:ILE:HA	1:H:156:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:GLU:HB3	1:K:190:PRO:CD	2.51	0.40
1:U:376:ASP:OD1	1:U:377:ARG:N	2.54	0.40
1:G:169:SER:HB2	1:G:280:ASN:HB3	2.03	0.40
1:H:318:ILE:HB	1:H:319:PRO:HD3	2.03	0.40
1:I:189:GLU:HB3	1:I:190:PRO:CD	2.51	0.40
1:I:308:PRO:HG2	1:I:313:ARG:HD2	2.03	0.40
1:M:170:GLY:H	2:M:400:08T:PB	2.45	0.40
1:N:195:ASN:O	1:N:197:ALA:N	2.50	0.40
1:V:189:GLU:HB3	1:V:190:PRO:CD	2.51	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 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%)	34	69
1	B	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	19	57
1	C	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	34	69
1	D	245/268 (91%)	233 (95%)	12 (5%)	0	100	100
1	E	256/268 (96%)	237 (93%)	16 (6%)	3 (1%)	13	48
1	F	245/268 (91%)	234 (96%)	10 (4%)	1 (0%)	34	69
1	G	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	34	69
1	H	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	19	57
1	I	246/268 (92%)	234 (95%)	11 (4%)	1 (0%)	34	69
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%)	13	48
1	M	245/268 (91%)	228 (93%)	15 (6%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	245/268 (91%)	234 (96%)	9 (4%)	2 (1%)	19	57
1	O	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	34	69
1	P	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	34	69
1	Q	245/268 (91%)	236 (96%)	9 (4%)	0	100	100
1	R	245/268 (91%)	233 (95%)	9 (4%)	3 (1%)	13	48
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	34	69
1	T	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	19	57
1	U	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	34	69
1	V	245/268 (91%)	235 (96%)	9 (4%)	1 (0%)	34	69
1	W	248/268 (92%)	238 (96%)	9 (4%)	1 (0%)	34	69
1	X	244/268 (91%)	232 (95%)	10 (4%)	2 (1%)	19	57
All	All	5893/6432 (92%)	5594 (95%)	267 (4%)	32 (0%)	29	66

All (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
1	T	196	VAL
1	V	216	PHE
1	H	352	TRP
1	L	314	LYS
1	P	219	ALA
1	R	309	PRO
1	S	352	TRP
1	X	216	PHE
1	X	309	PRO
1	A	352	TRP
1	B	352	TRP
1	G	352	TRP
1	M	352	TRP
1	N	352	TRP
1	O	213	LYS
1	C	307	ILE
1	E	134	LEU

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Mol	Chain	Res	Type
1	E	139	TYR
1	E	352	TRP
1	F	309	PRO
1	I	307	ILE
1	L	309	PRO
1	M	252	LEU
1	T	352	TRP
1	U	307	ILE
1	W	219	ALA
1	L	217	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	211 (100%)	1 (0%)	88	94
1	D	212/233 (91%)	212 (100%)	0	100	100
1	E	223/233 (96%)	222 (100%)	1 (0%)	91	95
1	F	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	G	212/233 (91%)	212 (100%)	0	100	100
1	H	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	I	213/233 (91%)	212 (100%)	1 (0%)	88	94
1	J	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	K	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	L	211/233 (91%)	211 (100%)	0	100	100
1	M	212/233 (91%)	212 (100%)	0	100	100
1	N	212/233 (91%)	212 (100%)	0	100	100
1	O	212/233 (91%)	210 (99%)	2 (1%)	78	90
1	P	212/233 (91%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	212/233 (91%)	210 (99%)	2 (1%)	78	90
1	R	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	S	212/233 (91%)	212 (100%)	0	100	100
1	T	212/233 (91%)	212 (100%)	0	100	100
1	U	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	V	212/233 (91%)	211 (100%)	1 (0%)	88	94
1	W	215/233 (92%)	214 (100%)	1 (0%)	88	94
1	X	211/233 (91%)	208 (99%)	3 (1%)	67	85
All	All	5101/5592 (91%)	5083 (100%)	18 (0%)	91	95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	186	ARG
1	E	216	PHE
1	F	216	PHE
1	H	350	TYR
1	I	141	PHE
1	J	216	PHE
1	K	216	PHE
1	O	216	PHE
1	O	267	LYS
1	Q	178	ARG
1	Q	216	PHE
1	R	227	PHE
1	U	274	ARG
1	V	295	ASP
1	W	216	PHE
1	X	216	PHE
1	X	237	LEU
1	X	280	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	E	400	3	26,33,33	3.34	10 (38%)	25,52,52	1.82	4 (16%)
2	08T	G	400	1,3	26,33,33	3.31	10 (38%)	25,52,52	2.21	6 (24%)
2	08T	H	400	1,3	26,33,33	3.31	10 (38%)	25,52,52	2.03	5 (20%)
2	08T	M	400	1	26,33,33	3.32	10 (38%)	25,52,52	2.05	5 (20%)
2	08T	P	400	1,3	26,33,33	3.30	10 (38%)	25,52,52	2.20	7 (28%)
2	08T	Q	400	1	26,33,33	3.23	10 (38%)	25,52,52	2.39	7 (28%)
2	08T	V	400	3	26,33,33	3.30	10 (38%)	25,52,52	2.16	5 (20%)
2	08T	W	400	3	26,33,33	3.35	10 (38%)	25,52,52	2.12	6 (24%)
2	08T	B	400	1,3	26,33,33	3.33	10 (38%)	25,52,52	1.96	4 (16%)
2	08T	C	400	3	26,33,33	3.32	10 (38%)	25,52,52	1.92	4 (16%)
2	08T	I	400	3	26,33,33	3.32	10 (38%)	25,52,52	1.88	4 (16%)
2	08T	J	400	3	26,33,33	3.36	10 (38%)	25,52,52	1.99	4 (16%)
4	ADP	L	400	-	24,29,29	1.01	2 (8%)	29,45,45	1.45	4 (13%)
2	08T	R	400	3	26,33,33	3.31	10 (38%)	25,52,52	2.04	4 (16%)
2	08T	T	400	1,3	26,33,33	3.31	10 (38%)	25,52,52	1.91	4 (16%)
2	08T	A	400	1,3	26,33,33	3.27	10 (38%)	25,52,52	2.11	4 (16%)
2	08T	K	400	1,3	26,33,33	3.32	10 (38%)	25,52,52	2.04	5 (20%)
2	08T	U	400	1,3	26,33,33	3.30	10 (38%)	25,52,52	1.87	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	08T	X	400	-	26,33,33	3.26	10 (38%)	25,52,52	2.12	7 (28%)
2	08T	D	400	1,3	26,33,33	3.30	10 (38%)	25,52,52	1.93	4 (16%)
2	08T	N	400	1,3	26,33,33	3.37	10 (38%)	25,52,52	1.96	6 (24%)
2	08T	O	400	3	26,33,33	3.33	10 (38%)	25,52,52	2.06	5 (20%)
2	08T	S	400	1,3	26,33,33	3.30	10 (38%)	25,52,52	2.22	6 (24%)
4	ADP	F	400	3	24,29,29	0.88	1 (4%)	29,45,45	1.57	5 (17%)

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	E	400	3	-	3/12/38/38	0/3/3/3
2	08T	G	400	1,3	-	4/12/38/38	0/3/3/3
2	08T	H	400	1,3	-	1/12/38/38	0/3/3/3
2	08T	M	400	1	-	3/12/38/38	0/3/3/3
2	08T	P	400	1,3	-	1/12/38/38	0/3/3/3
2	08T	Q	400	1	-	3/12/38/38	0/3/3/3
2	08T	V	400	3	-	3/12/38/38	0/3/3/3
2	08T	W	400	3	-	0/12/38/38	0/3/3/3
2	08T	B	400	1,3	-	3/12/38/38	0/3/3/3
2	08T	C	400	3	-	5/12/38/38	0/3/3/3
2	08T	I	400	3	-	5/12/38/38	0/3/3/3
2	08T	J	400	3	-	3/12/38/38	0/3/3/3
4	ADP	L	400	-	-	2/12/32/32	0/3/3/3
2	08T	R	400	3	-	5/12/38/38	0/3/3/3
2	08T	T	400	1,3	-	5/12/38/38	0/3/3/3
2	08T	A	400	1,3	-	1/12/38/38	0/3/3/3
2	08T	K	400	1,3	-	4/12/38/38	0/3/3/3
2	08T	U	400	1,3	-	5/12/38/38	0/3/3/3
2	08T	X	400	-	-	2/12/38/38	0/3/3/3
2	08T	D	400	1,3	-	8/12/38/38	0/3/3/3
2	08T	N	400	1,3	-	4/12/38/38	0/3/3/3
2	08T	O	400	3	-	4/12/38/38	0/3/3/3
2	08T	S	400	1,3	-	2/12/38/38	0/3/3/3
4	ADP	F	400	3	-	4/12/32/32	0/3/3/3

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	400	08T	F2-BE	-7.83	1.35	1.54
2	C	400	08T	F2-BE	-7.80	1.35	1.54
2	D	400	08T	F2-BE	-7.80	1.35	1.54
2	I	400	08T	F2-BE	-7.74	1.35	1.54
2	J	400	08T	F2-BE	-7.74	1.35	1.54
2	E	400	08T	F2-BE	-7.66	1.35	1.54
2	K	400	08T	F2-BE	-7.66	1.35	1.54
2	O	400	08T	F2-BE	-7.65	1.35	1.54
2	T	400	08T	F2-BE	-7.65	1.35	1.54
2	M	400	08T	F2-BE	-7.65	1.35	1.54
2	W	400	08T	F2-BE	-7.65	1.35	1.54
2	V	400	08T	F2-BE	-7.64	1.35	1.54
2	R	400	08T	F2-BE	-7.61	1.35	1.54
2	G	400	08T	F2-BE	-7.61	1.35	1.54
2	S	400	08T	F2-BE	-7.61	1.35	1.54
2	P	400	08T	F2-BE	-7.59	1.35	1.54
2	B	400	08T	F2-BE	-7.57	1.35	1.54
2	X	400	08T	F2-BE	-7.56	1.35	1.54
2	H	400	08T	F2-BE	-7.47	1.36	1.54
2	A	400	08T	F2-BE	-7.44	1.36	1.54
2	W	400	08T	F1-BE	-7.27	1.36	1.54
2	V	400	08T	F1-BE	-7.20	1.36	1.54
2	B	400	08T	F1-BE	-7.20	1.36	1.54
2	Q	400	08T	F2-BE	-7.18	1.36	1.54
2	E	400	08T	F1-BE	-7.16	1.36	1.54
2	G	400	08T	F1-BE	-7.14	1.36	1.54
2	N	400	08T	F3-BE	-7.13	1.36	1.54
2	I	400	08T	F1-BE	-7.12	1.36	1.54
2	K	400	08T	F1-BE	-7.12	1.36	1.54
2	C	400	08T	F1-BE	-7.11	1.36	1.54
2	U	400	08T	F3-BE	-7.10	1.36	1.54
2	U	400	08T	F2-BE	-7.10	1.36	1.54
2	J	400	08T	F1-BE	-7.10	1.36	1.54
2	N	400	08T	F1-BE	-7.10	1.36	1.54
2	S	400	08T	F1-BE	-7.08	1.36	1.54
2	O	400	08T	F3-BE	-7.01	1.37	1.54
2	H	400	08T	F1-BE	-7.01	1.37	1.54
2	A	400	08T	F1-BE	-7.01	1.37	1.54
2	M	400	08T	F1-BE	-6.99	1.37	1.54
2	S	400	08T	F3-BE	-6.98	1.37	1.54
2	R	400	08T	F3-BE	-6.98	1.37	1.54
2	M	400	08T	F3-BE	-6.97	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	400	08T	F1-BE	-6.96	1.37	1.54
2	R	400	08T	F1-BE	-6.96	1.37	1.54
2	G	400	08T	F3-BE	-6.96	1.37	1.54
2	B	400	08T	F3-BE	-6.94	1.37	1.54
2	W	400	08T	F3-BE	-6.94	1.37	1.54
2	J	400	08T	F3-BE	-6.93	1.37	1.54
2	H	400	08T	F3-BE	-6.93	1.37	1.54
2	X	400	08T	F1-BE	-6.93	1.37	1.54
2	U	400	08T	F1-BE	-6.92	1.37	1.54
2	A	400	08T	F3-BE	-6.91	1.37	1.54
2	Q	400	08T	F3-BE	-6.91	1.37	1.54
2	P	400	08T	F1-BE	-6.90	1.37	1.54
2	T	400	08T	F1-BE	-6.89	1.37	1.54
2	E	400	08T	F3-BE	-6.88	1.37	1.54
2	C	400	08T	F3-BE	-6.88	1.37	1.54
2	T	400	08T	F3-BE	-6.86	1.37	1.54
2	K	400	08T	F3-BE	-6.86	1.37	1.54
2	Q	400	08T	F1-BE	-6.85	1.37	1.54
2	D	400	08T	F1-BE	-6.82	1.37	1.54
2	I	400	08T	F3-BE	-6.81	1.37	1.54
2	P	400	08T	F3-BE	-6.77	1.37	1.54
2	X	400	08T	F3-BE	-6.75	1.37	1.54
2	V	400	08T	F3-BE	-6.70	1.37	1.54
2	J	400	08T	O4'-C1'	6.64	1.50	1.41
2	T	400	08T	O4'-C1'	6.63	1.50	1.41
2	D	400	08T	F3-BE	-6.60	1.38	1.54
2	D	400	08T	O4'-C1'	6.59	1.50	1.41
2	H	400	08T	O4'-C1'	6.58	1.50	1.41
2	U	400	08T	O4'-C1'	6.50	1.50	1.41
2	B	400	08T	O4'-C1'	6.45	1.50	1.41
2	R	400	08T	O4'-C1'	6.44	1.50	1.41
2	W	400	08T	O4'-C1'	6.42	1.50	1.41
2	N	400	08T	O4'-C1'	6.41	1.50	1.41
2	O	400	08T	O4'-C1'	6.41	1.50	1.41
2	P	400	08T	O4'-C1'	6.39	1.50	1.41
2	S	400	08T	O4'-C1'	6.39	1.50	1.41
2	E	400	08T	O4'-C1'	6.38	1.50	1.41
2	Q	400	08T	O4'-C1'	6.38	1.50	1.41
2	G	400	08T	O4'-C1'	6.32	1.49	1.41
2	V	400	08T	O4'-C1'	6.28	1.49	1.41
2	A	400	08T	O4'-C1'	6.26	1.49	1.41
2	X	400	08T	O4'-C1'	6.20	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	400	08T	O4'-C1'	6.19	1.49	1.41
2	C	400	08T	O4'-C1'	6.06	1.49	1.41
2	K	400	08T	O4'-C1'	6.06	1.49	1.41
2	M	400	08T	O4'-C1'	6.04	1.49	1.41
2	M	400	08T	C2'-C1'	-4.27	1.47	1.53
2	C	400	08T	C2'-C1'	-4.26	1.47	1.53
2	K	400	08T	C2'-C1'	-4.24	1.47	1.53
2	J	400	08T	C2'-C1'	-4.12	1.47	1.53
2	E	400	08T	C2'-C1'	-4.10	1.47	1.53
2	O	400	08T	C2'-C1'	-4.08	1.47	1.53
2	I	400	08T	C2'-C1'	-4.07	1.47	1.53
2	U	400	08T	C2'-C1'	-4.07	1.47	1.53
2	M	400	08T	C5-C4	-4.07	1.30	1.40
2	N	400	08T	C2'-C1'	-4.05	1.47	1.53
2	W	400	08T	C5-C4	-4.04	1.30	1.40
2	I	400	08T	C5-C4	-4.03	1.30	1.40
2	R	400	08T	C5-C4	-4.02	1.30	1.40
2	U	400	08T	C5-C4	-4.02	1.30	1.40
2	Q	400	08T	C5-C4	-3.98	1.30	1.40
2	C	400	08T	C5-C4	-3.98	1.30	1.40
2	B	400	08T	C5-C4	-3.96	1.30	1.40
2	A	400	08T	C5-C4	-3.96	1.30	1.40
2	N	400	08T	C2-N3	3.95	1.38	1.32
2	K	400	08T	C5-C4	-3.94	1.30	1.40
2	E	400	08T	C5-C4	-3.94	1.30	1.40
2	P	400	08T	C5-C4	-3.94	1.30	1.40
2	O	400	08T	C5-C4	-3.93	1.30	1.40
2	J	400	08T	C5-C4	-3.92	1.30	1.40
2	H	400	08T	C5-C4	-3.92	1.30	1.40
2	V	400	08T	C5-C4	-3.91	1.30	1.40
2	S	400	08T	C5-C4	-3.91	1.30	1.40
2	T	400	08T	C5-C4	-3.90	1.30	1.40
2	C	400	08T	C2-N3	3.89	1.38	1.32
2	N	400	08T	C5-C4	-3.88	1.30	1.40
2	G	400	08T	C2-N3	3.88	1.38	1.32
2	G	400	08T	C5-C4	-3.88	1.30	1.40
2	W	400	08T	C2'-C1'	-3.86	1.47	1.53
2	D	400	08T	C5-C4	-3.86	1.30	1.40
2	J	400	08T	C2-N3	3.84	1.38	1.32
2	K	400	08T	C2-N3	3.83	1.38	1.32
2	X	400	08T	C5-C4	-3.83	1.30	1.40
2	P	400	08T	C2-N3	3.82	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	400	08T	C2'-C1'	-3.81	1.48	1.53
2	P	400	08T	C2'-C1'	-3.81	1.48	1.53
2	X	400	08T	C2'-C1'	-3.81	1.48	1.53
2	Q	400	08T	C2-N3	3.81	1.38	1.32
2	H	400	08T	C2'-C1'	-3.79	1.48	1.53
2	M	400	08T	C2-N3	3.79	1.38	1.32
2	R	400	08T	C2'-C1'	-3.79	1.48	1.53
2	E	400	08T	C2-N3	3.78	1.38	1.32
2	A	400	08T	C2-N3	3.78	1.38	1.32
2	V	400	08T	C2-N3	3.77	1.38	1.32
2	T	400	08T	C2-N3	3.77	1.38	1.32
2	B	400	08T	C2'-C1'	-3.76	1.48	1.53
2	R	400	08T	C2-N3	3.74	1.38	1.32
2	D	400	08T	C2'-C1'	-3.70	1.48	1.53
2	B	400	08T	C2-N3	3.70	1.38	1.32
2	O	400	08T	C2-N3	3.69	1.38	1.32
2	A	400	08T	C2'-C1'	-3.68	1.48	1.53
2	W	400	08T	C2-N3	3.68	1.38	1.32
2	G	400	08T	C2'-C1'	-3.67	1.48	1.53
2	I	400	08T	C2-N3	3.67	1.38	1.32
2	S	400	08T	C2-N3	3.67	1.38	1.32
2	T	400	08T	C2'-C1'	-3.66	1.48	1.53
2	H	400	08T	C2-N3	3.66	1.38	1.32
2	U	400	08T	C2-N3	3.65	1.38	1.32
2	D	400	08T	C2-N3	3.62	1.37	1.32
2	X	400	08T	C2-N3	3.59	1.37	1.32
2	S	400	08T	C2'-C1'	-3.52	1.48	1.53
2	U	400	08T	C2'-C3'	-3.33	1.44	1.53
2	X	400	08T	C5-N7	-3.33	1.27	1.39
2	P	400	08T	C5-N7	-3.32	1.27	1.39
2	E	400	08T	C2'-C3'	-3.32	1.44	1.53
2	G	400	08T	C5-N7	-3.28	1.27	1.39
2	M	400	08T	C5-N7	-3.28	1.27	1.39
2	V	400	08T	C5-N7	-3.27	1.27	1.39
2	K	400	08T	C5-N7	-3.27	1.27	1.39
2	W	400	08T	C5-N7	-3.27	1.27	1.39
2	B	400	08T	C5-N7	-3.27	1.27	1.39
2	P	400	08T	C2'-C3'	-3.26	1.44	1.53
2	S	400	08T	C5-N7	-3.26	1.27	1.39
2	N	400	08T	C5-N7	-3.24	1.28	1.39
2	I	400	08T	C2'-C3'	-3.24	1.44	1.53
2	H	400	08T	C5-N7	-3.24	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	400	08T	C2'-C1'	-3.24	1.48	1.53
2	Q	400	08T	C5-N7	-3.23	1.28	1.39
2	O	400	08T	C2'-C3'	-3.22	1.44	1.53
2	W	400	08T	C2'-C3'	-3.22	1.44	1.53
2	A	400	08T	C5-N7	-3.20	1.28	1.39
2	J	400	08T	C2'-C3'	-3.19	1.44	1.53
2	D	400	08T	C5-N7	-3.19	1.28	1.39
2	E	400	08T	C5-N7	-3.19	1.28	1.39
2	J	400	08T	C5-N7	-3.19	1.28	1.39
2	T	400	08T	C5-N7	-3.19	1.28	1.39
2	O	400	08T	C5-N7	-3.18	1.28	1.39
2	I	400	08T	C5-N7	-3.17	1.28	1.39
2	U	400	08T	C5-N7	-3.17	1.28	1.39
2	V	400	08T	C2'-C3'	-3.17	1.44	1.53
2	C	400	08T	C2'-C3'	-3.17	1.44	1.53
2	R	400	08T	C5-N7	-3.16	1.28	1.39
2	D	400	08T	C2'-C3'	-3.15	1.44	1.53
2	C	400	08T	C5-N7	-3.14	1.28	1.39
2	T	400	08T	C2'-C3'	-3.14	1.44	1.53
2	B	400	08T	C2'-C3'	-3.14	1.44	1.53
2	A	400	08T	C2'-C3'	-3.13	1.44	1.53
2	H	400	08T	C2'-C3'	-3.09	1.44	1.53
2	G	400	08T	C2'-C3'	-3.02	1.45	1.53
2	R	400	08T	C2'-C3'	-3.02	1.45	1.53
2	X	400	08T	C2'-C3'	-3.01	1.45	1.53
2	M	400	08T	C2'-C3'	-3.00	1.45	1.53
2	K	400	08T	C2'-C3'	-3.00	1.45	1.53
2	Q	400	08T	C2'-C3'	-2.96	1.45	1.53
2	S	400	08T	C2'-C3'	-2.96	1.45	1.53
2	N	400	08T	C2'-C3'	-2.81	1.45	1.53
2	D	400	08T	C6-N6	2.54	1.43	1.34
2	P	400	08T	C6-N6	2.47	1.43	1.34
2	J	400	08T	C6-N6	2.45	1.43	1.34
2	W	400	08T	C6-N6	2.45	1.43	1.34
2	B	400	08T	C6-N6	2.45	1.43	1.34
2	H	400	08T	C6-N6	2.45	1.43	1.34
2	V	400	08T	C6-N6	2.44	1.42	1.34
2	A	400	08T	C6-N6	2.43	1.42	1.34
2	E	400	08T	C6-N6	2.43	1.42	1.34
4	L	400	ADP	C5-C4	2.42	1.47	1.40
2	N	400	08T	C6-N6	2.41	1.42	1.34
2	X	400	08T	C6-N6	2.41	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	400	08T	C6-N6	2.41	1.42	1.34
2	O	400	08T	C6-N6	2.40	1.42	1.34
2	K	400	08T	C6-N6	2.39	1.42	1.34
2	Q	400	08T	C6-N6	2.39	1.42	1.34
2	S	400	08T	C6-N6	2.38	1.42	1.34
2	G	400	08T	C6-N6	2.36	1.42	1.34
2	M	400	08T	C6-N6	2.36	1.42	1.34
2	R	400	08T	C6-N6	2.35	1.42	1.34
2	C	400	08T	C6-N6	2.33	1.42	1.34
2	I	400	08T	C6-N6	2.32	1.42	1.34
2	U	400	08T	C6-N6	2.31	1.42	1.34
4	F	400	ADP	C5-C4	2.21	1.46	1.40
4	L	400	ADP	C2-N3	2.05	1.35	1.32

