



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:13 PM EDT

PDB ID : 4LY6 / pdb_00004ly6
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 : 2013-07-30
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

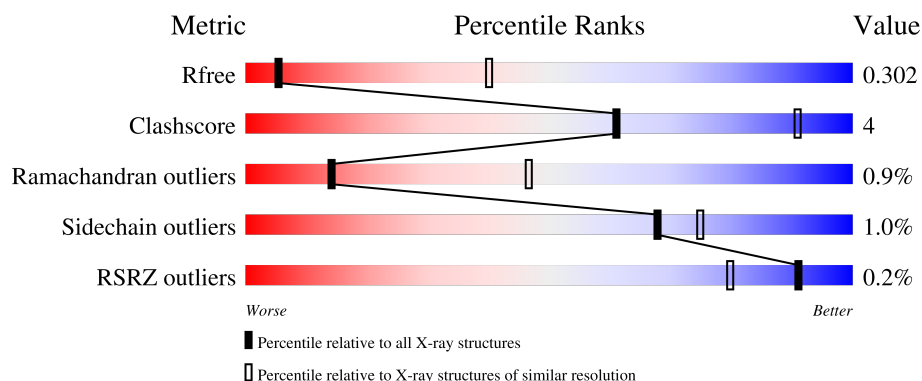
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



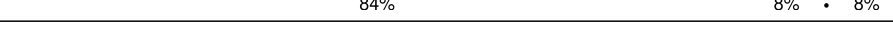
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	268	 83% 9% 8%
1	B	268	 84% 8% 8%
1	C	268	 84% 8% 8%
1	D	268	 78% 13% 8%
1	E	268	 82% 10% 8%

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Mol	Chain	Length	Quality of chain
1	F	268	 80% 11% • 8%
1	G	268	 82% 9% • 8%
1	H	268	 85% 6% • 8%
1	I	268	 80% 12% • 8%
1	J	268	 78% 13% • 8%
1	K	268	 82% 9% • 8%
1	L	268	 % 79% 11% • 8%
1	M	268	 81% 10% • 8%
1	N	268	 85% 5% • 8%
1	O	268	 79% 13% • 8%
1	P	268	 78% 13% 8%
1	Q	268	 81% 10% 8%
1	R	268	 74% 16% • 8%
1	S	268	 84% 8% • 8%
1	T	268	 82% 10% • 8%
1	U	268	 81% 10% • 8%
1	V	268	 81% 9% • 8%
1	W	268	 84% 8% 8%
1	X	268	 % 75% 16% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 97439 atoms, of which 49249 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
			4021	1278	2042	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
			4021	1278	2042	333	364	4			
1	E	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	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
			4021	1278	2042	333	364	4			
1	H	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	I	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	333	364	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
			4021	1278	2042	333	364	4			
1	L	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	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
			4021	1278	2042	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
			4021	1278	2042	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
			4021	1278	2042	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
			4021	1278	2042	333	364	4			
1	T	247	Total	C	H	N	O	S	0	0	0
			4020	1278	2041	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	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			
1	X	247	Total	C	H	N	O	S	0	0	0
			4021	1278	2042	333	364	4			

There are 24 discrepancies between the modelled and reference sequences:

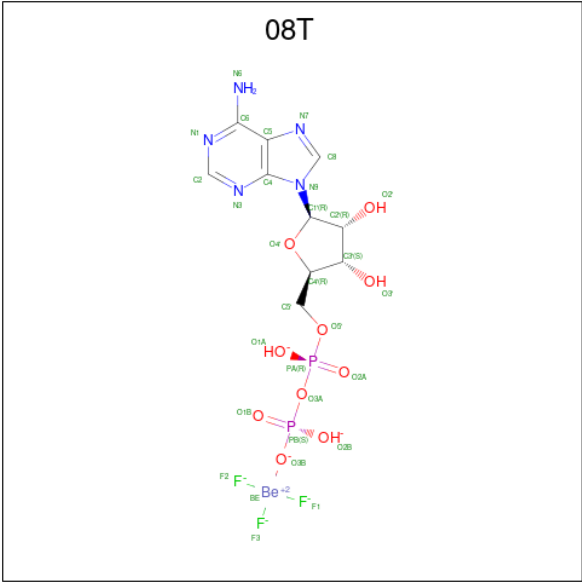
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	initiating methionine	UNP O67198
B	120	MET	-	initiating methionine	UNP O67198
C	120	MET	-	initiating methionine	UNP O67198
D	120	MET	-	initiating methionine	UNP O67198
E	120	MET	-	initiating methionine	UNP O67198
F	120	MET	-	initiating methionine	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-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (CCD ID: 08T) (formula: C₁₀H₁₄BeF₃N₅O₁₀P₂).



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	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		

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

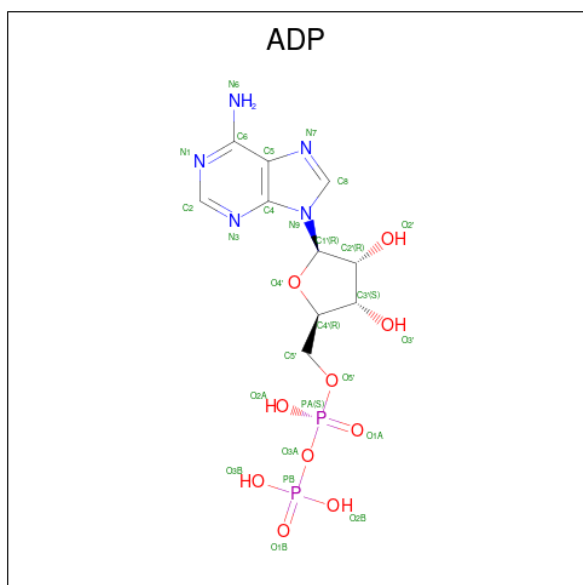
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	P	1	Total	Mg	0	0
			1	1		
3	Q	1	Total	Mg	0	0
			1	1		
3	S	1	Total	Mg	0	0
			1	1		
3	T	1	Total	Mg	0	0
			1	1		
3	U	1	Total	Mg	0	0
			1	1		
3	V	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		