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	400	08T	C4-C5-N7	5.96	115.61	109.40
2	V	400	08T	C4-C5-N7	5.73	115.37	109.40
2	P	400	08T	C4-C5-N7	5.72	115.36	109.40
2	D	400	08T	N3-C2-N1	-5.71	119.75	128.68
2	R	400	08T	N3-C2-N1	-5.67	119.82	128.68
2	I	400	08T	N3-C2-N1	-5.65	119.85	128.68
2	S	400	08T	N3-C2-N1	-5.60	119.92	128.68
2	Q	400	08T	N3-C2-N1	-5.58	119.95	128.68
2	C	400	08T	N3-C2-N1	-5.58	119.96	128.68
2	O	400	08T	N3-C2-N1	-5.57	119.98	128.68
2	Q	400	08T	C4-C5-N7	5.56	115.19	109.40
2	W	400	08T	N3-C2-N1	-5.56	119.99	128.68
2	A	400	08T	N3-C2-N1	-5.55	120.00	128.68
2	M	400	08T	C4-C5-N7	5.55	115.19	109.40
2	K	400	08T	N3-C2-N1	-5.55	120.00	128.68
2	J	400	08T	C4-C5-N7	5.54	115.17	109.40
2	J	400	08T	N3-C2-N1	-5.53	120.04	128.68
2	E	400	08T	N3-C2-N1	-5.52	120.05	128.68
2	H	400	08T	N3-C2-N1	-5.52	120.05	128.68
2	D	400	08T	C4-C5-N7	5.51	115.14	109.40
2	S	400	08T	C4-C5-N7	5.51	115.14	109.40
2	V	400	08T	N3-C2-N1	-5.50	120.07	128.68
2	M	400	08T	N3-C2-N1	-5.46	120.15	128.68
2	T	400	08T	N3-C2-N1	-5.46	120.15	128.68
2	U	400	08T	N3-C2-N1	-5.44	120.17	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	400	08T	N3-C2-N1	-5.43	120.19	128.68
2	B	400	08T	N3-C2-N1	-5.41	120.22	128.68
2	G	400	08T	C4-C5-N7	5.38	115.00	109.40
2	A	400	08T	C4-C5-N7	5.36	114.99	109.40
2	N	400	08T	N3-C2-N1	-5.35	120.31	128.68
2	H	400	08T	C4-C5-N7	5.29	114.91	109.40
2	K	400	08T	C4-C5-N7	5.29	114.91	109.40
2	O	400	08T	C4-C5-N7	5.26	114.88	109.40
2	C	400	08T	C4-C5-N7	5.24	114.86	109.40
2	I	400	08T	C4-C5-N7	5.24	114.86	109.40
2	G	400	08T	N3-C2-N1	-5.23	120.50	128.68
2	X	400	08T	N3-C2-N1	-5.23	120.50	128.68
2	U	400	08T	C4-C5-N7	5.21	114.83	109.40
2	B	400	08T	C4-C5-N7	5.20	114.81	109.40
2	E	400	08T	C4-C5-N7	5.18	114.80	109.40
2	X	400	08T	C4-C5-N7	5.16	114.77	109.40
2	R	400	08T	C4-C5-N7	5.08	114.70	109.40
2	T	400	08T	C4-C5-N7	4.95	114.56	109.40
2	S	400	08T	C3'-C2'-C1'	4.76	108.14	100.98
2	G	400	08T	C3'-C2'-C1'	4.68	108.02	100.98
2	N	400	08T	C4-C5-N7	4.63	114.23	109.40
2	Q	400	08T	O4'-C4'-C3'	4.61	114.24	105.11
2	Q	400	08T	C3'-C2'-C1'	4.60	107.90	100.98
2	P	400	08T	C3'-C2'-C1'	4.52	107.79	100.98
2	V	400	08T	C3'-C2'-C1'	4.46	107.70	100.98
2	A	400	08T	C3'-C2'-C1'	4.39	107.59	100.98
2	R	400	08T	C3'-C2'-C1'	4.29	107.43	100.98
2	O	400	08T	PB-O3A-PA	-4.20	118.42	132.83
2	H	400	08T	C3'-C2'-C1'	4.18	107.28	100.98
2	X	400	08T	C3'-C2'-C1'	4.14	107.21	100.98
2	W	400	08T	C3'-C2'-C1'	3.81	106.71	100.98
4	L	400	ADP	N3-C2-N1	-3.68	122.93	128.68
2	Q	400	08T	O4'-C4'-C5'	3.62	121.28	109.37
2	U	400	08T	PB-O3A-PA	-3.59	120.51	132.83
2	M	400	08T	C3'-C2'-C1'	3.51	106.26	100.98
4	F	400	ADP	N3-C2-N1	-3.46	123.27	128.68
2	T	400	08T	C3'-C2'-C1'	3.44	106.16	100.98
4	F	400	ADP	O4'-C1'-C2'	-3.42	101.94	106.93
2	V	400	08T	PB-O3A-PA	-3.35	121.34	132.83
2	K	400	08T	PB-O3A-PA	-3.28	121.56	132.83
2	G	400	08T	PB-O3A-PA	-3.28	121.58	132.83
2	J	400	08T	C3'-C2'-C1'	3.26	105.89	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	400	ADP	C4-C5-N7	-3.25	106.02	109.40
4	L	400	ADP	C3'-C2'-C1'	3.24	105.86	100.98
2	O	400	08T	C3'-C2'-C1'	3.21	105.81	100.98
2	A	400	08T	PB-O3A-PA	-3.20	121.83	132.83
2	S	400	08T	PB-O3A-PA	-3.19	121.86	132.83
2	J	400	08T	PB-O3A-PA	-3.18	121.90	132.83
2	P	400	08T	PB-O3A-PA	-3.18	121.92	132.83
2	B	400	08T	C3'-C2'-C1'	3.18	105.76	100.98
2	X	400	08T	C1'-N9-C4	3.16	132.19	126.64
4	F	400	ADP	PA-O3A-PB	-3.11	122.14	132.83
2	N	400	08T	PB-O3A-PA	-2.99	122.55	132.83
2	C	400	08T	PB-O3A-PA	-2.97	122.64	132.83
4	L	400	ADP	PA-O3A-PB	-2.95	122.70	132.83
2	X	400	08T	PB-O3A-PA	-2.92	122.80	132.83
2	R	400	08T	PB-O3A-PA	-2.90	122.87	132.83
2	D	400	08T	C3'-C2'-C1'	2.86	105.29	100.98
2	B	400	08T	PB-O3A-PA	-2.84	123.08	132.83
2	H	400	08T	PB-O3A-PA	-2.80	123.21	132.83
2	I	400	08T	PB-O3A-PA	-2.79	123.24	132.83
2	M	400	08T	PB-O3A-PA	-2.79	123.26	132.83
4	L	400	ADP	C4-C5-N7	-2.75	106.53	109.40
2	G	400	08T	C2'-C3'-C4'	2.73	107.95	102.64
4	F	400	ADP	C3'-C2'-C1'	2.62	104.92	100.98
2	G	400	08T	C1'-N9-C4	2.61	131.23	126.64
2	W	400	08T	PB-O3A-PA	-2.56	124.03	132.83
2	N	400	08T	C1'-N9-C4	2.55	131.13	126.64
2	M	400	08T	C2'-C3'-C4'	2.52	107.55	102.64
2	N	400	08T	C3'-C2'-C1'	2.47	104.70	100.98
2	X	400	08T	C2'-C3'-C4'	2.42	107.34	102.64
2	S	400	08T	C2'-C3'-C4'	2.38	107.27	102.64
2	W	400	08T	N6-C6-N1	2.31	123.37	118.57
2	Q	400	08T	PB-O3A-PA	-2.22	125.22	132.83
2	P	400	08T	C2'-C3'-C4'	2.21	106.93	102.64
2	H	400	08T	C5-C6-N1	-2.20	115.38	120.35
2	K	400	08T	C1'-N9-C4	2.18	130.47	126.64
2	K	400	08T	C3'-C2'-C1'	2.18	104.26	100.98
2	E	400	08T	C3'-C2'-C1'	2.17	104.24	100.98
2	D	400	08T	C5-C6-N1	-2.17	115.44	120.35
2	T	400	08T	O3B-PB-O1B	-2.15	105.51	111.52
2	P	400	08T	C5-C6-N1	-2.14	115.50	120.35
2	V	400	08T	C5-C6-N1	-2.12	115.54	120.35
2	S	400	08T	C5-C6-N1	-2.11	115.56	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	400	08T	C5-C6-N1	-2.10	115.59	120.35
2	O	400	08T	C5-C6-N1	-2.10	115.59	120.35
2	N	400	08T	C5'-C4'-C3'	-2.10	107.33	115.18
2	E	400	08T	PB-O3A-PA	-2.09	125.65	132.83
2	X	400	08T	C5-C6-N1	-2.08	115.63	120.35
2	P	400	08T	N6-C6-N1	2.05	122.84	118.57
2	C	400	08T	C2'-C3'-C4'	2.02	106.56	102.64
2	Q	400	08T	C5-C6-N1	-2.01	115.79	120.35
2	I	400	08T	C5-C6-N1	-2.00	115.81	120.35

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	400	08T	C5'-O5'-PA-O1A
2	G	400	08T	C5'-O5'-PA-O2A
2	G	400	08T	C5'-O5'-PA-O3A
2	C	400	08T	C5'-O5'-PA-O3A
2	I	400	08T	C5'-O5'-PA-O2A
2	I	400	08T	C5'-O5'-PA-O3A
2	R	400	08T	C5'-O5'-PA-O1A
2	R	400	08T	C5'-O5'-PA-O3A
2	R	400	08T	O4'-C4'-C5'-O5'
2	R	400	08T	C3'-C4'-C5'-O5'
2	K	400	08T	O4'-C4'-C5'-O5'
2	K	400	08T	C3'-C4'-C5'-O5'
2	U	400	08T	C5'-O5'-PA-O1A
2	U	400	08T	C5'-O5'-PA-O3A
2	D	400	08T	C5'-O5'-PA-O1A
2	D	400	08T	C5'-O5'-PA-O2A
2	N	400	08T	C5'-O5'-PA-O2A
2	S	400	08T	O4'-C4'-C5'-O5'
2	S	400	08T	C3'-C4'-C5'-O5'
4	F	400	ADP	C5'-O5'-PA-O1A
4	L	400	ADP	C3'-C4'-C5'-O5'
2	E	400	08T	C3'-C4'-C5'-O5'
2	E	400	08T	O4'-C4'-C5'-O5'
2	U	400	08T	O4'-C4'-C5'-O5'
2	U	400	08T	C3'-C4'-C5'-O5'
4	L	400	ADP	O4'-C4'-C5'-O5'
2	M	400	08T	C4'-C5'-O5'-PA
2	B	400	08T	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	G	400	08T	O4'-C4'-C5'-O5'
2	Q	400	08T	O4'-C4'-C5'-O5'
2	B	400	08T	O4'-C4'-C5'-O5'
2	I	400	08T	C3'-C4'-C5'-O5'
2	I	400	08T	O4'-C4'-C5'-O5'
2	J	400	08T	O4'-C4'-C5'-O5'
2	T	400	08T	O4'-C4'-C5'-O5'
2	O	400	08T	O4'-C4'-C5'-O5'
2	N	400	08T	PA-O3A-PB-O3B
2	C	400	08T	O4'-C4'-C5'-O5'
4	F	400	ADP	C4'-C5'-O5'-PA
2	D	400	08T	PA-O3A-PB-O1B
2	T	400	08T	C3'-C4'-C5'-O5'
2	O	400	08T	C3'-C4'-C5'-O5'
2	V	400	08T	C4'-C5'-O5'-PA
2	N	400	08T	C4'-C5'-O5'-PA
2	O	400	08T	C4'-C5'-O5'-PA
2	V	400	08T	PB-O3A-PA-O5'
2	J	400	08T	C3'-C4'-C5'-O5'
2	D	400	08T	C5'-O5'-PA-O3A
2	N	400	08T	C5'-O5'-PA-O3A
2	T	400	08T	PA-O3A-PB-O2B
2	K	400	08T	PA-O3A-PB-O2B
2	O	400	08T	PB-O3A-PA-O1A
2	C	400	08T	C5'-O5'-PA-O1A
2	C	400	08T	C5'-O5'-PA-O2A
2	I	400	08T	C5'-O5'-PA-O1A
2	R	400	08T	C5'-O5'-PA-O2A
2	U	400	08T	C5'-O5'-PA-O2A
2	C	400	08T	C3'-C4'-C5'-O5'
2	A	400	08T	O4'-C4'-C5'-O5'
2	X	400	08T	PA-O3A-PB-O2B
2	B	400	08T	C4'-C5'-O5'-PA
2	J	400	08T	C4'-C5'-O5'-PA
2	D	400	08T	O4'-C4'-C5'-O5'
2	M	400	08T	PA-O3A-PB-O3B
2	P	400	08T	C4'-C5'-O5'-PA
2	Q	400	08T	PB-O3A-PA-O2A
2	X	400	08T	PA-O3A-PB-O1B
2	D	400	08T	PA-O3A-PB-O2B
4	F	400	ADP	C5'-O5'-PA-O3A
2	D	400	08T	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	T	400	08T	PB-O3A-PA-O1A
2	E	400	08T	C4'-C5'-O5'-PA
2	H	400	08T	C4'-C5'-O5'-PA
2	Q	400	08T	C4'-C5'-O5'-PA
2	K	400	08T	C4'-C5'-O5'-PA
2	V	400	08T	C5'-O5'-PA-O2A
2	M	400	08T	O4'-C4'-C5'-O5'
4	F	400	ADP	O4'-C4'-C5'-O5'
2	T	400	08T	C4'-C5'-O5'-PA
2	D	400	08T	C4'-C5'-O5'-PA

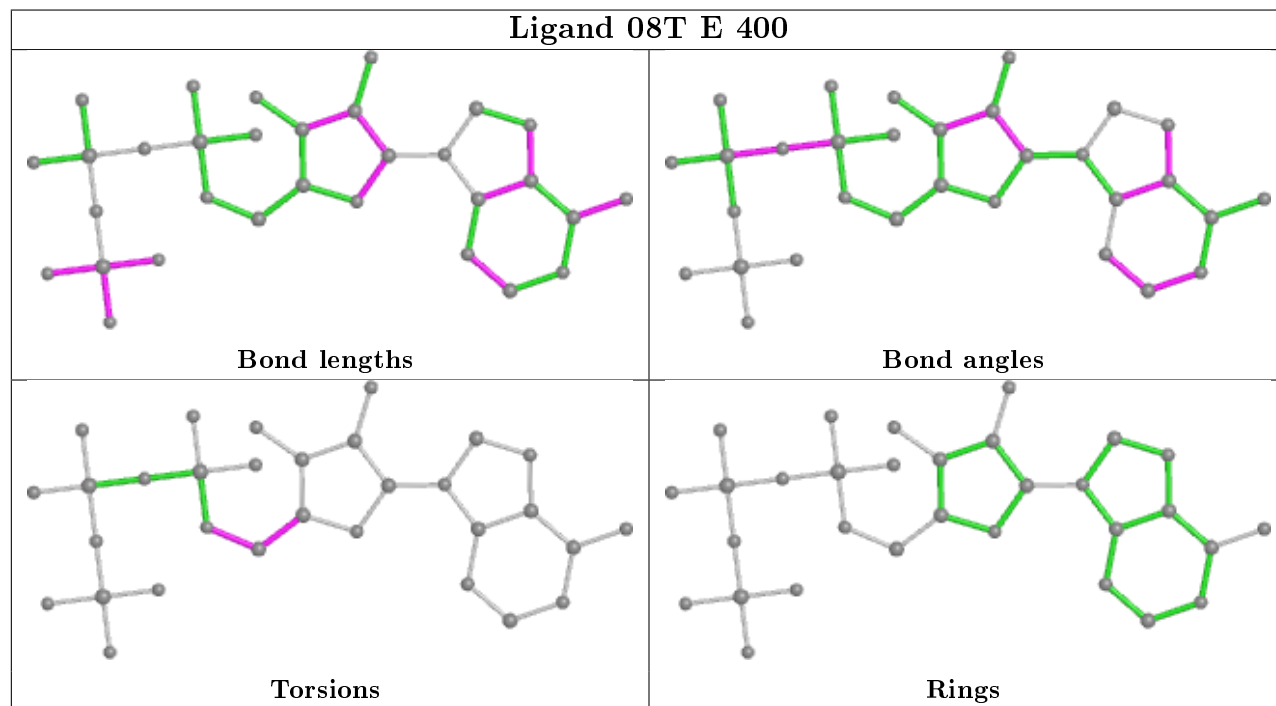
There are no ring outliers.