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

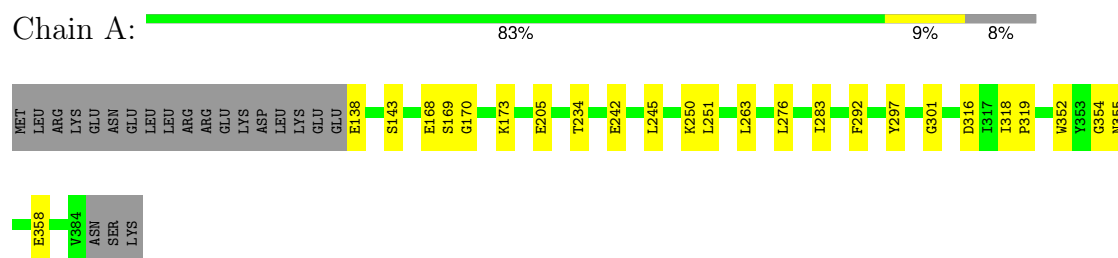


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	L	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
4	X	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

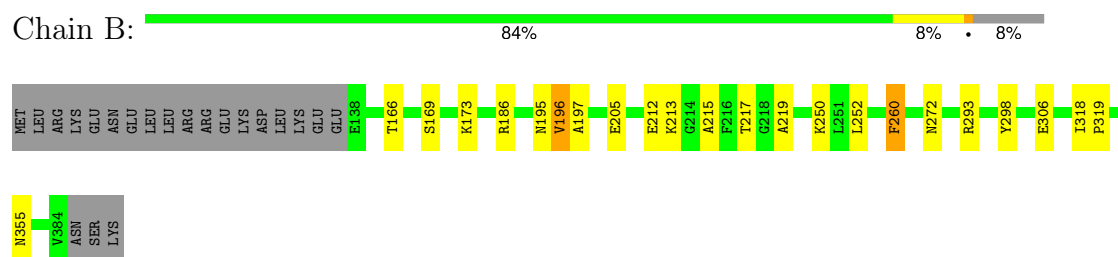
3 Residue-property plots

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

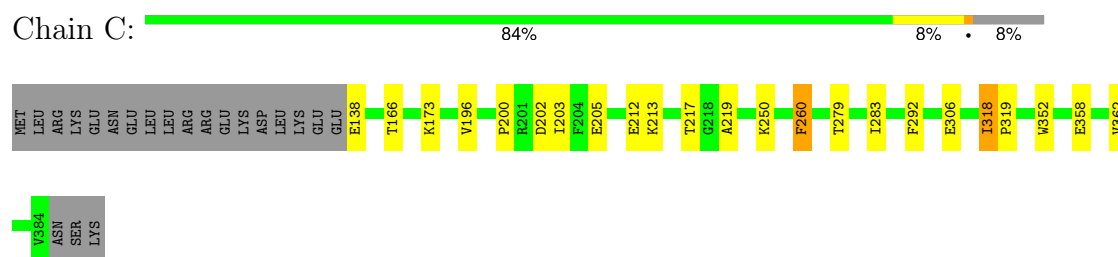
- Molecule 1: Transcriptional regulator (NtrC family)



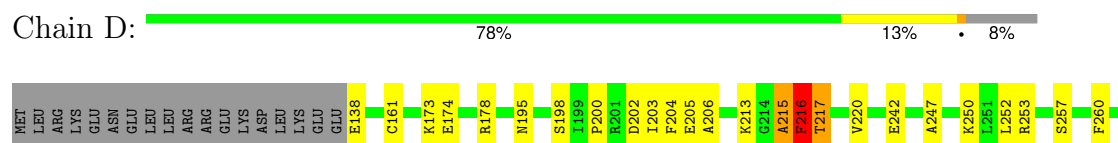
- Molecule 1: Transcriptional regulator (NtrC family)

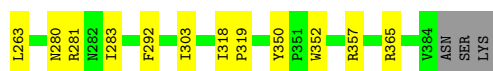


- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)





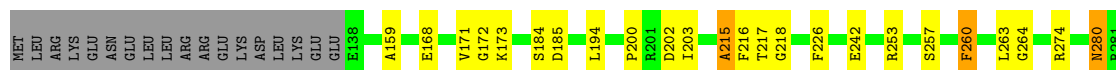
- Molecule 1: Transcriptional regulator (NtrC family)

Chain E: 82% 10% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain F: 80% 11% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain G: 82% 9% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain H: 85% 6% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

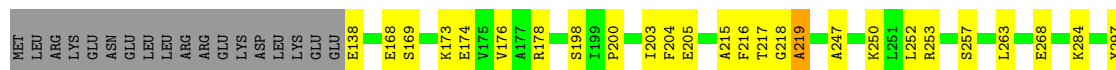
Chain I: 80% 12% 8%





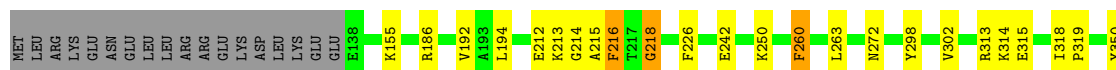
- Molecule 1: Transcriptional regulator (NtrC family)

Chain J: 78% 13% • 8%



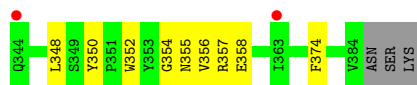
- Molecule 1: Transcriptional regulator (NtrC family)

Chain K: 82% 9% • 8%



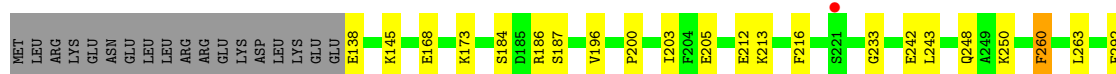
- Molecule 1: Transcriptional regulator (NtrC family)

Chain L: 79% 11% • 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain M: 81% 10% • 8%



- Molecule 1: Transcriptional regulator (NtrC family)

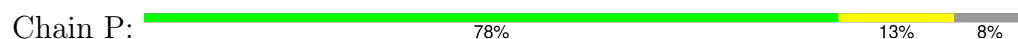
Chain N: 85% 5% • 8%



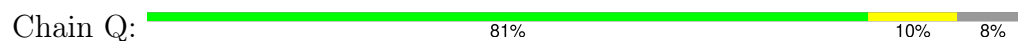
- Molecule 1: Transcriptional regulator (NtrC family)



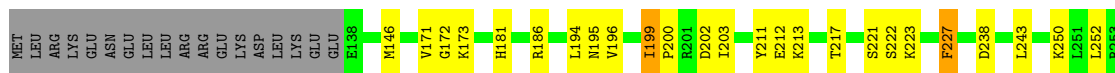
- Molecule 1: Transcriptional regulator (NtrC family)



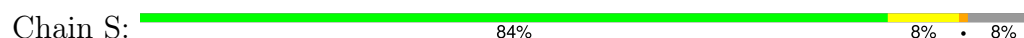
- Molecule 1: Transcriptional regulator (NtrC family)

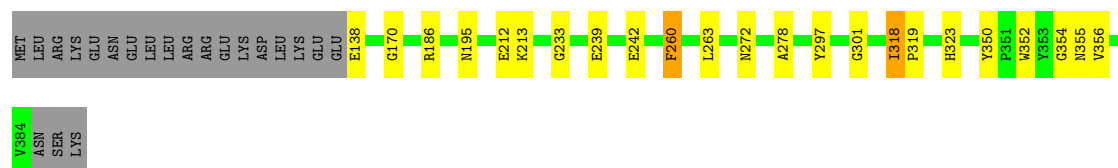


- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)





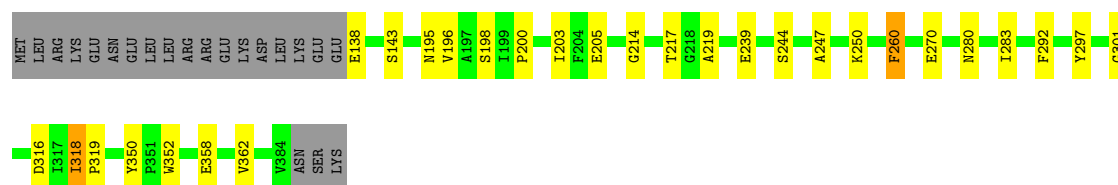
- Molecule 1: Transcriptional regulator (NtrC family)

Chain T: 82% 10% 8%



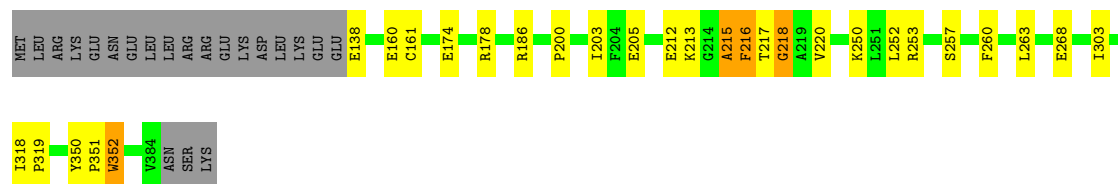
- Molecule 1: Transcriptional regulator (NtrC family)

Chain U: 81% 10% 8%



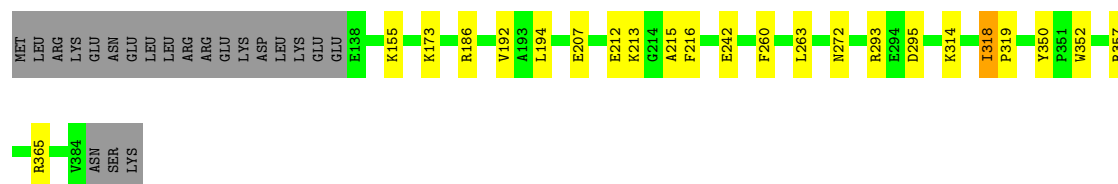
- Molecule 1: Transcriptional regulator (NtrC family)

Chain V: 81% 9% 8%



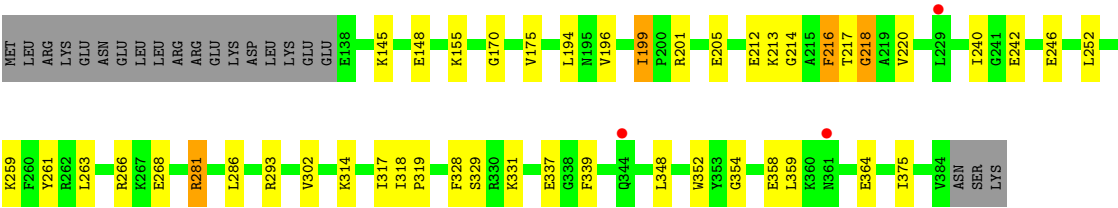
- Molecule 1: Transcriptional regulator (NtrC family)