24 monomers are involved in 63 short contacts:

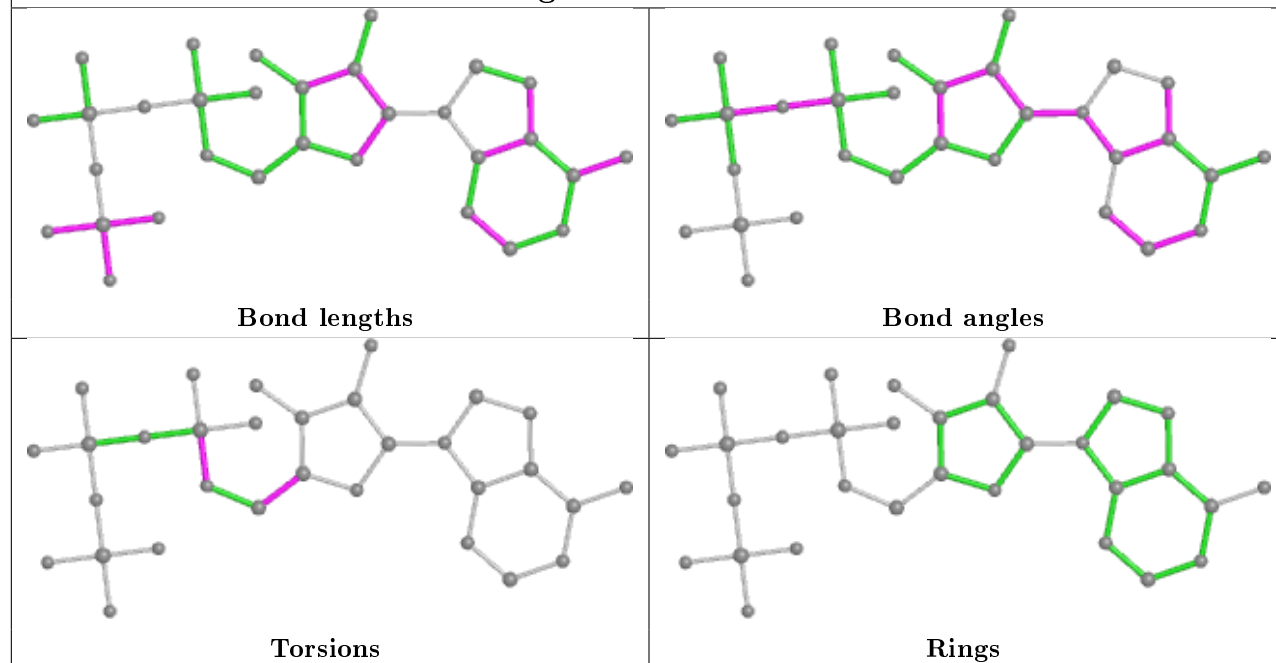
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	400	08T	2	0
2	G	400	08T	1	0
2	H	400	08T	2	0
2	M	400	08T	3	0
2	P	400	08T	2	0
2	Q	400	08T	2	0
2	V	400	08T	3	0
2	W	400	08T	2	0
2	B	400	08T	2	0
2	C	400	08T	2	0
2	I	400	08T	1	0
2	J	400	08T	2	0
4	L	400	ADP	1	0
2	R	400	08T	4	0
2	T	400	08T	7	0
2	A	400	08T	1	0
2	K	400	08T	3	0
2	U	400	08T	2	0
2	X	400	08T	4	0
2	D	400	08T	5	0
2	N	400	08T	4	0
2	O	400	08T	2	0
2	S	400	08T	3	0
4	F	400	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

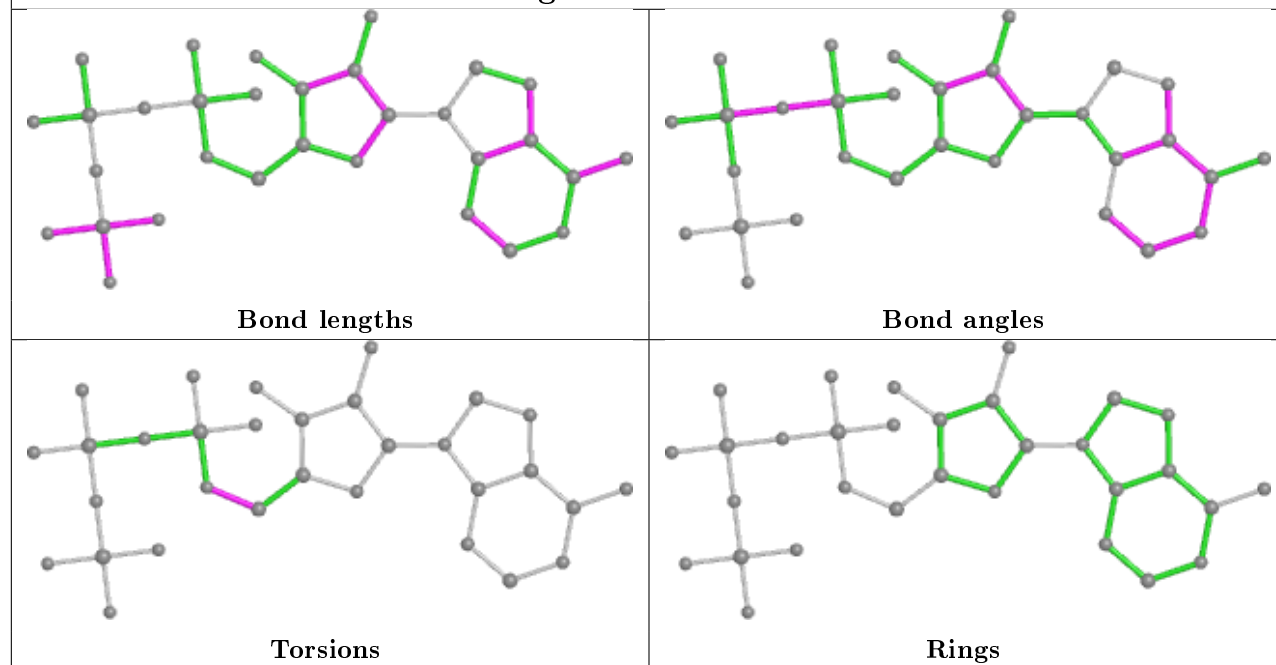
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