Chain W: 84% 8% 8%



- Molecule 1: Transcriptional regulator (NtrC family)

Chain X: 75% 16% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	119.34Å 130.04Å 206.37Å 90.00° 89.73° 89.90°	Depositor
Resolution (Å)	37.85 – 3.60 37.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	76.2 (37.85-3.60) 69.7 (37.85-3.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.258 , 0.308 0.257 , 0.302	Depositor DCC
R_{free} test set	5533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.943	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 123.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l 0.319 for -h,k,-l 0.219 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	97439	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/2013	0.77	1/2700 (0.0%)
1	B	0.32	0/2013	0.79	1/2700 (0.0%)
1	C	0.34	0/2013	0.81	1/2700 (0.0%)
1	D	0.33	0/2013	0.83	4/2700 (0.1%)
1	E	0.33	0/2013	0.81	2/2700 (0.1%)
1	F	0.35	0/2013	0.84	0/2700
1	G	0.30	0/2013	0.78	4/2700 (0.1%)
1	H	0.33	0/2013	0.81	3/2700 (0.1%)
1	I	0.34	0/2013	0.83	4/2700 (0.1%)
1	J	0.34	0/2013	0.84	6/2700 (0.2%)
1	K	0.34	0/2013	0.82	3/2700 (0.1%)
1	L	0.34	0/2013	0.85	8/2700 (0.3%)
1	M	0.31	0/2013	0.79	1/2700 (0.0%)
1	N	0.32	0/2013	0.79	3/2700 (0.1%)
1	O	0.34	0/2013	0.83	1/2700 (0.0%)
1	P	0.34	0/2013	0.85	3/2700 (0.1%)
1	Q	0.33	0/2013	0.81	2/2700 (0.1%)
1	R	0.37	0/2013	1.05	11/2700 (0.4%)
1	S	0.31	0/2013	0.78	4/2700 (0.1%)
1	T	0.33	0/2013	0.82	3/2700 (0.1%)
1	U	0.32	0/2013	0.82	3/2700 (0.1%)
1	V	0.32	0/2013	0.82	5/2700 (0.2%)
1	W	0.33	0/2013	0.82	3/2700 (0.1%)
1	X	0.37	0/2013	1.01	4/2700 (0.1%)
All	All	0.33	0/48312	0.84	80/64800 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	F	0	1
1	K	0	1
1	L	0	1
1	N	0	1
1	O	0	1
1	U	0	1
1	V	0	2
1	X	0	1
All	All	0	11

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	218	GLY	N-CA-C	12.10	125.78	110.29
1	R	252	LEU	N-CA-C	10.34	122.13	111.07
1	J	252	LEU	N-CA-C	7.64	120.34	111.02
1	T	252	LEU	N-CA-C	6.48	118.92	111.02
1	X	252	LEU	N-CA-C	6.44	118.88	111.02
1	V	252	LEU	N-CA-C	6.39	118.81	111.02
1	R	199	ILE	CA-C-N	6.32	126.27	119.76
1	R	199	ILE	C-N-CA	6.32	126.27	119.76
1	J	219	ALA	N-CA-C	6.13	117.08	108.00
1	D	252	LEU	N-CA-C	6.09	118.45	111.02
1	R	254	VAL	N-CA-C	6.08	117.62	111.00
1	L	317	ILE	CA-C-N	6.03	124.04	120.24
1	L	317	ILE	C-N-CA	6.03	124.04	120.24
1	R	300	LEU	N-CA-C	5.95	119.73	112.23
1	P	252	LEU	N-CA-C	5.92	118.25	111.02
1	V	350	TYR	CA-C-N	-5.92	112.44	119.84
1	V	350	TYR	C-N-CA	-5.92	112.44	119.84
1	Q	350	TYR	CA-C-N	-5.86	112.52	119.84
1	Q	350	TYR	C-N-CA	-5.86	112.52	119.84
1	D	350	TYR	CA-C-N	-5.83	112.55	119.84
1	D	350	TYR	C-N-CA	-5.83	112.55	119.84
1	W	350	TYR	CA-C-N	-5.71	112.70	119.84
1	W	350	TYR	C-N-CA	-5.71	112.70	119.84
1	I	350	TYR	CA-C-N	-5.68	112.73	119.84
1	I	350	TYR	C-N-CA	-5.68	112.73	119.84
1	B	252	LEU	N-CA-C	5.65	117.92	111.02
1	D	217	THR	N-CA-C	-5.65	103.59	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	350	TYR	CA-C-N	-5.61	112.83	119.84
1	J	350	TYR	C-N-CA	-5.61	112.83	119.84
1	L	306	GLU	N-CA-C	5.60	117.19	111.14
1	R	301	GLY	N-CA-C	5.53	124.57	115.34
1	U	318	ILE	CB-CA-C	-5.49	108.53	114.35
1	L	350	TYR	CA-C-N	-5.49	112.98	119.84
1	L	350	TYR	C-N-CA	-5.49	112.98	119.84
1	E	350	TYR	CA-C-N	-5.45	113.03	119.84
1	E	350	TYR	C-N-CA	-5.45	113.03	119.84
1	H	350	TYR	CA-C-N	-5.44	113.04	119.84
1	H	350	TYR	C-N-CA	-5.44	113.04	119.84
1	M	318	ILE	CB-CA-C	-5.41	108.61	114.35
1	V	215	ALA	CA-C-N	5.41	131.44	121.70
1	V	215	ALA	C-N-CA	5.41	131.44	121.70
1	R	283	ILE	N-CA-C	5.41	116.19	110.72
1	G	350	TYR	CA-C-N	-5.39	113.10	119.84
1	G	350	TYR	C-N-CA	-5.39	113.10	119.84
1	R	258	GLY	N-CA-C	5.33	122.56	114.61
1	I	318	ILE	CB-CA-C	-5.33	108.70	114.35
1	S	318	ILE	CB-CA-C	-5.33	108.70	114.35
1	L	355	ASN	N-CA-C	5.33	117.08	108.08
1	N	252	LEU	N-CA-C	5.32	117.51	111.02
1	A	355	ASN	CB-CA-C	-5.28	110.51	116.63
1	R	307	ILE	CA-C-N	-5.27	114.95	120.38
1	R	307	ILE	C-N-CA	-5.27	114.95	120.38
1	L	355	ASN	CB-CA-C	-5.25	110.54	116.63
1	G	318	ILE	CB-CA-C	-5.23	108.80	114.35
1	J	318	ILE	CB-CA-C	-5.21	108.83	114.35
1	J	215	ALA	CB-CA-C	-5.21	110.15	117.23
1	L	318	ILE	CB-CA-C	-5.20	108.83	114.35
1	K	218	GLY	N-CA-C	-5.18	100.90	113.18
1	I	358	GLU	N-CA-C	5.16	116.91	111.28
1	S	350	TYR	CA-C-N	-5.16	113.39	119.84
1	S	350	TYR	C-N-CA	-5.16	113.39	119.84
1	S	355	ASN	CB-CA-C	-5.16	110.64	116.63
1	W	318	ILE	CB-CA-C	-5.16	108.88	114.35
1	R	238	ASP	N-CA-C	5.15	118.50	110.32
1	P	350	TYR	CA-C-N	-5.15	113.41	119.84
1	P	350	TYR	C-N-CA	-5.15	113.41	119.84
1	C	318	ILE	CB-CA-C	-5.14	108.90	114.35
1	H	318	ILE	CB-CA-C	-5.14	108.90	114.35
1	N	355	ASN	CB-CA-C	-5.11	110.71	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	350	TYR	CA-C-N	-5.06	113.51	119.84
1	T	350	TYR	C-N-CA	-5.06	113.51	119.84
1	X	337	GLU	N-CA-C	5.06	118.91	112.12
1	N	318	ILE	CB-CA-C	-5.06	108.99	114.35
1	K	350	TYR	CA-C-N	-5.04	113.55	119.84
1	K	350	TYR	C-N-CA	-5.04	113.55	119.84
1	U	350	TYR	CA-C-N	-5.03	113.55	119.84
1	U	350	TYR	C-N-CA	-5.03	113.55	119.84
1	X	199	ILE	N-CA-C	5.02	113.87	108.95
1	O	211	TYR	N-CA-C	5.02	116.47	108.79
1	G	140	VAL	N-CA-C	5.02	115.08	107.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	ALA	Peptide
1	D	216	PHE	Peptide
1	F	215	ALA	Peptide
1	K	214	GLY	Peptide
1	L	216	PHE	Peptide