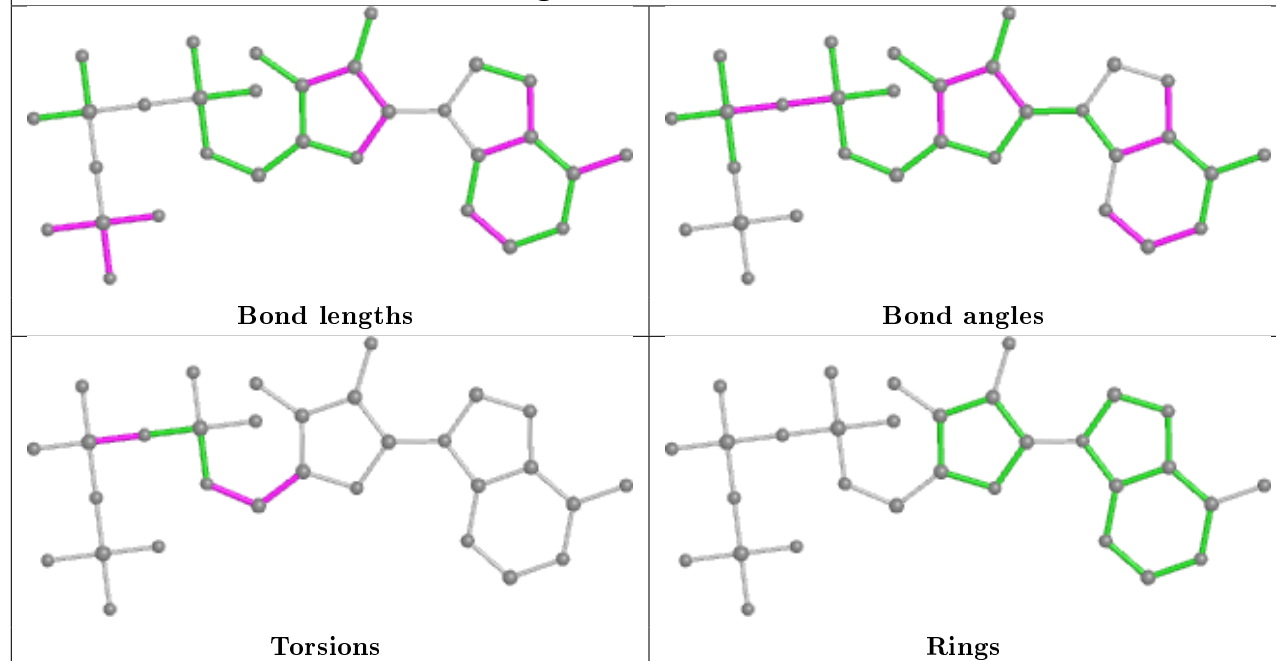
## Ligand 08T G 400



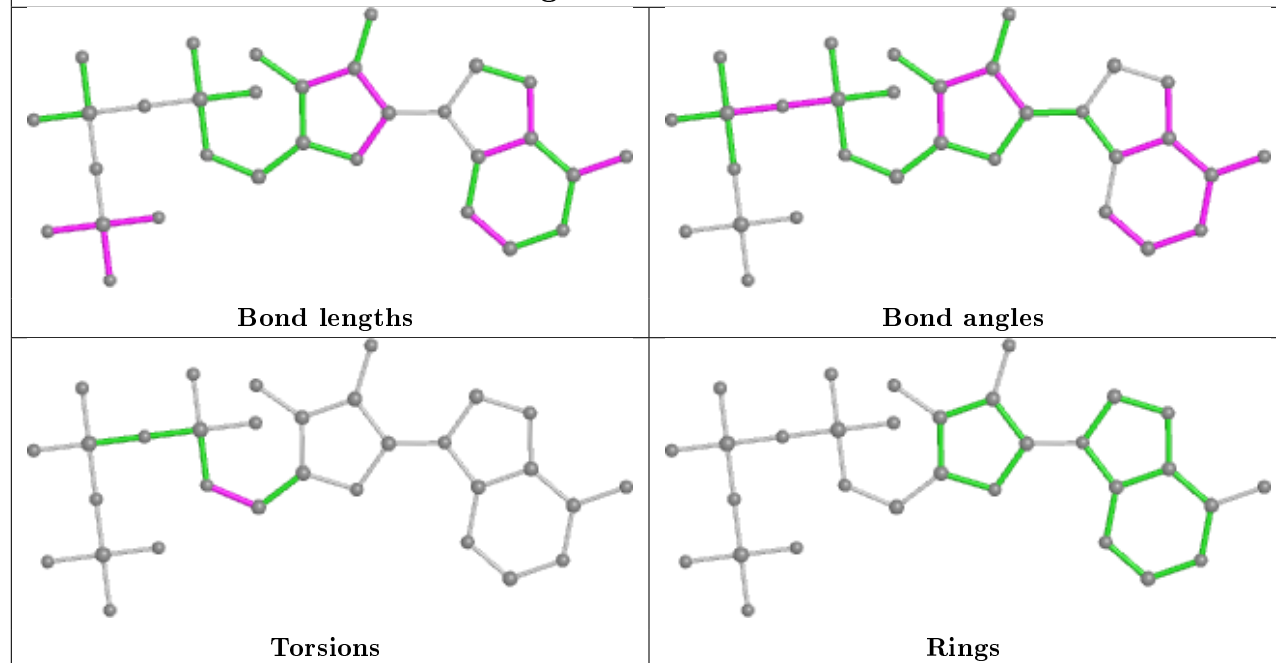
## Ligand 08T H 400



## Ligand 08T M 400

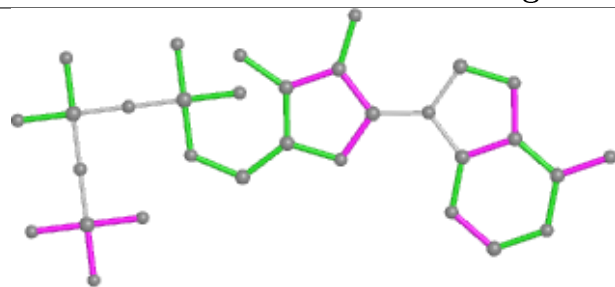


## Ligand 08T P 400

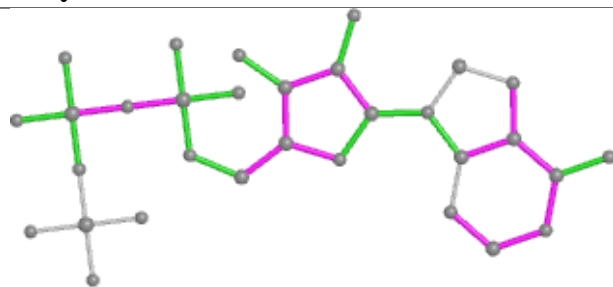




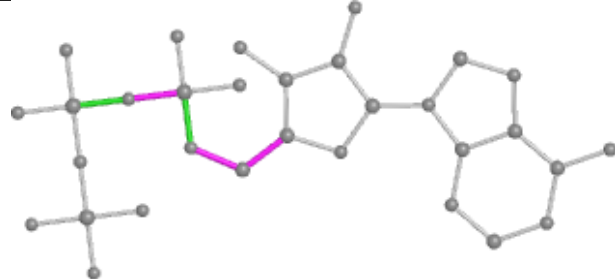
## Ligand 08T Q 400



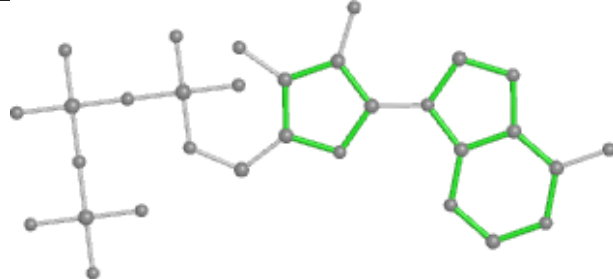
Bond lengths



Bond angles

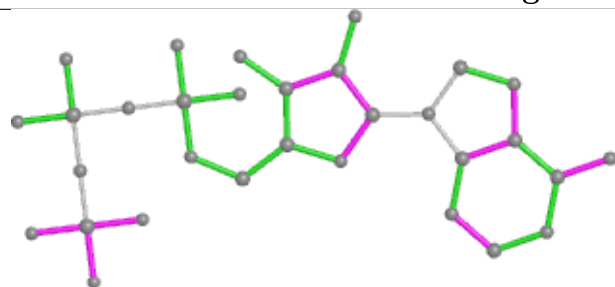


Torsions

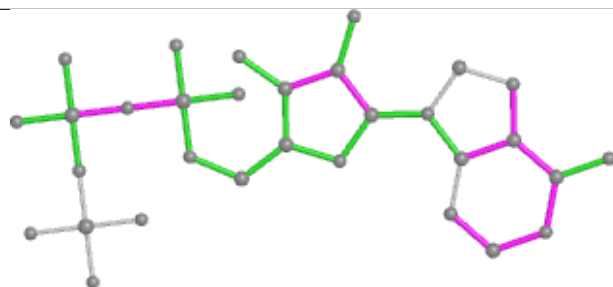


Rings

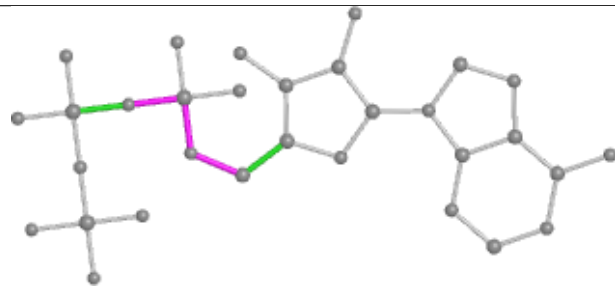
## Ligand 08T V 400



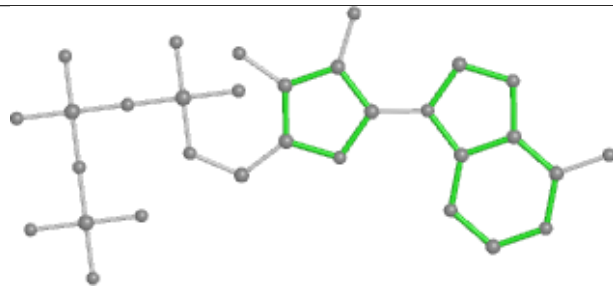
Bond lengths



Bond angles

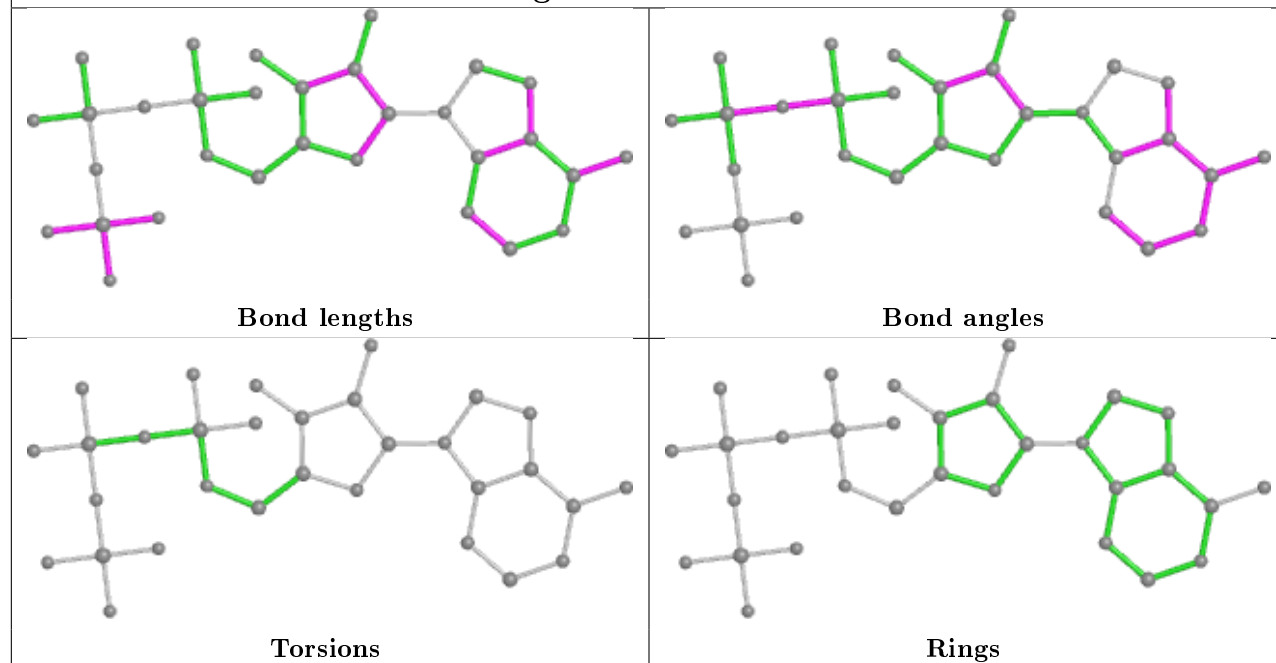


Torsions

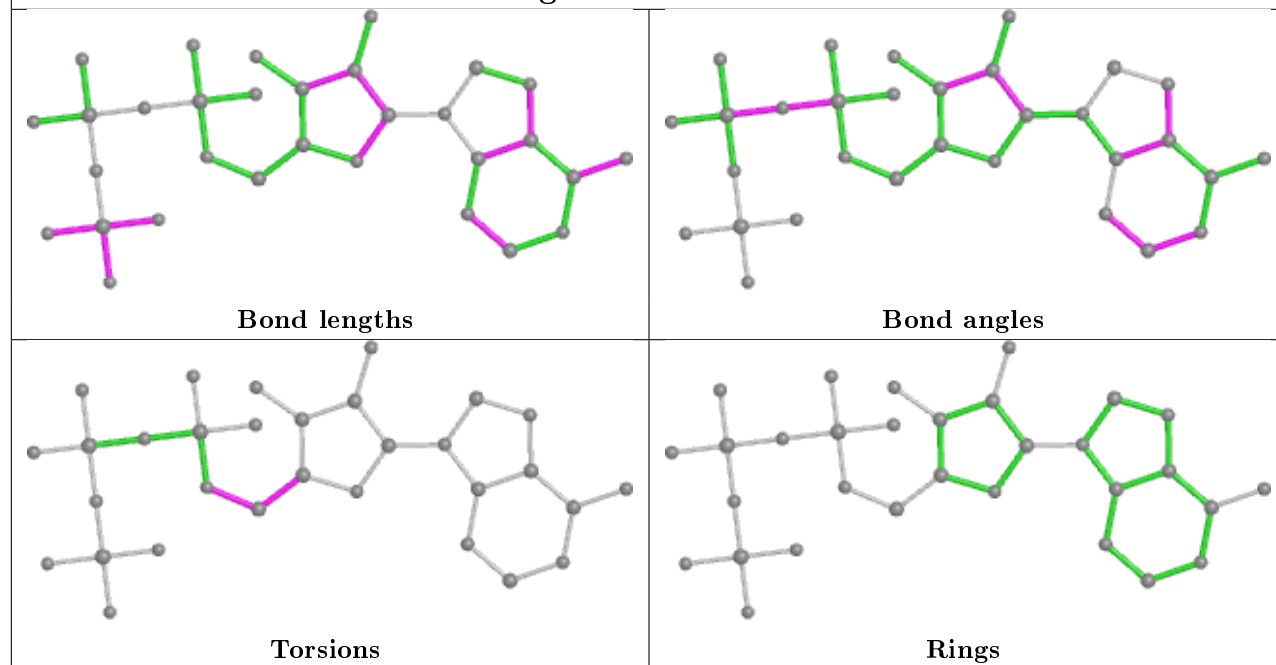


Rings

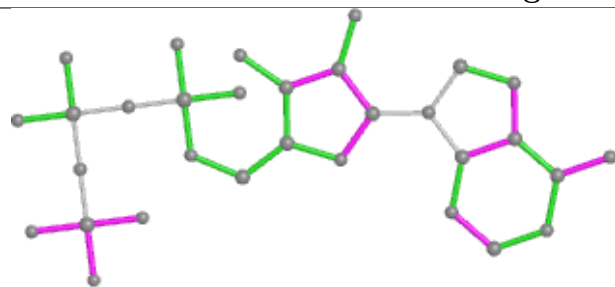
## Ligand 08T W 400



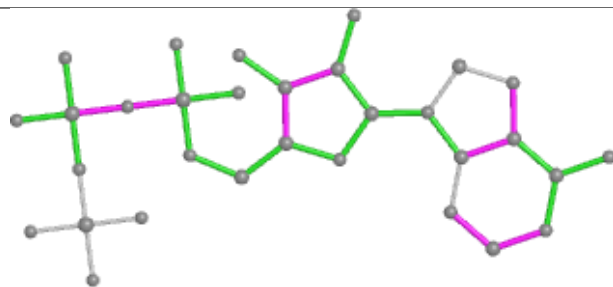
## Ligand 08T B 400



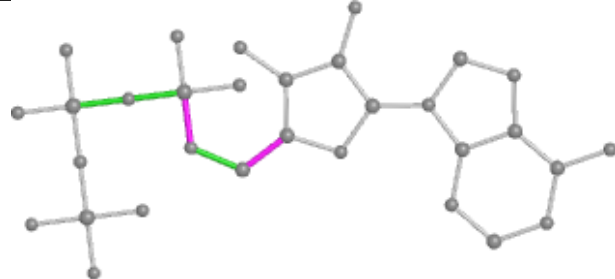
## Ligand 08T C 400



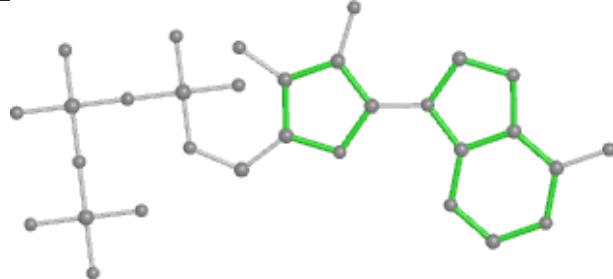
Bond lengths



Bond angles

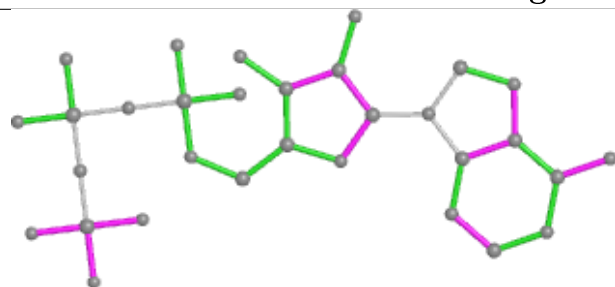


Torsions

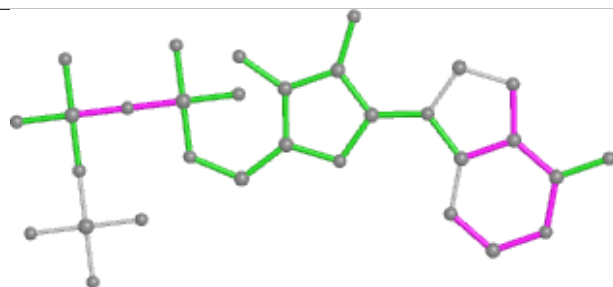


Rings

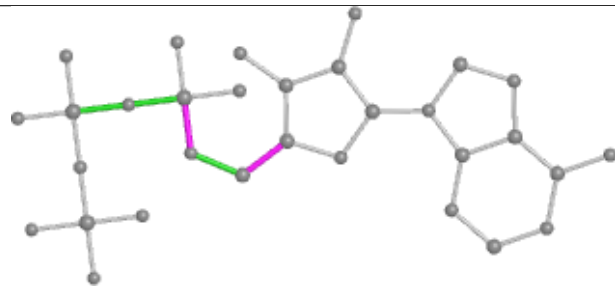
## Ligand 08T I 400



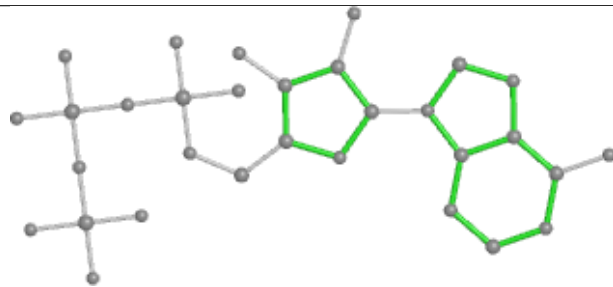
Bond lengths



Bond angles

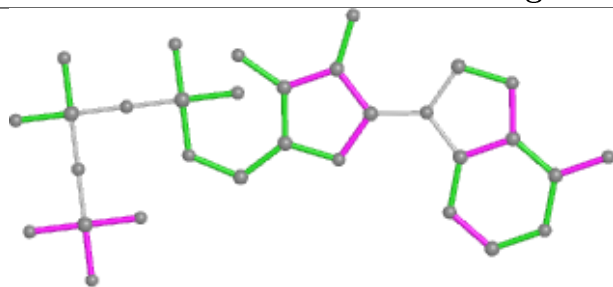


Torsions

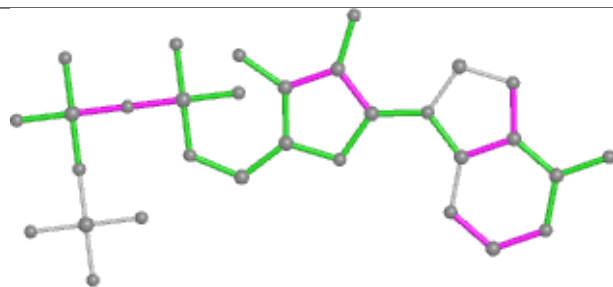


Rings

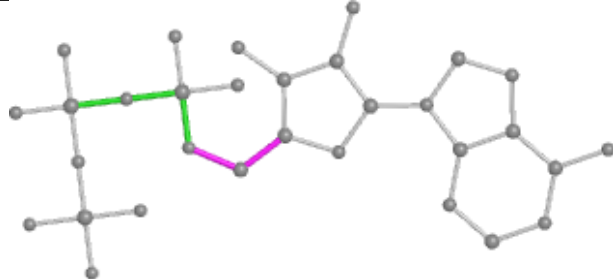
## Ligand 08T J 400



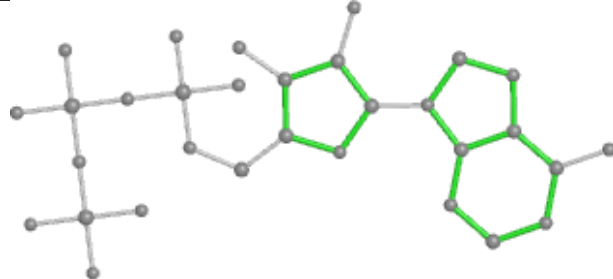
Bond lengths



Bond angles

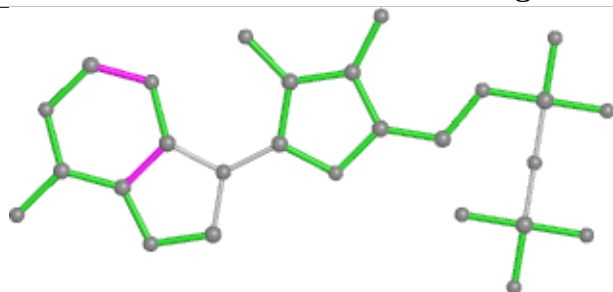


Torsions

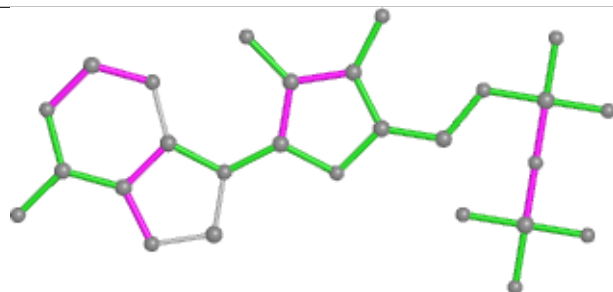


Rings

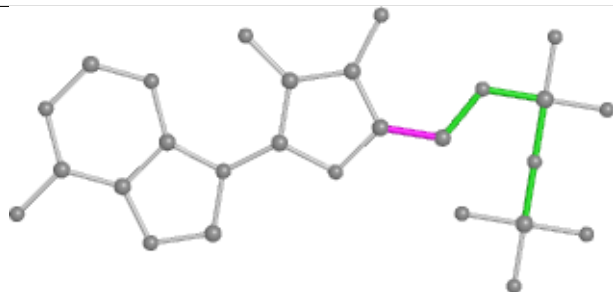
## Ligand ADP L 400



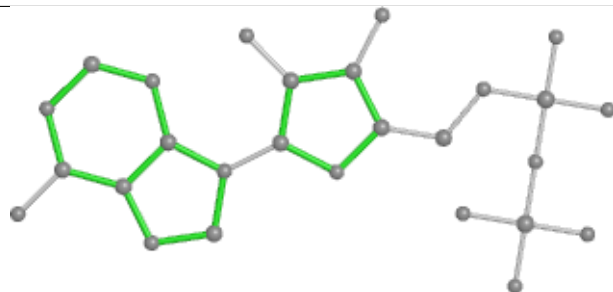
Bond lengths



Bond angles

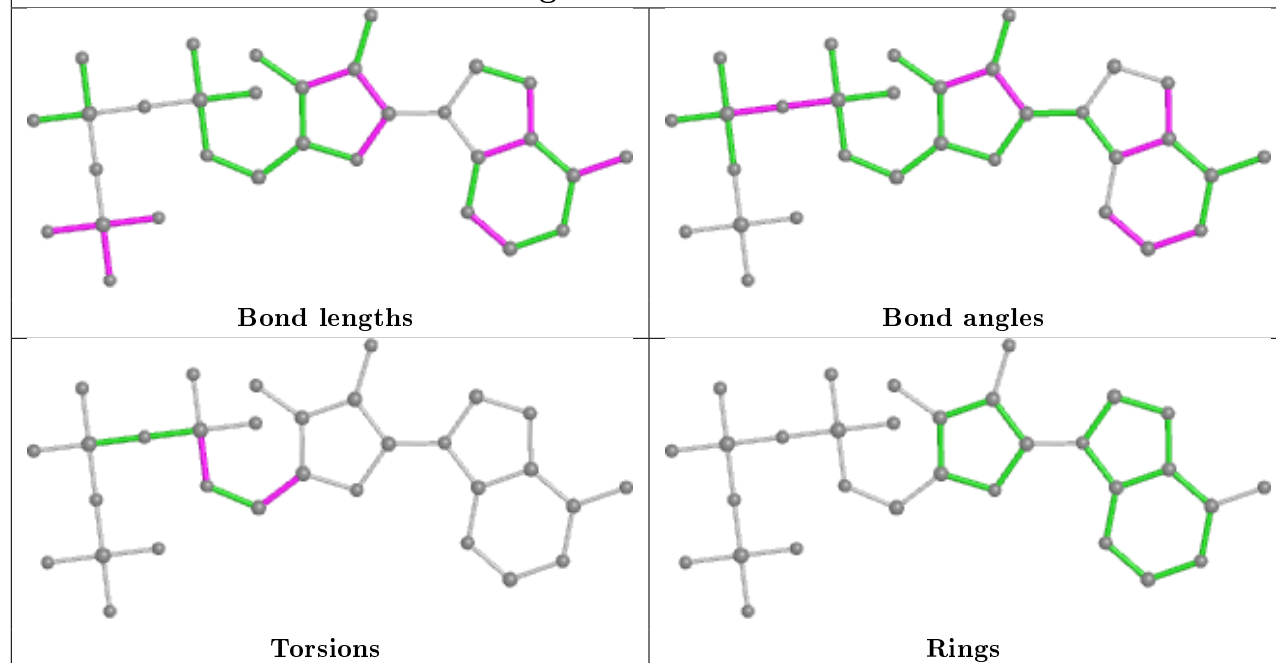


Torsions

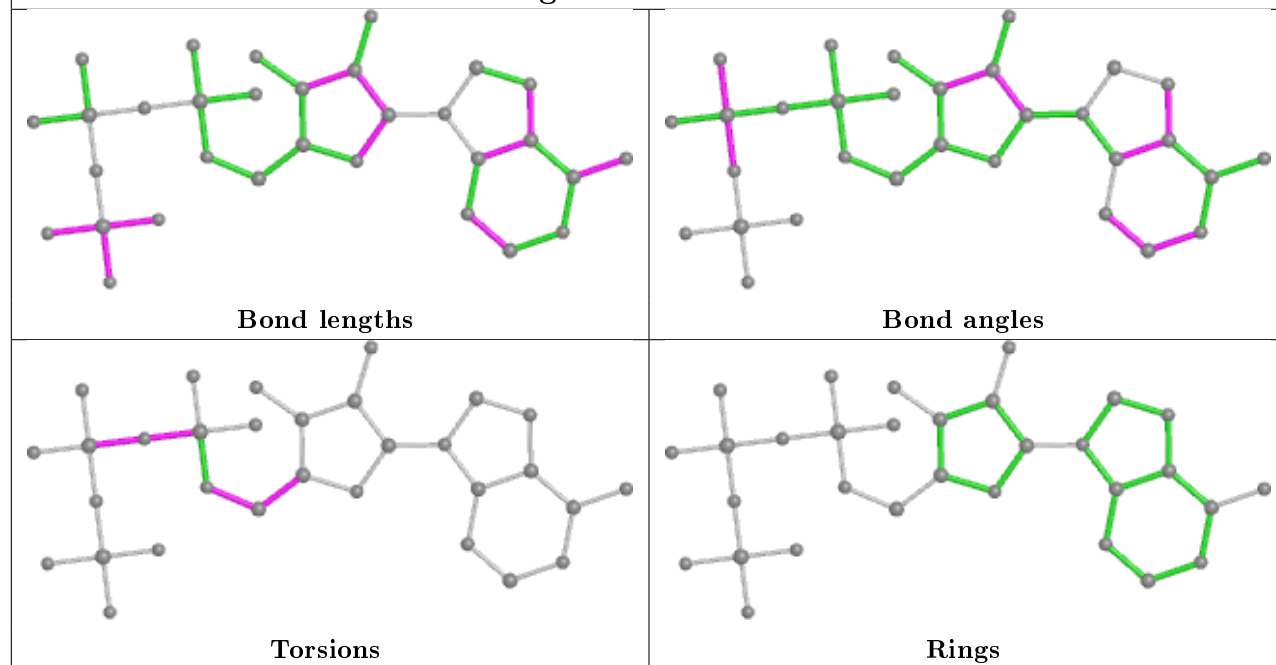


Rings

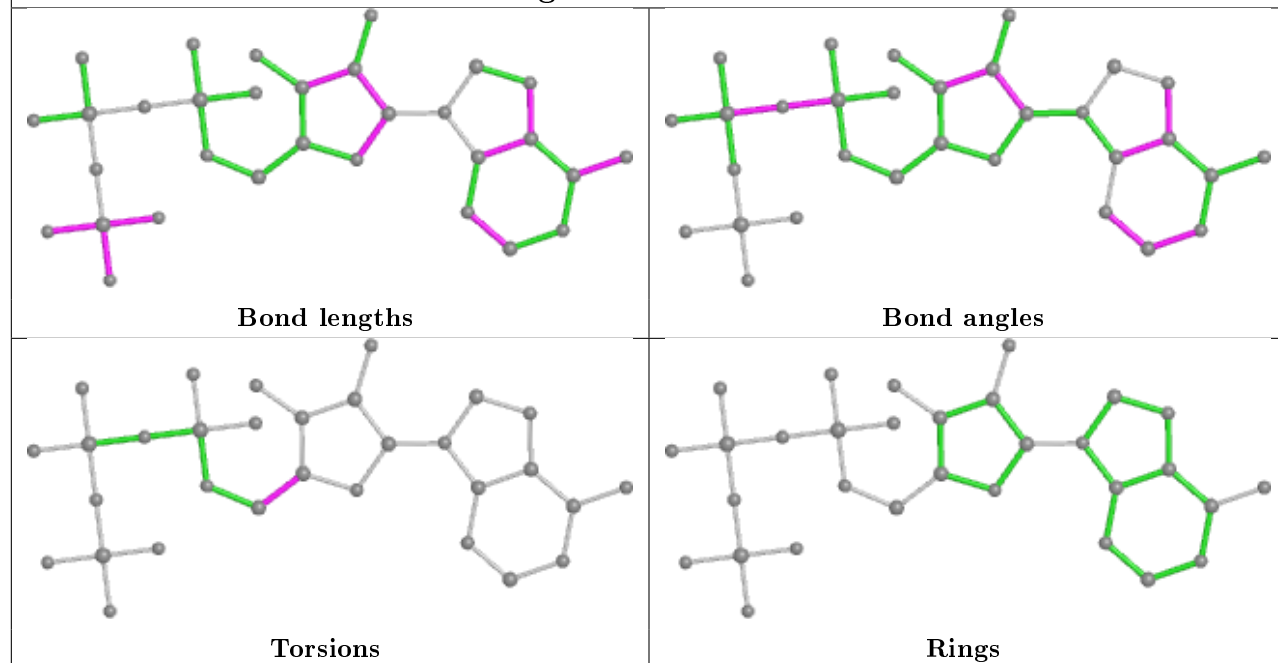
## Ligand 08T R 400



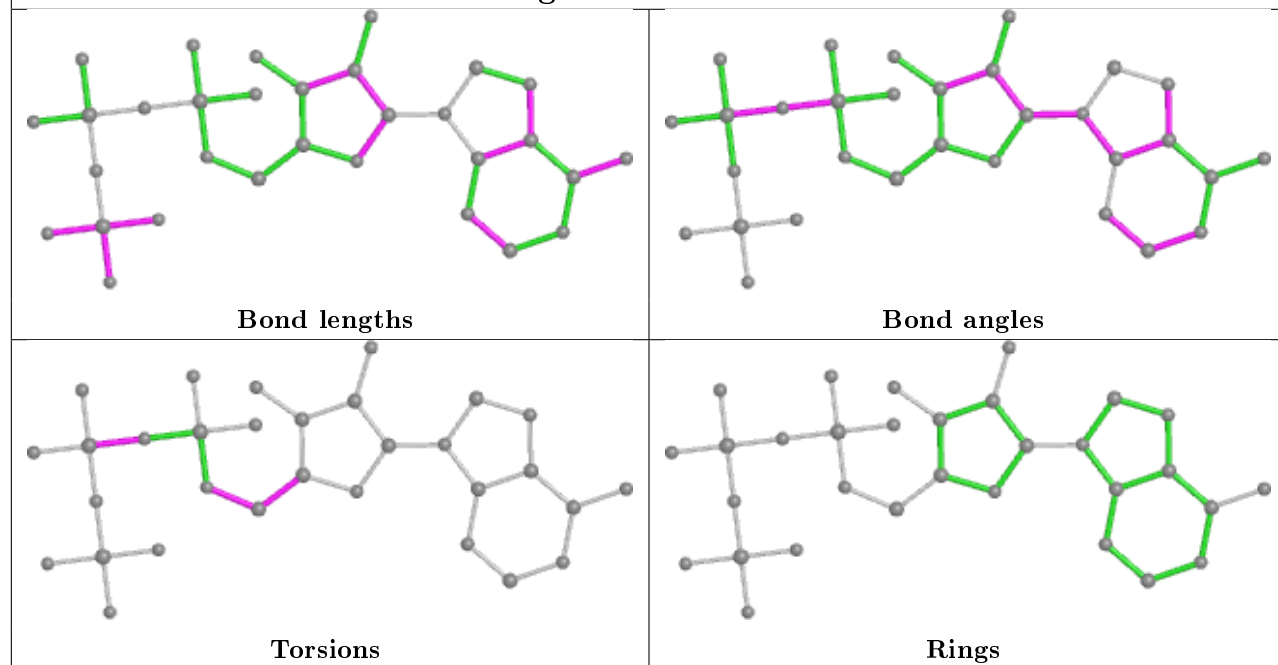
## Ligand 08T T 400



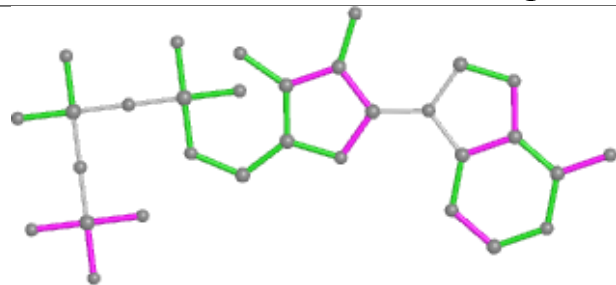
## Ligand 08T A 400



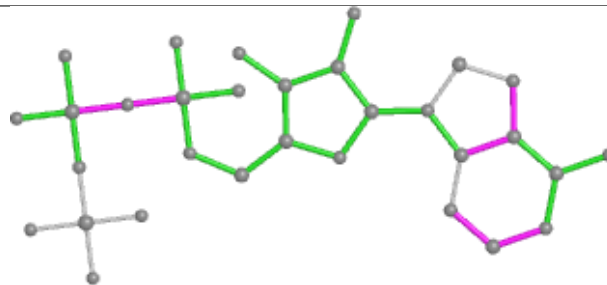
## Ligand 08T K 400



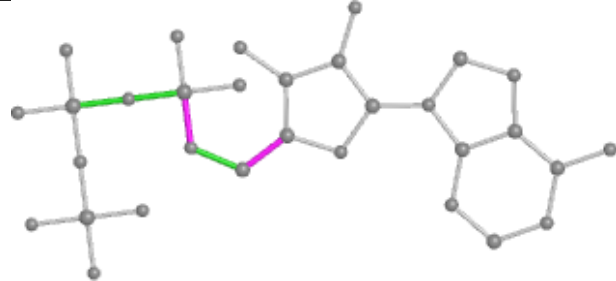
## Ligand 08T U 400



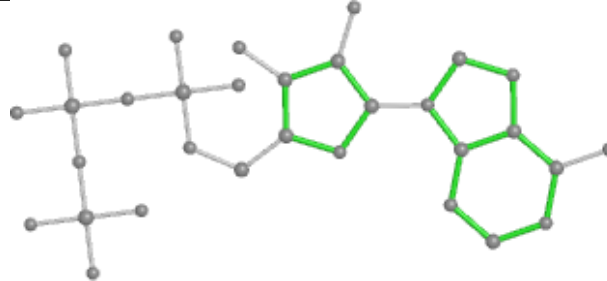
Bond lengths



Bond angles

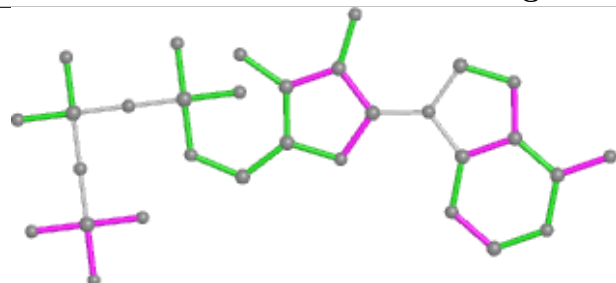


Torsions

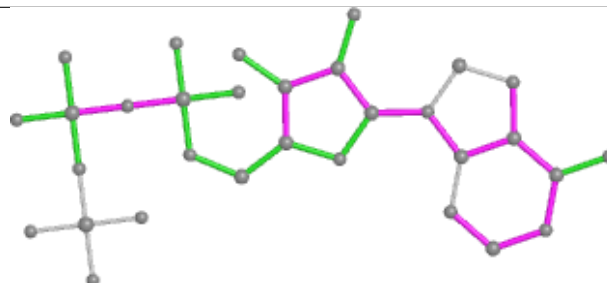


Rings

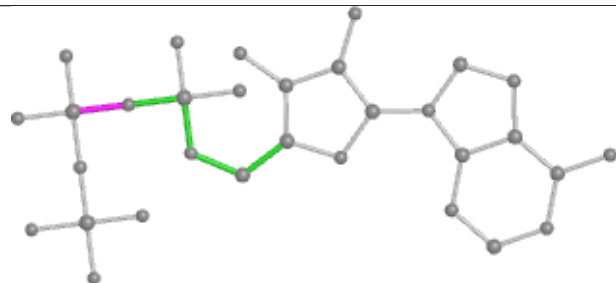
## Ligand 08T X 400



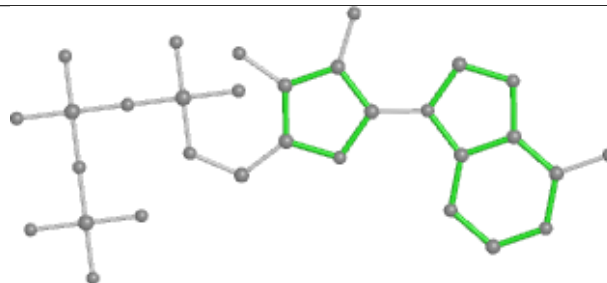
Bond lengths



Bond angles

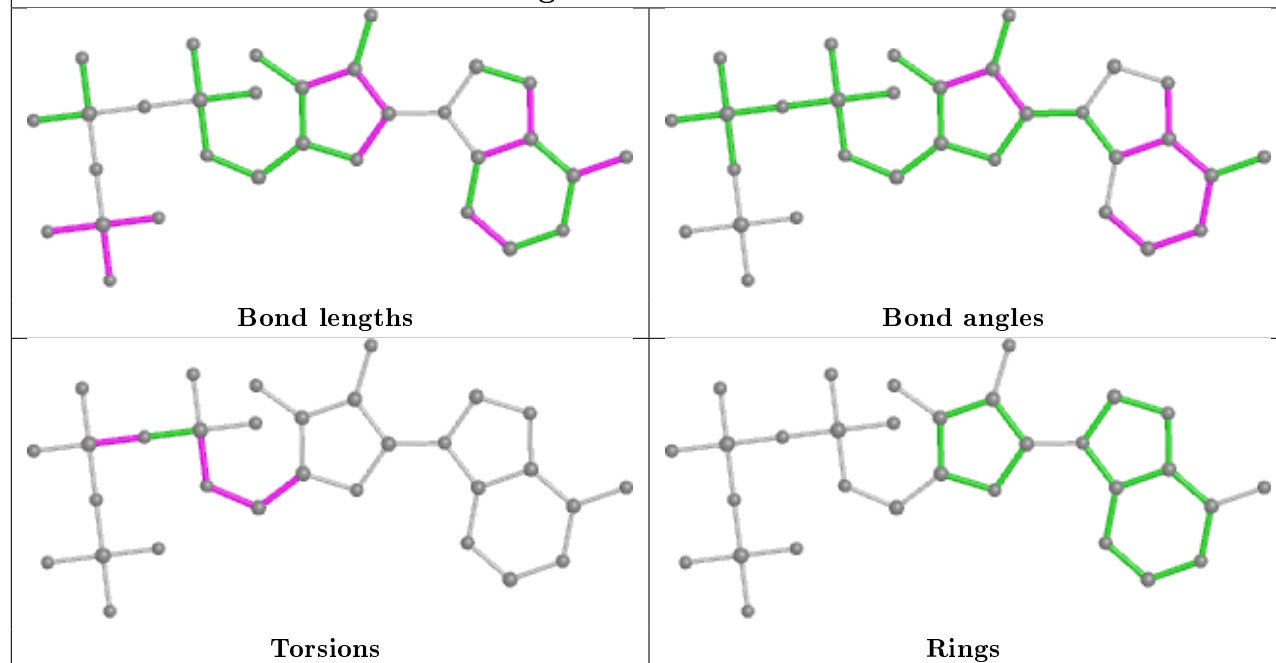


Torsions

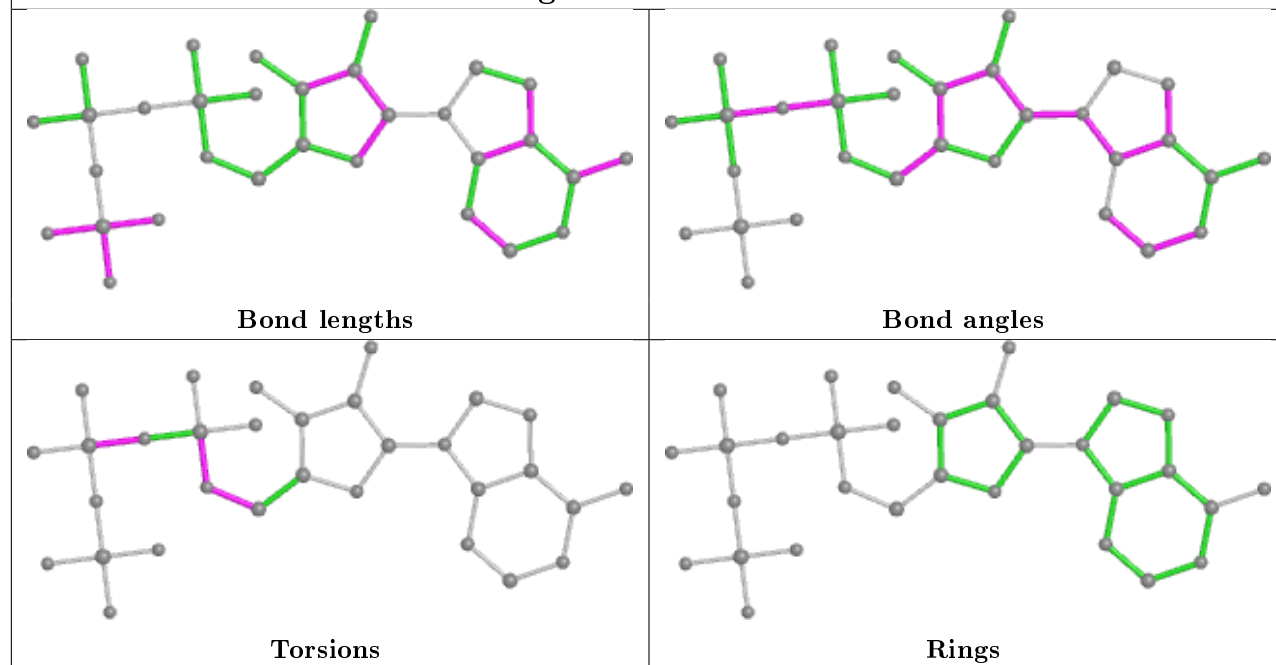


Rings

## Ligand 08T D 400

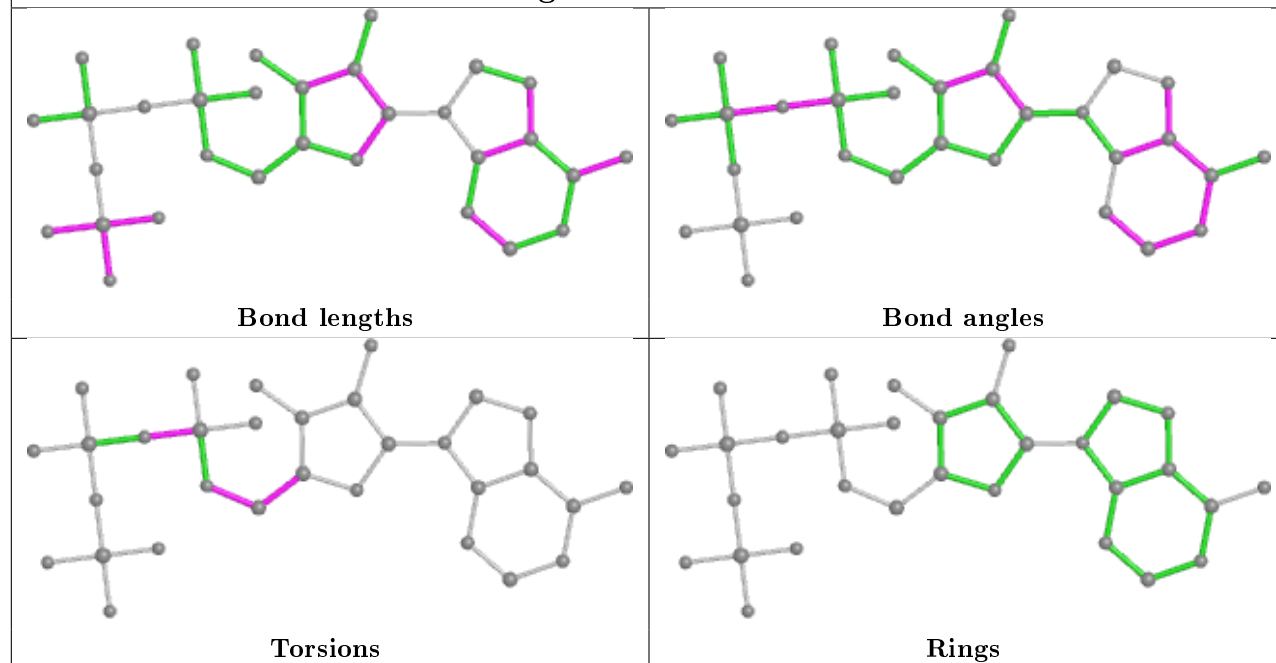


## Ligand 08T N 400

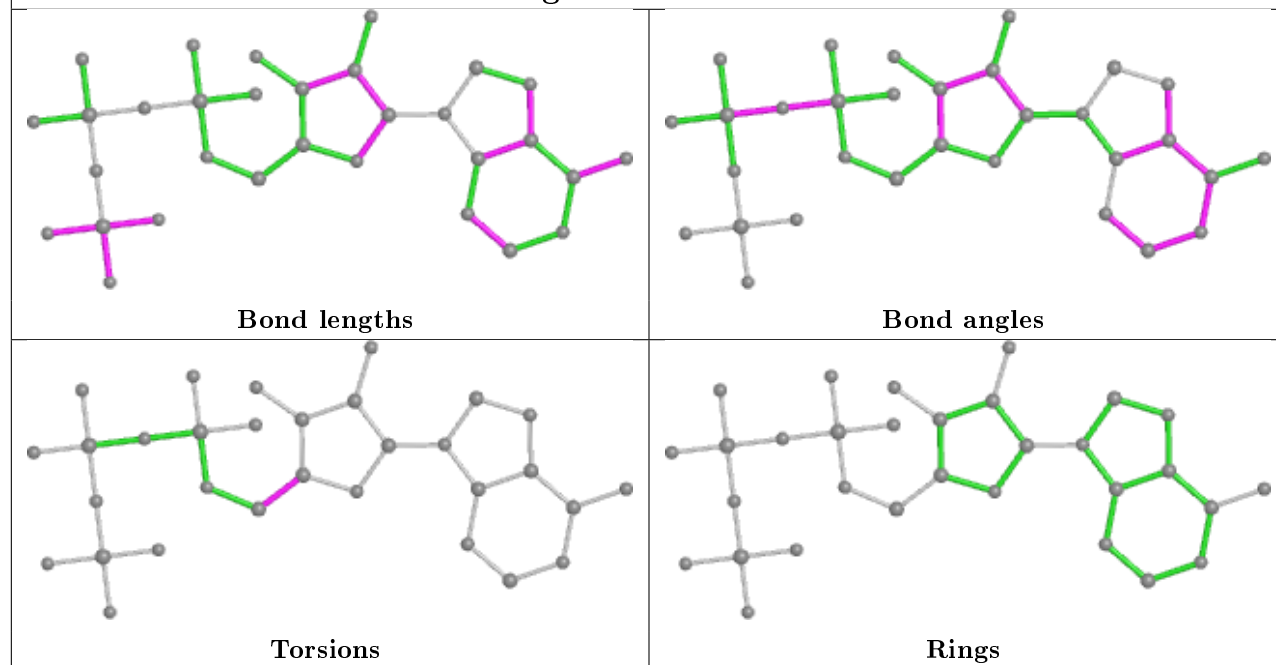


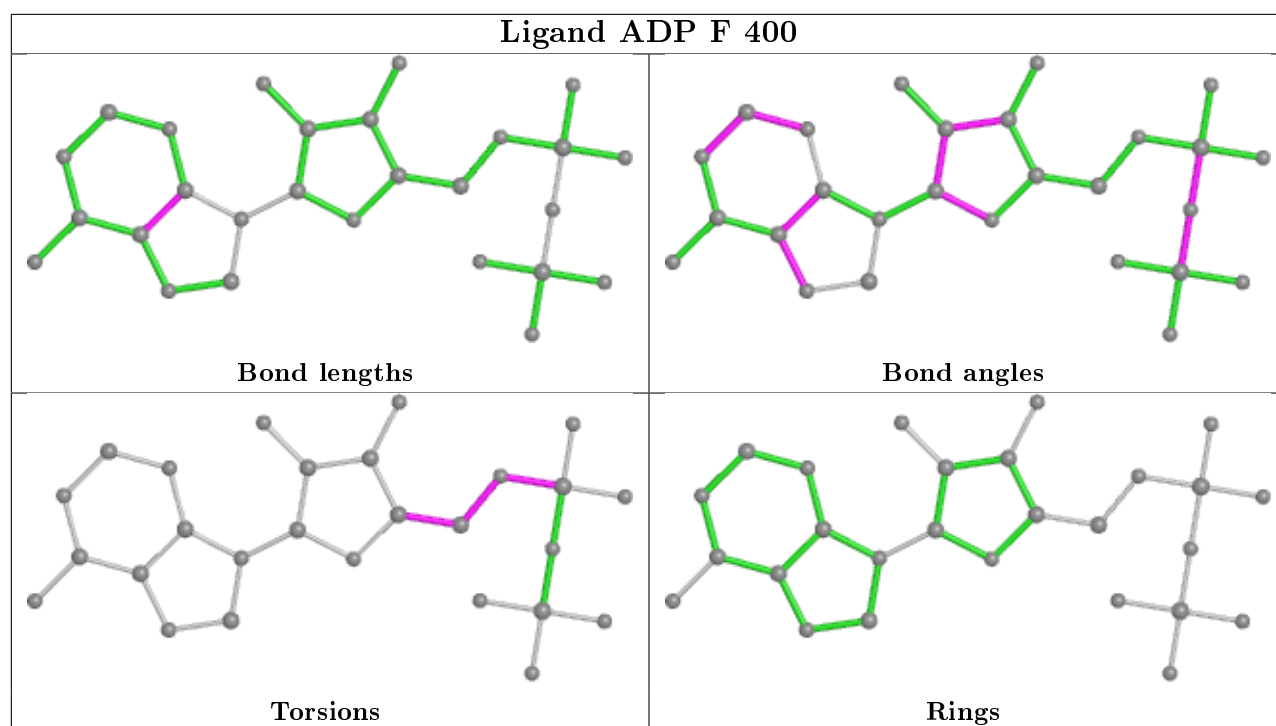


## Ligand 08T O 400



## Ligand 08T S 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	247/268 (92%)	0.29	10 (4%) 38 26	84, 119, 143, 157	0
1	B	247/268 (92%)	0.19	4 (1%) 72 60	44, 88, 117, 132	0
1	C	247/268 (92%)	0.09	1 (0%) 92 89	38, 73, 116, 139	0