1	N	215	ALA	Peptide
1	O	216	PHE	Peptide
1	U	214	GLY	Peptide
1	V	216	PHE	Peptide
1	V	218	GLY	Peptide
1	X	216	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1979	2041	2039	15	0
1	B	1979	2042	2040	13	0
1	C	1979	2042	2040	14	0
1	D	1979	2042	2040	23	0
1	E	1979	2042	2040	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1979	2042	2040	24	0
1	G	1979	2042	2040	14	0
1	H	1979	2042	2040	14	0
1	I	1979	2041	2039	19	0
1	J	1979	2042	2040	22	0
1	K	1979	2042	2040	18	0
1	L	1979	2042	2040	21	0
1	M	1979	2042	2040	18	0
1	N	1979	2042	2040	12	0
1	O	1979	2042	2040	27	0
1	P	1979	2042	2040	27	0
1	Q	1979	2042	2040	17	0
1	R	1979	2042	2040	22	0
1	S	1979	2042	2040	15	0
1	T	1979	2041	2039	17	0
1	U	1979	2042	2040	15	0
1	V	1979	2042	2040	19	0
1	W	1979	2042	2040	12	0
1	X	1979	2042	2040	29	0
2	A	31	11	13	2	0
2	B	31	11	13	1	0
2	C	31	11	13	0	0
2	D	31	11	13	3	0
2	E	31	11	13	2	0
2	G	31	11	13	4	0
2	H	31	11	13	1	0
2	I	31	11	13	0	0
2	J	31	11	13	2	0
2	K	31	11	13	1	0
2	M	31	11	13	2	0
2	N	31	11	13	4	0
2	O	31	11	13	7	0
2	P	31	11	13	2	0
2	Q	31	11	13	0	0
2	S	31	11	13	2	0
2	T	31	11	13	1	0
2	U	31	11	13	0	0
2	V	31	11	13	0	0
2	W	31	11	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	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	M	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	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
4	L	27	12	12	3	0
4	X	27	12	12	2	0
All	All	48190	49249	49241	408	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 (408) 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:B:205:GLU:OE1	1:B:250:LYS:NZ	2.11	0.84
1:K:242:GLU:OE2	1:L:293:ARG:NH2	2.13	0.81
1:V:205:GLU:OE1	1:V:250:LYS:NZ	2.12	0.81
1:A:242:GLU:OE2	1:B:293:ARG:NH1	2.14	0.81
1:C:205:GLU:OE2	1:C:250:LYS:NZ	2.13	0.81
1:P:213:LYS:NZ	1:U:270:GLU:O	2.15	0.80
1:I:205:GLU:OE2	1:I:250:LYS:NZ	2.15	0.79
1:O:205:GLU:OE2	1:O:250:LYS:NZ	2.18	0.76
1:V:216:PHE:O	1:V:218:GLY:N	2.18	0.75
1:L:205:GLU:OE2	1:L:250:LYS:NZ	2.20	0.74
1:P:205:GLU:OE1	1:P:250:LYS:NZ	2.20	0.74
1:R:334:LYS:NZ	1:R:367:VAL:O	2.20	0.74
1:D:242:GLU:OE1	1:D:281:ARG:NE	2.21	0.74
1:O:280:ASN:ND2	2:O:400:08T:F3	2.12	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:242:GLU:OE2	1:X:293:ARG:NH2	2.21	0.73
1:G:173:LYS:NZ	2:G:400:08T:O2B	2.22	0.72
1:P:365:ARG:NE	1:Q:302:VAL:O	2.21	0.72
1:F:334:LYS:NZ	1:F:367:VAL:O	2.24	0.71
1:U:205:GLU:OE2	1:U:250:LYS:NZ	2.19	0.71
1:J:205:GLU:OE1	1:J:250:LYS:NZ	2.23	0.69
1:L:357:ARG:NH2	4:L:400:ADP:O1B	2.24	0.69
1:F:168:GLU:O	1:F:173:LYS:NZ	2.24	0.69
1:J:217:THR:O	1:J:219:ALA:N	2.25	0.69
1:T:173:LYS:NZ	2:T:400:08T:O1B	2.17	0.69
1:M:145:LYS:NZ	1:M:312:GLU:O	2.25	0.69
1:S:242:GLU:OE2	1:T:293:ARG:NH2	2.27	0.68
1:E:242:GLU:OE1	1:F:293:ARG:NH1	2.27	0.68
1:D:173:LYS:NZ	2:D:400:08T:O2B	2.26	0.67
1:V:215:ALA:HB3	1:V:216:PHE:HB2	1.76	0.67
1:P:242:GLU:OE1	1:P:281:ARG:NE	2.28	0.67
1:N:168:GLU:O	1:N:173:LYS:NZ	2.27	0.67
1:D:205:GLU:OE1	1:D:250:LYS:NZ	2.28	0.66
1:D:365:ARG:NE	1:E:302:VAL:O	2.28	0.66
1:A:138:GLU:N	1:A:138:GLU:OE2	2.28	0.66
1:I:166:THR:OG1	1:I:306:GLU:OE2	2.13	0.66
1:S:186:ARG:NH1	1:S:233:GLY:O	2.27	0.66
1:V:174:GLU:OE2	1:V:178:ARG:NH1	2.28	0.66
1:E:173:LYS:N	2:E:400:08T:O1A	2.29	0.65
1:E:280:ASN:OD1	1:E:281:ARG:NH1	2.29	0.65
1:D:215:ALA:O	1:D:217:THR:N	2.29	0.65
1:M:242:GLU:OE2	1:N:293:ARG:NH1	2.28	0.64
1:O:166:THR:OG1	1:O:306:GLU:OE2	2.15	0.64
1:I:169:SER:OG	1:I:357:ARG:NH1	2.30	0.64
1:J:174:GLU:OE2	1:J:178:ARG:NH1	2.29	0.64
1:R:146:MET:SD	1:R:313:ARG:NH2	2.71	0.63
1:H:205:GLU:OE2	1:H:250:LYS:NZ	2.32	0.63
1:P:253:ARG:O	1:P:257:SER:OG	2.15	0.63
1:A:205:GLU:OE1	1:A:250:LYS:NZ	2.32	0.62
1:P:215:ALA:O	1:P:216:PHE:HB2	1.99	0.61
1:J:314:LYS:NZ	1:J:348:LEU:O	2.33	0.61
1:B:169:SER:O	1:B:355:ASN:ND2	2.30	0.61
1:E:239:GLU:OE2	1:E:280:ASN:ND2	2.34	0.60
1:M:297:TYR:O	1:M:301:GLY:N	2.34	0.60
1:U:195:ASN:ND2	1:U:239:GLU:OE2	2.34	0.60
1:W:186:ARG:NH2	1:W:272:ASN:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:N	1:C:138:GLU:OE2	2.35	0.60
1:M:138:GLU:N	1:M:138:GLU:OE2	2.34	0.60
1:F:283:ILE:HG23	1:F:284:LYS:H	1.67	0.59
1:F:202:ASP:OD1	1:F:203:ILE:N	2.34	0.59
1:O:138:GLU:N	1:O:138:GLU:OE2	2.36	0.59
1:O:173:LYS:NZ	2:O:400:08T:O1B	2.34	0.59
1:L:354:GLY:HA3	1:L:358:GLU:HB2	1.83	0.59
1:E:173:LYS:NZ	2:E:400:08T:O2B	2.23	0.59
1:V:160:GLU:OE2	1:V:186:ARG:NH2	2.36	0.58
1:S:138:GLU:OE2	1:S:138:GLU:N	2.37	0.58
1:G:138:GLU:OE2	1:G:138:GLU:N	2.36	0.58
1:C:203:ILE:HG21	1:D:215:ALA:HB1	1.84	0.58
1:A:297:TYR:O	1:A:301:GLY:N	2.36	0.58
1:R:213:LYS:N	1:R:222:SER:OG	2.37	0.58
1:G:357:ARG:NH2	2:G:400:08T:O1B	2.34	0.57
1:V:138:GLU:OE2	1:V:138:GLU:N	2.37	0.57
1:C:202:ASP:OD1	1:C:203:ILE:N	2.37	0.57
1:D:253:ARG:O	1:D:257:SER:OG	2.21	0.57
1:P:168:GLU:O	1:P:173:LYS:NZ	2.38	0.57
1:K:186:ARG:NH2	1:K:272:ASN:OD1	2.37	0.57
1:U:138:GLU:N	1:U:138:GLU:OE2	2.38	0.57
1:X:155:LYS:HE2	1:X:155:LYS:HA	1.87	0.57
1:Q:159:ALA:O	1:Q:274:ARG:NH1	2.37	0.57
1:O:173:LYS:N	2:O:400:08T:O1A	2.38	0.57
1:G:186:ARG:NH1	1:G:233:GLY:O	2.38	0.56
1:N:173:LYS:N	2:N:400:08T:O1A	2.38	0.56
1:C:173:LYS:NZ	1:C:279:THR:O	2.37	0.56
1:D:138:GLU:N	1:D:138:GLU:OE2	2.38	0.56
1:M:168:GLU:O	1:M:173:LYS:NZ	2.38	0.56
1:I:138:GLU:OE2	1:I:138:GLU:N	2.39	0.56
1:J:138:GLU:OE2	1:J:138:GLU:N	2.38	0.56
1:D:202:ASP:OD1	1:D:203:ILE:N	2.39	0.56
1:Q:242:GLU:OE1	1:Q:281:ARG:NH2	2.38	0.56
1:F:216:PHE:HB3	1:F:217:THR:C	2.31	0.55
1:P:217:THR:O	1:P:217:THR:OG1	2.24	0.55
1:F:216:PHE:HB3	1:F:217:THR:HB	1.89	0.55
1:E:361:ASN:ND2	1:F:298:TYR:O	2.40	0.55
1:I:169:SER:O	1:I:355:ASN:ND2	2.39	0.55
1:F:171:VAL:HG12	1:F:355:ASN:CB	2.37	0.54
1:I:242:GLU:OE2	1:I:281:ARG:NH1	2.41	0.54
1:O:216:PHE:HB3	1:P:217:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:173:LYS:NZ	2:M:400:08T:O2B	2.26	0.54
1:O:175:VAL:O	1:O:179:LEU:N	2.41	0.54
1:N:172:GLY:HA2	2:N:400:08T:H14	1.90	0.53
1:J:253:ARG:O	1:J:257:SER:OG	2.24	0.53
1:A:169:SER:CB	2:A:400:08T:F3	2.31	0.53
1:G:297:TYR:O	1:G:301:GLY:N	2.41	0.53
1:F:253:ARG:O	1:F:257:SER:OG	2.26	0.52
1:P:365:ARG:NH2	1:Q:301:GLY:O	2.40	0.52
1:I:186:ARG:NH1	1:I:272:ASN:OD1	2.42	0.52
1:K:365:ARG:NH2	1:L:302:VAL:O	2.43	0.52
1:J:253:ARG:NH2	1:J:268:GLU:OE2	2.43	0.52
1:K:155:LYS:HA	1:K:155:LYS:HE2	1.92	0.52
1:D:357:ARG:NH2	2:D:400:08T:O3A	2.43	0.51
1:O:169:SER:O	1:O:355:ASN:ND2	2.39	0.51
1:R:202:ASP:OD1	1:R:203:ILE:N	2.42	0.51
1:Q:155:LYS:HE2	1:Q:155:LYS:HA	1.92	0.51
1:J:284:LYS:NZ	1:J:297:TYR:OH	2.33	0.51
1:B:166:THR:OG1	1:B:306:GLU:OE1	2.22	0.51
1:O:168:GLU:O	1:O:173:LYS:NZ	2.43	0.51
1:V:200:PRO:HG2	1:V:203:ILE:HG12	1.93	0.51
1:P:212:GLU:HG3	1:P:213:LYS:H	1.76	0.51
1:I:253:ARG:O	1:I:257:SER:OG	2.25	0.50
1:K:216:PHE:C	1:K:218:GLY:H	2.18	0.50
1:L:155:LYS:HE2	1:L:155:LYS:HA	1.93	0.50
1:C:358:GLU:O	1:C:362:VAL:N	2.38	0.50
1:L:216:PHE:HA	1:L:217:THR:HB	1.93	0.50
1:X:242:GLU:OE1	1:X:281:ARG:NH2	2.44	0.50
1:T:169:SER:OG	1:T:357:ARG:NH1	2.45	0.50
1:B:173:LYS:N	2:B:400:08T:O2A	2.45	0.50
2:J:400:08T:PA	2:J:400:08T:H4	2.52	0.50
1:B:195:ASN:C	1:B:197:ALA:H	2.20	0.49
1:F:242:GLU:OE2	1:F:280:ASN:ND2	2.46	0.49