1	D	247/268 (92%)	0.08	0 100 100	32, 61, 90, 113	0
1	E	258/268 (96%)	0.15	0 100 100	33, 64, 92, 132	8 (3%)
1	F	247/268 (92%)	0.19	7 (2%) 53 39	41, 83, 142, 177	0
1	G	247/268 (92%)	0.71	34 (13%) 2 2	95, 136, 162, 175	0
1	H	247/268 (92%)	0.15	2 (0%) 86 79	51, 88, 115, 136	0
1	I	248/268 (92%)	0.13	1 (0%) 92 89	33, 76, 110, 127	0
1	J	247/268 (92%)	0.12	0 100 100	42, 70, 96, 105	0
1	K	247/268 (92%)	0.10	0 100 100	38, 64, 91, 122	0
1	L	246/268 (91%)	0.42	18 (7%) 15 9	41, 87, 165, 193	0
1	M	247/268 (92%)	0.76	32 (12%) 3 2	101, 134, 159, 181	0
1	N	247/268 (92%)	0.16	1 (0%) 92 89	49, 88, 121, 137	0
1	O	247/268 (92%)	0.12	1 (0%) 92 89	35, 72, 113, 134	0
1	P	247/268 (92%)	0.11	1 (0%) 92 89	40, 69, 98, 121	0
1	Q	247/268 (92%)	0.10	0 100 100	41, 68, 92, 117	0
1	R	247/268 (92%)	0.34	13 (5%) 26 15	48, 91, 164, 182	0
1	S	247/268 (92%)	0.20	6 (2%) 59 45	86, 115, 140, 153	0
1	T	247/268 (92%)	0.16	3 (1%) 79 68	45, 90, 123, 143	0
1	U	247/268 (92%)	0.16	0 100 100	39, 77, 116, 135	0
1	V	247/268 (92%)	0.10	0 100 100	36, 62, 95, 121	0
1	W	250/268 (93%)	0.15	0 100 100	33, 63, 95, 116	1 (0%)
1	X	246/268 (91%)	0.23	8 (3%) 46 32	40, 85, 146, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5941/6432 (92%)	0.22	142 (2%)	59	45	32, 81, 142, 193	9 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	372	GLY	10.7
1	M	221	SER	10.4
1	X	348	LEU	7.7
1	G	216	PHE	6.9
1	G	149	ILE	6.5
1	L	347	LEU	6.2
1	M	220	VAL	6.1
1	L	349	SER	6.0
1	L	332	TYR	5.6
1	M	149	ILE	5.2
1	M	371	GLU	4.9
1	F	348	LEU	4.8
1	R	347	LEU	4.8
1	A	339	PHE	4.6
1	L	333	ALA	4.6
1	M	369	PHE	4.5
1	R	333	ALA	4.5
1	X	384	VAL	4.5
1	G	363	ILE	4.3
1	R	351	PRO	4.1
1	M	219	ALA	4.1
1	G	164	LEU	3.9
1	G	369	PHE	3.8
1	A	288	LYS	3.8
1	T	216	PHE	3.8
1	M	255	ILE	3.7
1	R	324	PHE	3.7
1	L	324	PHE	3.7
1	G	277	ALA	3.6
1	F	347	LEU	3.6
1	S	350	TYR	3.6
1	B	139	TYR	3.5
1	L	348	LEU	3.5
1	R	368	LEU	3.4
1	G	160	GLU	3.3
1	M	192	VAL	3.3
1	M	302	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	212	GLU	3.2
1	G	196	VAL	3.2
1	G	303	ILE	3.2
1	I	139	TYR	3.2
1	L	337	GLU	3.2
1	G	255	ILE	3.2
1	L	327	LYS	3.1
1	F	332	TYR	3.1
1	B	141	PHE	3.0
1	L	368	LEU	3.0
1	H	139	TYR	3.0
1	G	235	LEU	3.0
1	S	216	PHE	2.9
1	G	236	PHE	2.9
1	A	215	ALA	2.9
1	B	216	PHE	2.9
1	L	300	LEU	2.9
1	N	139	TYR	2.9
1	L	146	MET	2.9
1	A	216	PHE	2.9
1	G	197	ALA	2.9
1	F	329	SER	2.8
1	S	339	PHE	2.8
1	G	365	ARG	2.8
1	M	164	LEU	2.8
1	M	347	LEU	2.8
1	L	328	PHE	2.7
1	L	350	TYR	2.7
1	M	367	VAL	2.7
1	G	347	LEU	2.7
1	M	238	ASP	2.7
1	A	277	ALA	2.7
1	M	264	GLY	2.7
1	R	382	CYS	2.7
1	G	212	GLU	2.7
1	A	292	PHE	2.7
1	G	213	LYS	2.7
1	M	139	TYR	2.6
1	R	350	TYR	2.6
1	T	139	TYR	2.6
1	F	331	LYS	2.6
1	G	367	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	249	ALA	2.6
1	L	384	VAL	2.6
1	G	178	ARG	2.5
1	G	252	LEU	2.5
1	M	293	ARG	2.5
1	G	194	LEU	2.5
1	L	346	LEU	2.5
1	M	382	CYS	2.5
1	X	350	TYR	2.5
1	G	161	CYS	2.5
1	R	383	LEU	2.4
1	X	329	SER	2.4
1	G	264	GLY	2.4
1	A	382	CYS	2.4
1	F	234	THR	2.4
1	C	359	LEU	2.4
1	G	221	SER	2.4
1	G	339	PHE	2.4
1	R	332	TYR	2.4
1	G	368	LEU	2.4
1	M	236	PHE	2.4
1	H	216	PHE	2.3
1	G	304	GLU	2.3
1	M	158	CYS	2.3
1	M	310	LEU	2.3
1	G	185	ASP	2.3
1	P	219	ALA	2.3
1	M	368	LEU	2.3
1	S	332	TYR	2.3
1	X	320	LEU	2.3
1	M	256	GLU	2.3
1	L	275	ILE	2.3
1	R	337	GLU	2.3
1	A	212	GLU	2.3
1	M	176	VAL	2.3
1	R	349	SER	2.2
1	M	375	ILE	2.2
1	S	302	VAL	2.2
1	G	192	VAL	2.2
1	G	237	LEU	2.2
1	M	292	PHE	2.2
1	M	337	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	350	TYR	2.2
1	A	240	ILE	2.2
1	X	275	ILE	2.2
1	X	282	ASN	2.1
1	M	235	LEU	2.1
1	L	361	ASN	2.1
1	X	341	LYS	2.1
1	R	327	LYS	2.1
1	M	193	ALA	2.1
1	M	308	PRO	2.1
1	A	246	GLU	2.1
1	M	153	ILE	2.1
1	G	215	ALA	2.1
1	G	372	GLY	2.0
1	L	320	LEU	2.0
1	B	322	ASN	2.0
1	S	237	LEU	2.0
1	O	380	LEU	2.0
1	G	300	LEU	2.0
1	T	337	GLU	2.0
1	R	348	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ADP	F	400	27/27	0.83	0.30	71,91,118,119	38
2	08T	G	400	31/31	0.86	0.38	93,105,129,132	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	Q	401	1/1	0.86	0.20	57,57,57,57	1
3	MG	F	401	1/1	0.87	0.16	79,79,79,79	1
3	MG	B	401	1/1	0.89	0.20	62,62,62,62	1
3	MG	G	401	1/1	0.90	0.26	98,98,98,98	1
3	MG	U	401	1/1	0.91	0.24	70,70,70,70	1
2	08T	N	400	31/31	0.91	0.28	51,76,92,99	42
2	08T	X	400	31/31	0.91	0.21	74,98,116,126	0
3	MG	O	401	1/1	0.92	0.16	71,71,71,71	1
3	MG	R	401	1/1	0.92	0.16	100,100,100,100	1
2	08T	T	400	31/31	0.92	0.27	45,81,97,100	42
2	08T	O	400	31/31	0.92	0.30	46,61,78,82	42
2	08T	M	400	31/31	0.92	0.27	88,102,120,128	42
2	08T	S	400	31/31	0.93	0.26	72,95,115,119	42
2	08T	A	400	31/31	0.93	0.26	77,92,110,125	42
3	MG	J	401	1/1	0.93	0.14	57,57,57,57	0
2	08T	B	400	31/31	0.94	0.26	50,70,87,94	42
2	08T	R	400	31/31	0.94	0.20	93,110,133,149	0
2	08T	I	400	31/31	0.94	0.28	50,63,78,85	42
3	MG	I	401	1/1	0.94	0.21	61,61,61,61	1
4	ADP	L	400	27/27	0.94	0.22	76,95,114,139	0
2	08T	D	400	31/31	0.95	0.23	42,63,82,85	0
3	MG	P	401	1/1	0.95	0.19	56,56,56,56	1
2	08T	H	400	31/31	0.95	0.27	62,73,87,90	42
3	MG	L	401	1/1	0.95	0.20	63,63,63,63	0
2	08T	U	400	31/31	0.95	0.26	48,68,82,83	42
2	08T	C	400	31/31	0.95	0.27	39,63,75,88	42
3	MG	D	401	1/1	0.95	0.17	57,57,57,57	1
3	MG	C	401	1/1	0.95	0.17	51,51,51,51	1
2	08T	J	400	31/31	0.96	0.23	51,64,77,87	0
3	MG	H	401	1/1	0.96	0.18	51,51,51,51	0
2	08T	Q	400	31/31	0.96	0.24	36,65,79,83	0
2	08T	E	400	31/31	0.96	0.26	44,57,69,80	42
2	08T	W	400	31/31	0.97	0.24	40,55,70,74	42
2	08T	K	400	31/31	0.97	0.27	42,59,74,81	42
3	MG	S	401	1/1	0.97	0.15	64,64,64,64	0
3	MG	T	401	1/1	0.97	0.21	68,68,68,68	1
3	MG	N	401	1/1	0.98	0.26	62,62,62,62	1
3	MG	X	401	1/1	0.98	0.13	77,77,77,77	1
2	08T	V	400	31/31	0.98	0.22	34,56,71,75	0
3	MG	A	401	1/1	0.98	0.17	54,54,54,54	0
2	08T	P	400	31/31	0.98	0.23	47,59,75,81	0
3	MG	E	401	1/1	0.98	0.25	55,55,55,55	0

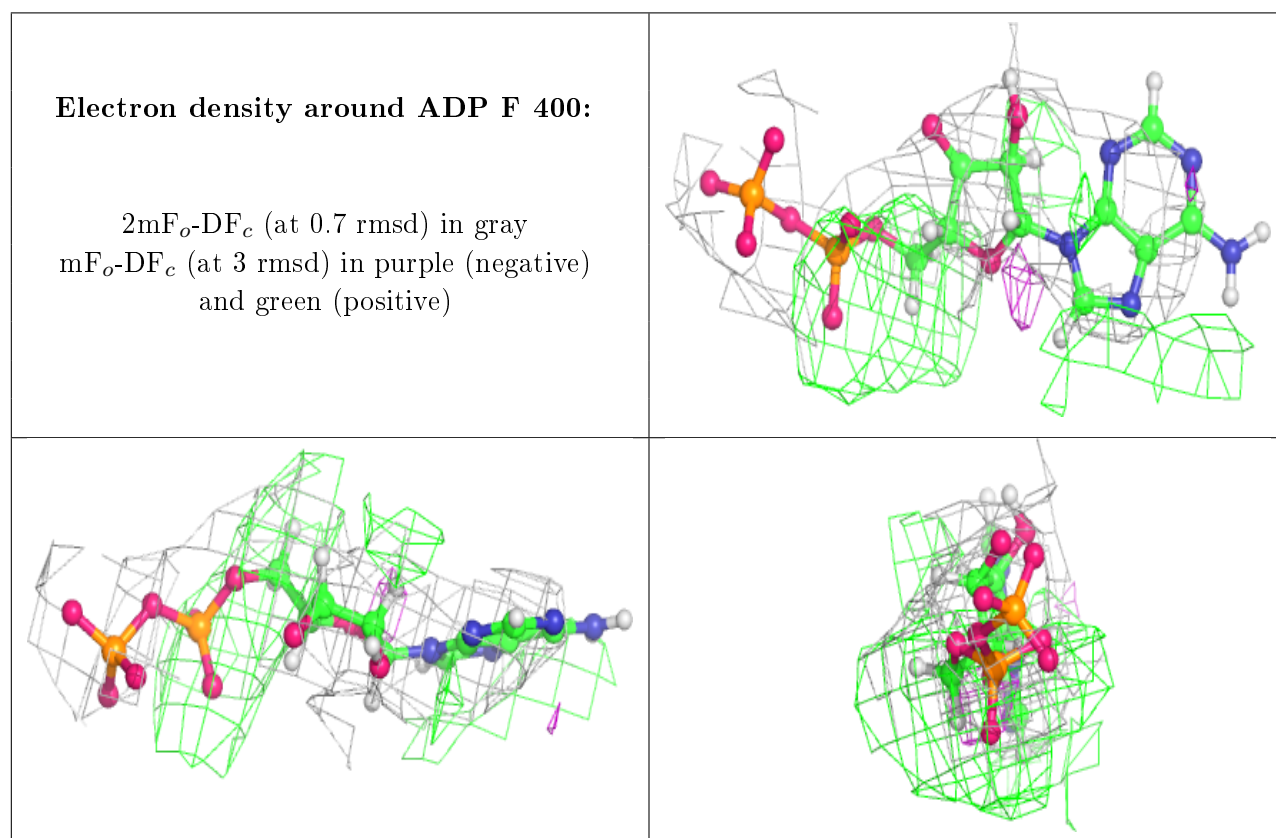
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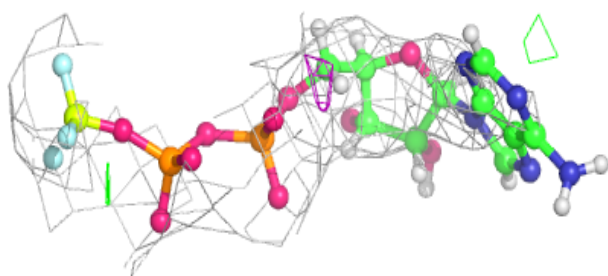
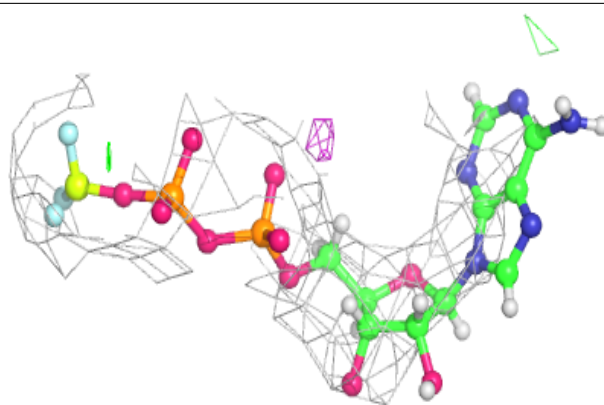
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	K	401	1/1	0.99	0.33	46,46,46,46	0
3	MG	V	401	1/1	0.99	0.16	53,53,53,53	1
3	MG	W	401	1/1	0.99	0.22	51,51,51,51	1

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.

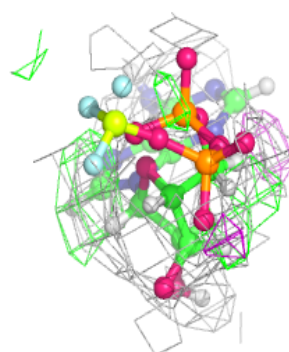
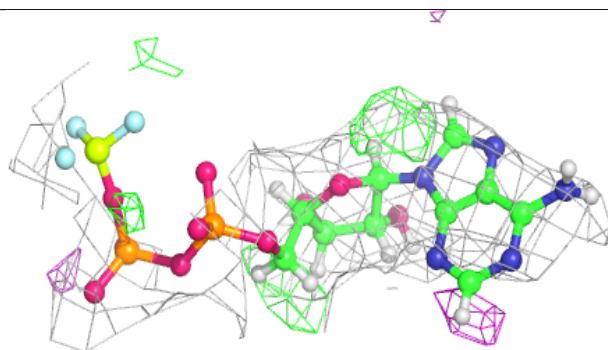
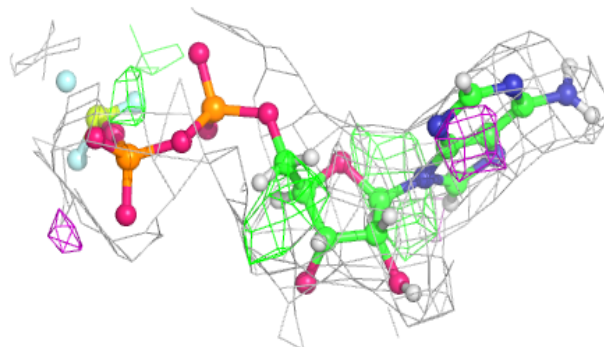


**Electron density around 08T G 400:**

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

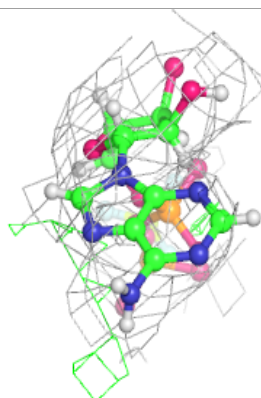
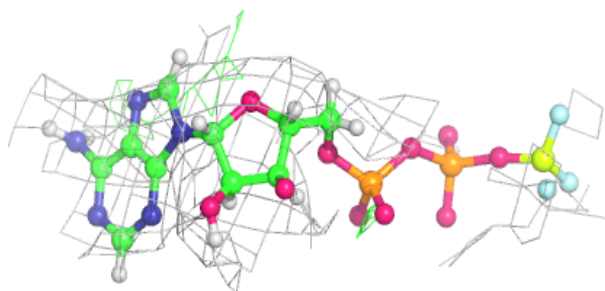
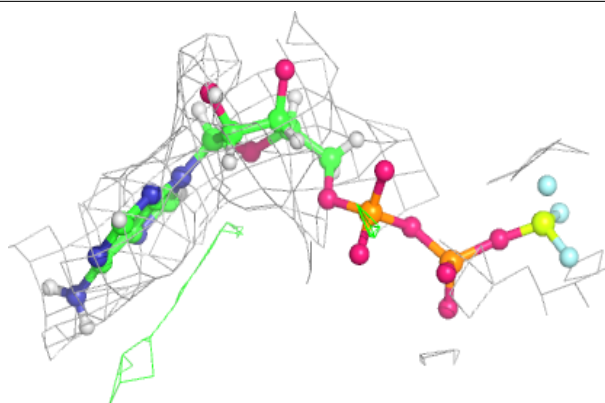
**Electron density around 08T N 400:**

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

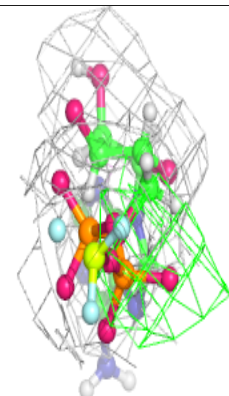
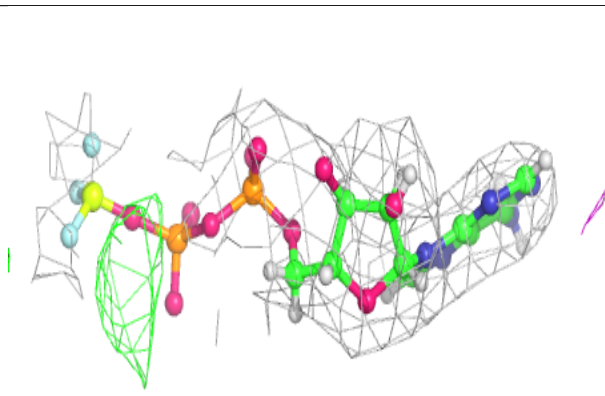
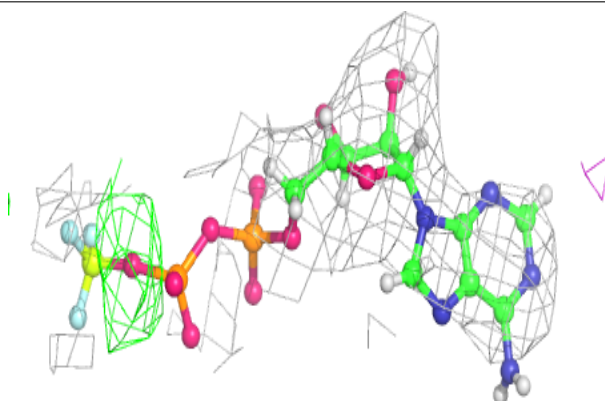


**Electron density around 08T X 400:**

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

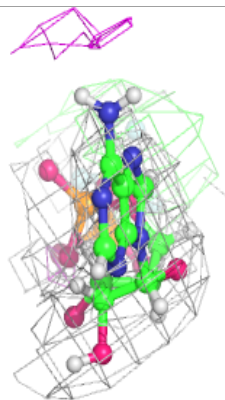
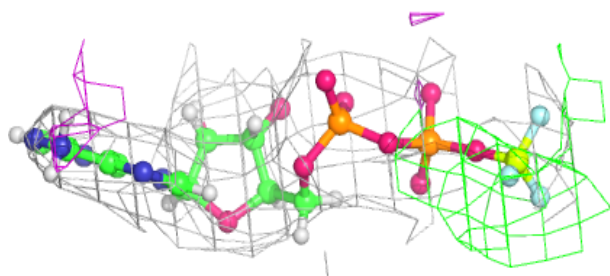
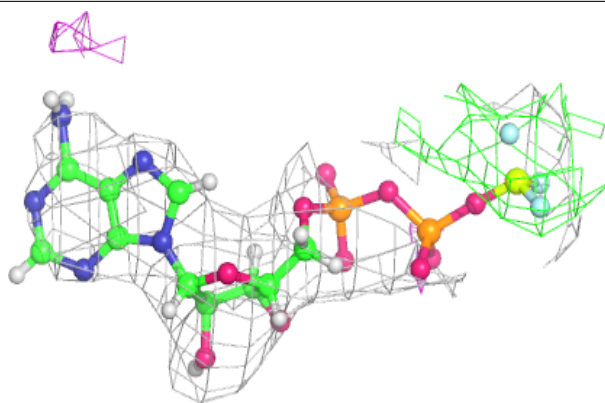
**Electron density around 08T T 400:**

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

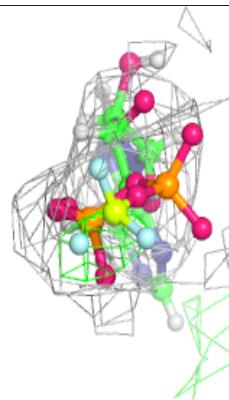
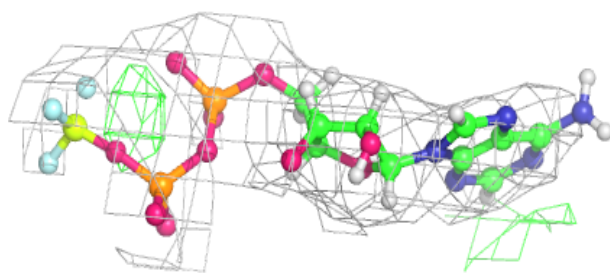
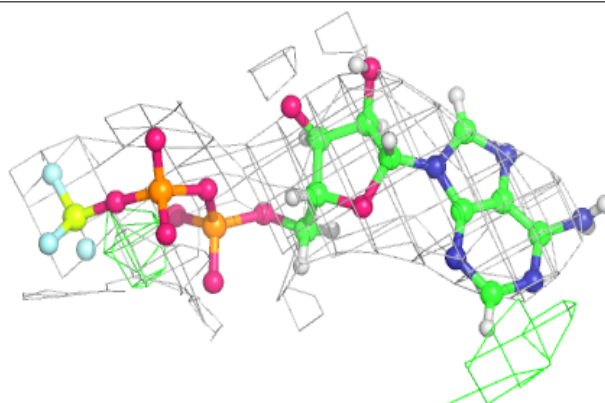


**Electron density around 08T O 400:**

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

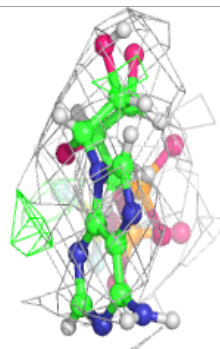
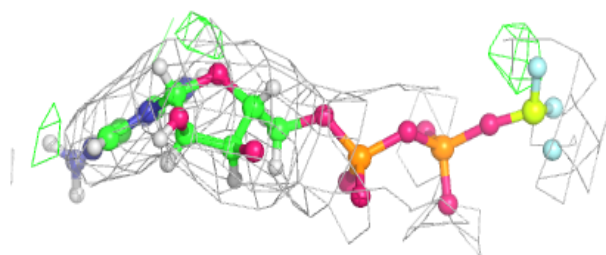
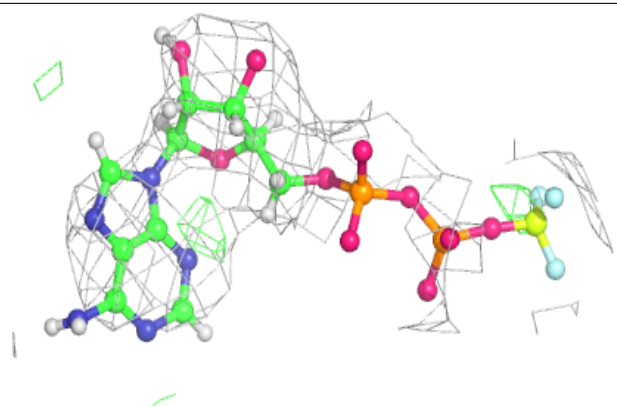
**Electron density around 08T M 400:**

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

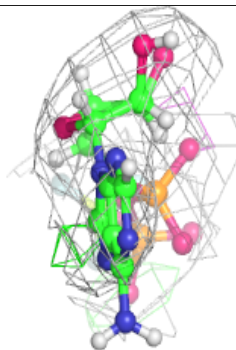
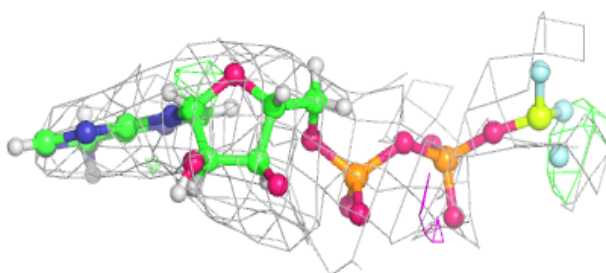
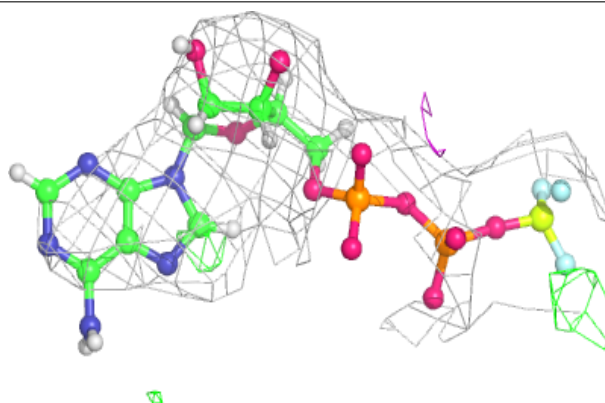


**Electron density around 08T S 400:**

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

**Electron density around 08T A 400:**

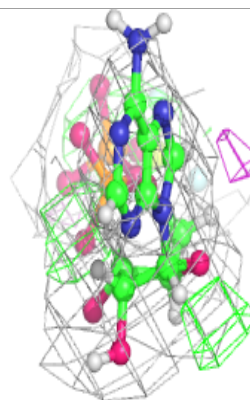
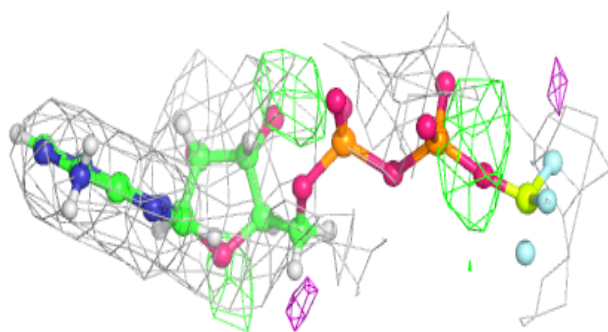
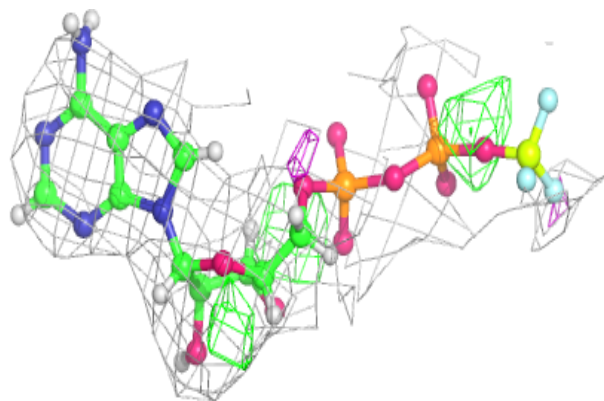
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



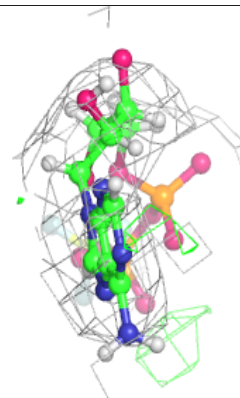
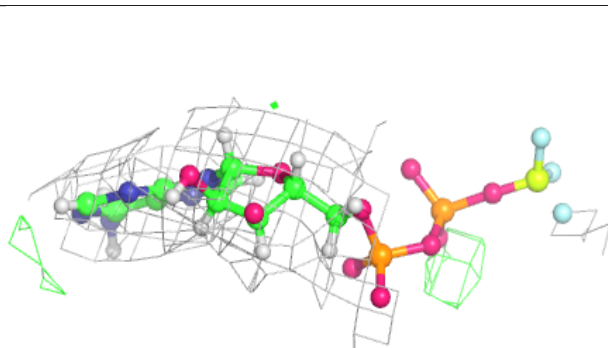
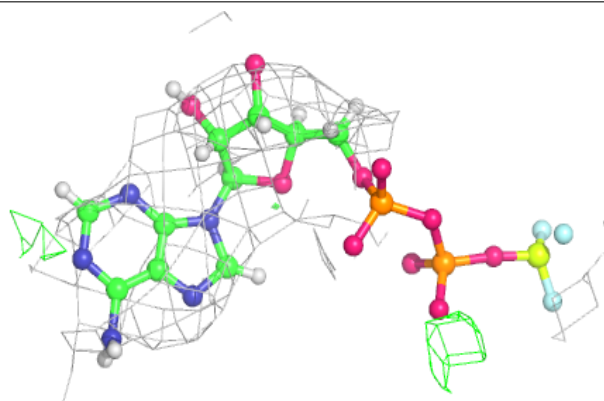


**Electron density around 08T B 400:**

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

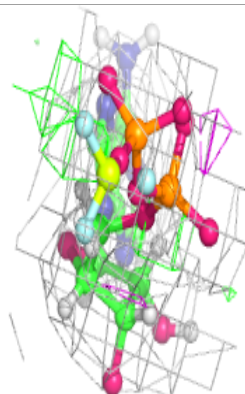
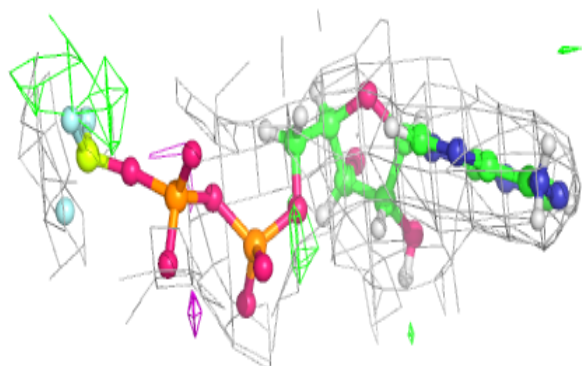
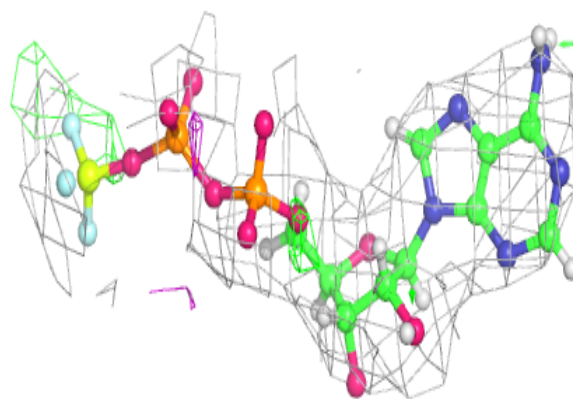
**Electron density around 08T R 400:**

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

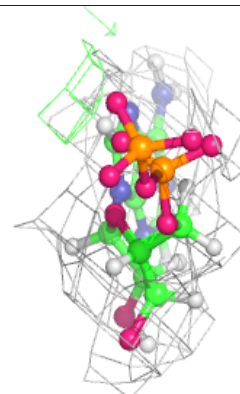
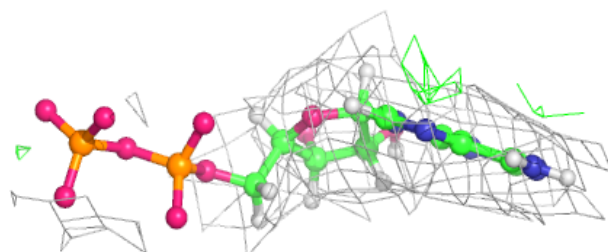
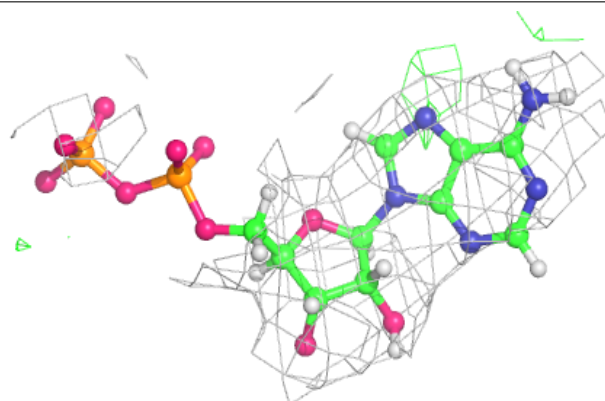


**Electron density around 08T I 400:**

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

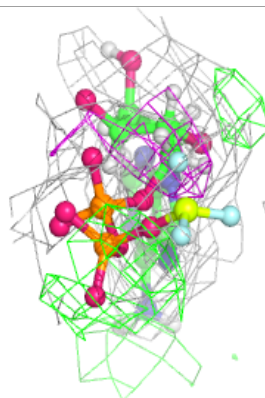
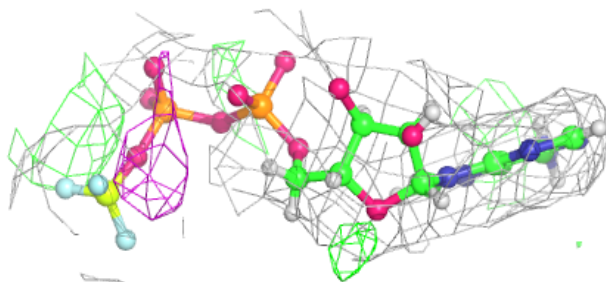
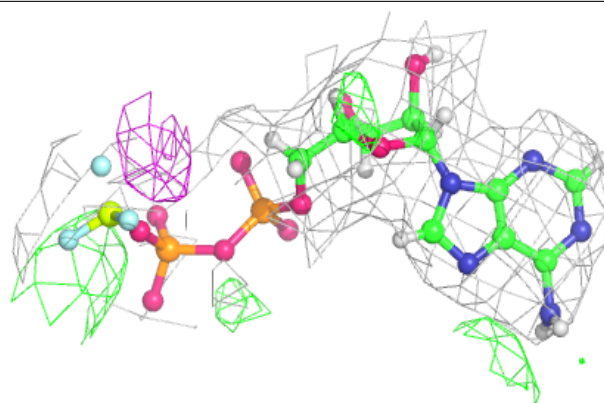
**Electron density around ADP L 400:**

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

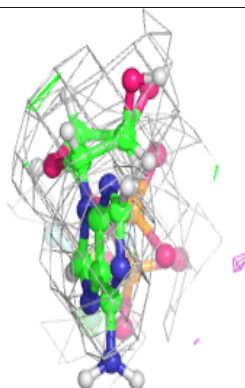
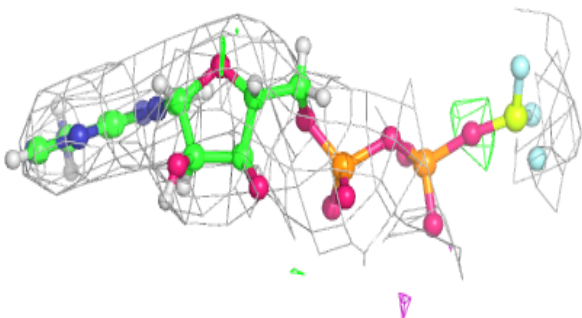
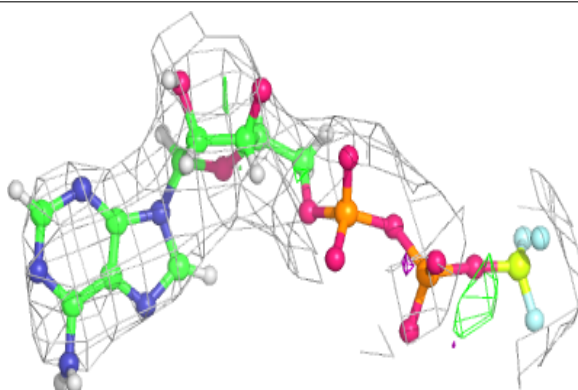


**Electron density around 08T D 400:**

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

**Electron density around 08T H 400:**

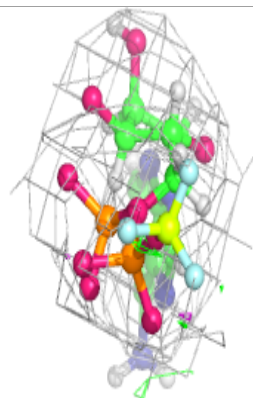
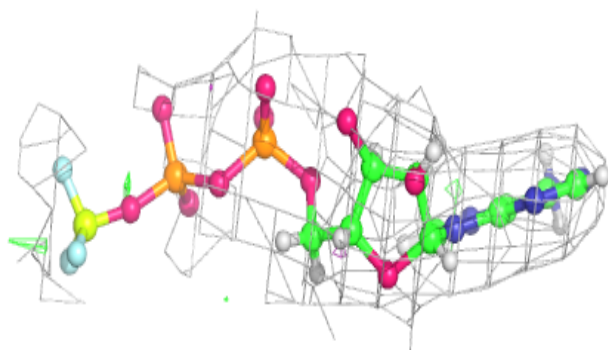
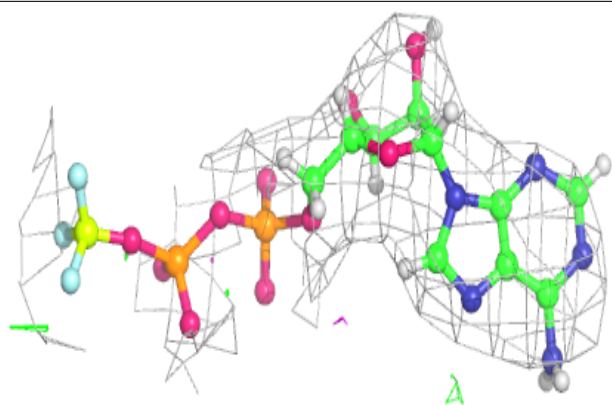
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



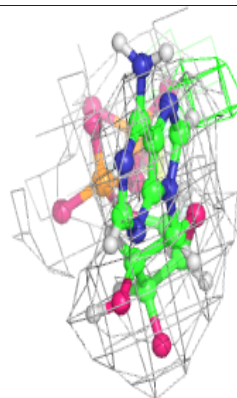
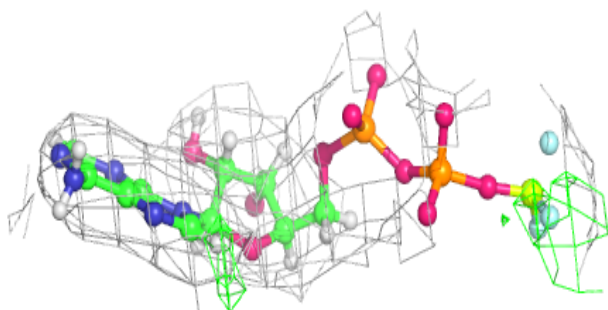
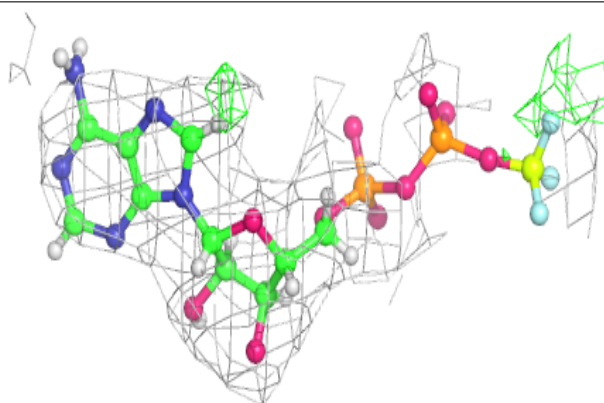


**Electron density around 08T U 400:**

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

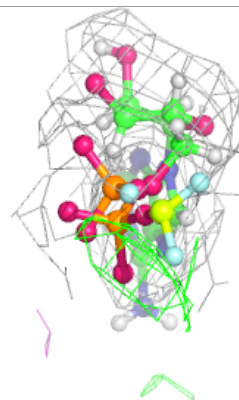
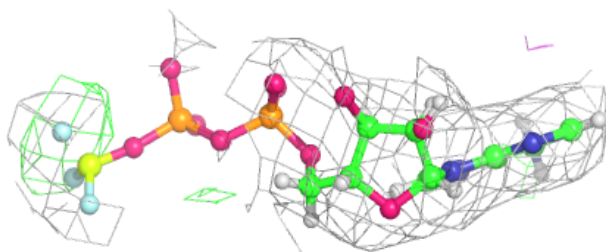
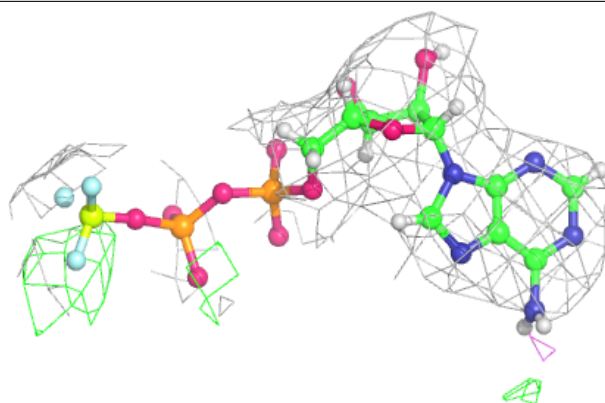
**Electron density around 08T C 400:**

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

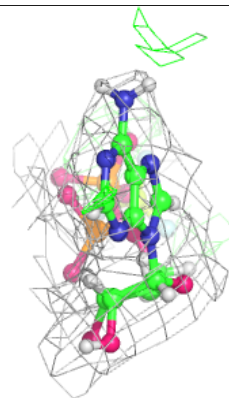
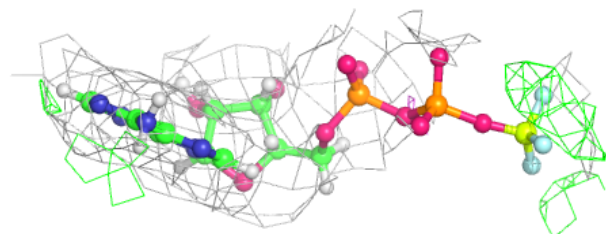
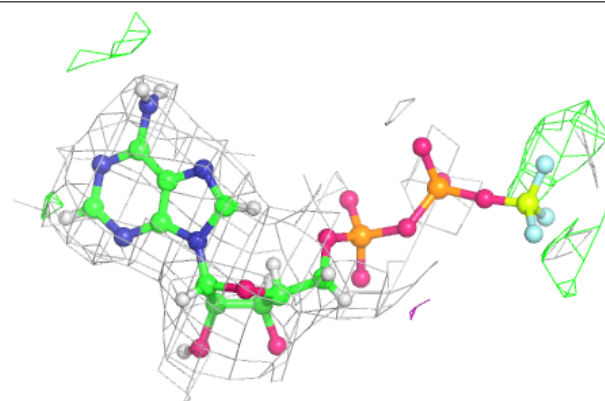


**Electron density around 08T J 400:**

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

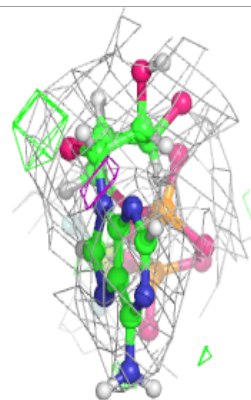
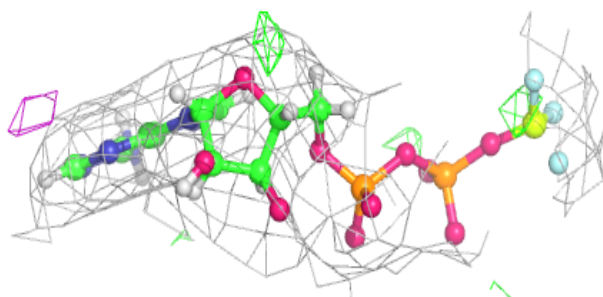
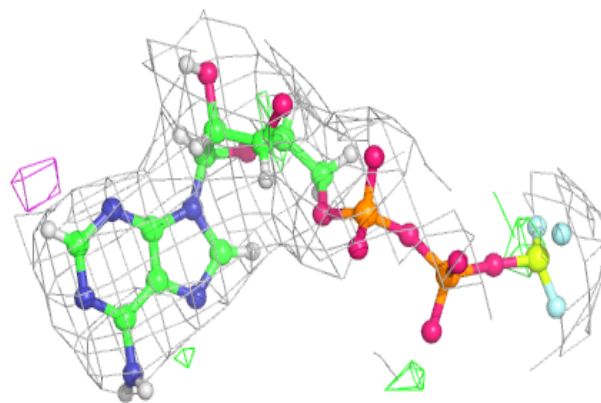
**Electron density around 08T Q 400:**

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

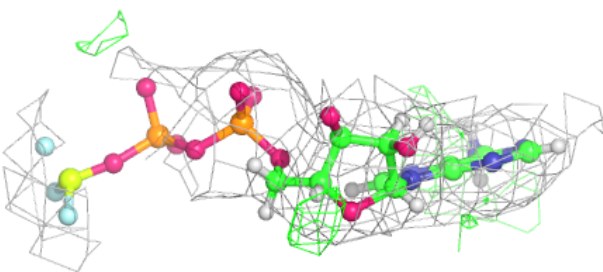
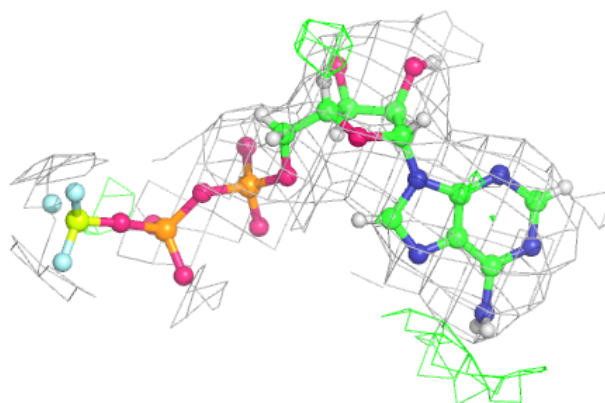


**Electron density around 08T E 400:**

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

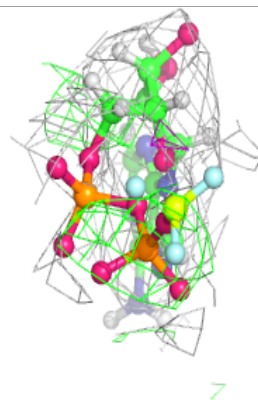
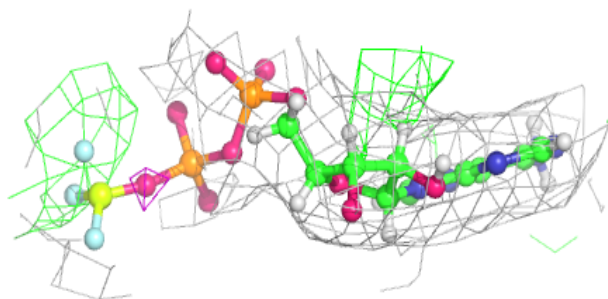
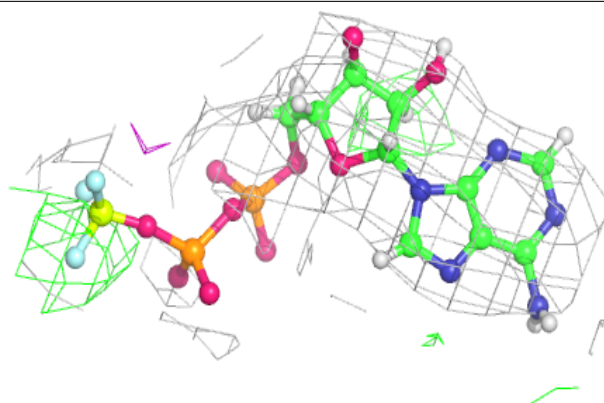
**Electron density around 08T W 400:**

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

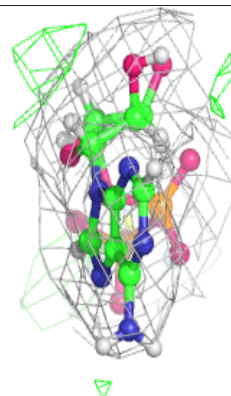
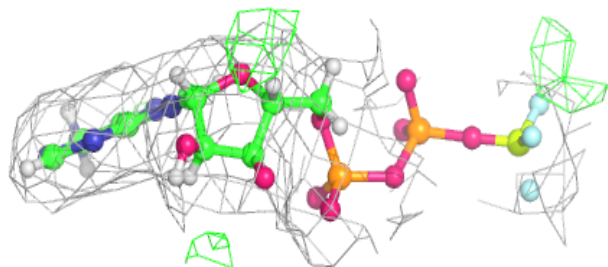
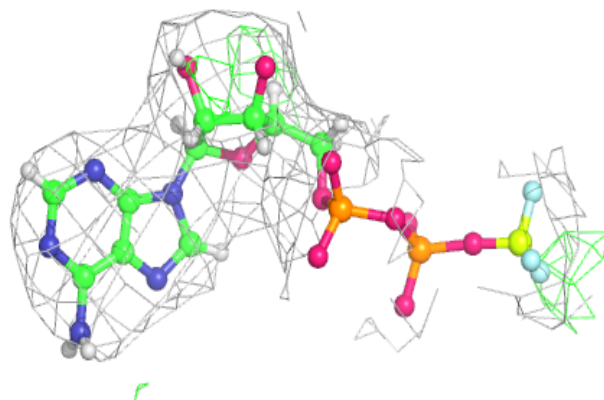


**Electron density around 08T K 400:**

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

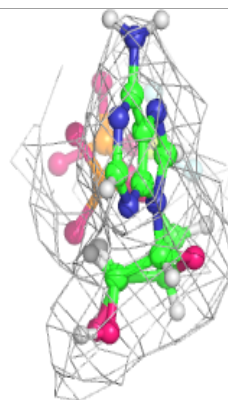
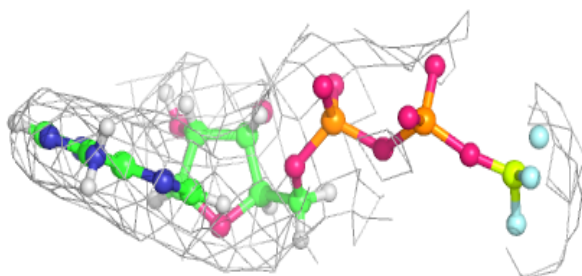
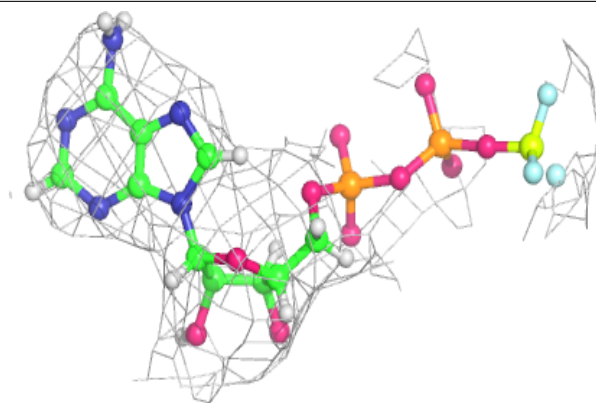
**Electron density around 08T V 400:**

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



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.