1:L:221:SER:OG	1:L:222:SER:N	2.45	0.49
1:E:155:LYS:HE2	1:E:155:LYS:HA	1.95	0.49
1:L:216:PHE:HA	1:L:217:THR:CB	2.43	0.49
1:H:357:ARG:NH2	2:H:400:08T:O3A	2.45	0.48
1:B:195:ASN:O	1:B:196:VAL:HG12	2.12	0.48
1:H:195:ASN:O	1:H:196:VAL:HG12	2.12	0.48
1:A:168:GLU:O	1:A:173:LYS:NZ	2.46	0.48
1:V:253:ARG:O	1:V:257:SER:OG	2.25	0.48
1:W:155:LYS:HA	1:W:155:LYS:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:PHE:CD1	1:D:260:PHE:C	2.91	0.48
1:J:217:THR:C	1:J:219:ALA:H	2.20	0.48
1:Q:332:TYR:OH	1:Q:364:GLU:OE2	2.31	0.48
1:R:171:VAL:O	1:R:173:LYS:N	2.46	0.48
1:T:195:ASN:C	1:T:197:ALA:H	2.21	0.48
1:V:260:PHE:CD1	1:V:260:PHE:C	2.91	0.48
1:A:245:LEU:HB2	1:F:200:PRO:HG3	1.96	0.48
1:N:195:ASN:O	1:N:196:VAL:HG12	2.14	0.48
1:T:195:ASN:O	1:T:196:VAL:HG12	2.13	0.48
1:T:181:HIS:NE2	1:T:189:GLU:O	2.46	0.48
1:E:242:GLU:OE2	1:F:293:ARG:NH2	2.47	0.47
1:M:173:LYS:N	2:M:400:08T:O2A	2.47	0.47
1:G:170:GLY:N	2:G:400:08T:O1B	2.48	0.47
1:W:293:ARG:NE	1:W:295:ASP:OD2	2.42	0.47
1:R:171:VAL:O	1:R:171:VAL:HG23	2.14	0.47
1:D:206:ALA:HB2	1:D:216:PHE:CE2	2.50	0.47
1:P:204:PHE:HE2	1:P:247:ALA:HB1	1.80	0.47
1:X:354:GLY:HA3	1:X:358:GLU:HB2	1.96	0.47
1:C:200:PRO:HG2	1:C:203:ILE:HG12	1.96	0.47
1:G:212:GLU:HG3	1:G:213:LYS:H	1.80	0.47
1:M:212:GLU:HG3	1:M:213:LYS:H	1.79	0.47
1:J:200:PRO:HG2	1:J:203:ILE:HG12	1.97	0.47
1:L:172:GLY:N	4:L:400:ADP:O1A	2.39	0.47
1:S:195:ASN:HB2	1:T:253:ARG:HD2	1.97	0.47
1:X:216:PHE:CB	1:X:218:GLY:N	2.78	0.47
1:K:357:ARG:NH2	2:K:400:08T:O3A	2.47	0.47
1:T:182:LYS:O	1:T:187:SER:OG	2.24	0.47
1:I:159:ALA:O	1:I:274:ARG:NH1	2.48	0.46
1:N:318:ILE:N	1:N:319:PRO:CD	2.78	0.46
1:P:174:GLU:H	2:P:400:08T:H9	1.63	0.46
1:D:174:GLU:OE2	1:D:178:ARG:NH1	2.48	0.46
1:G:182:LYS:O	1:G:187:SER:OG	2.32	0.46
1:O:217:THR:C	1:O:219:ALA:H	2.22	0.46
1:R:200:PRO:HD2	1:R:203:ILE:HD11	1.97	0.46
1:S:260:PHE:CD1	1:S:260:PHE:C	2.93	0.46
1:W:318:ILE:N	1:W:319:PRO:CD	2.79	0.46
1:F:171:VAL:HG12	1:F:355:ASN:HB2	1.97	0.46
1:R:318:ILE:HB	1:R:319:PRO:HD3	1.97	0.46
1:V:212:GLU:HG3	1:V:213:LYS:H	1.80	0.46
1:W:212:GLU:HG3	1:W:213:LYS:N	2.31	0.46
1:X:212:GLU:O	1:X:214:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:HE2	1:D:247:ALA:HB1	1.81	0.46
1:U:217:THR:C	1:U:219:ALA:H	2.24	0.46
1:Q:216:PHE:HB3	1:Q:218:GLY:H	1.81	0.46
1:S:170:GLY:N	2:S:400:08T:O2B	2.43	0.46
1:C:217:THR:C	1:C:219:ALA:H	2.24	0.46
1:H:205:GLU:OE1	1:H:205:GLU:N	2.43	0.46
1:J:176:VAL:HG21	1:J:307:ILE:HD11	1.98	0.46
1:A:250:LYS:O	1:A:251:LEU:HB3	2.16	0.45
1:B:212:GLU:HG3	1:B:213:LYS:H	1.81	0.45
1:L:340:THR:HG22	1:L:374:PHE:HB3	1.98	0.45
1:T:260:PHE:CD1	1:T:260:PHE:C	2.94	0.45
1:D:200:PRO:HG2	1:D:203:ILE:HG12	1.97	0.45
1:K:212:GLU:HG3	1:K:213:LYS:H	1.81	0.45
1:V:215:ALA:HB3	1:V:216:PHE:CB	2.45	0.45
1:C:166:THR:OG1	1:C:306:GLU:OE2	2.33	0.45
1:J:173:LYS:NZ	2:J:400:08T:O1B	2.40	0.45
1:J:200:PRO:HG2	1:J:203:ILE:CG1	2.47	0.45
1:Q:318:ILE:N	1:Q:319:PRO:CD	2.79	0.45
1:T:328:PHE:CE2	1:T:364:GLU:HB2	2.51	0.45
1:W:192:VAL:HG12	1:W:194:LEU:CD1	2.46	0.45
1:X:201:ARG:NH1	1:X:246:GLU:OE1	2.48	0.45
1:E:194:LEU:HD21	1:E:226:PHE:CD2	2.52	0.45
1:P:216:PHE:C	1:P:217:THR:HG23	2.42	0.45
1:K:260:PHE:C	1:K:260:PHE:CD1	2.95	0.45
1:Q:198:SER:HA	1:R:250:LYS:HD3	1.98	0.45
1:R:349:SER:O	1:R:350:TYR:HB2	2.17	0.45
1:X:216:PHE:HB3	1:X:217:THR:C	2.42	0.45
1:E:318:ILE:N	1:E:319:PRO:CD	2.80	0.45
1:H:195:ASN:C	1:H:197:ALA:H	2.24	0.45
1:X:281:ARG:HG2	1:X:286:LEU:HD11	1.98	0.45
1:X:216:PHE:HB3	1:X:217:THR:HB	1.97	0.45
1:F:171:VAL:HG23	1:F:171:VAL:O	2.17	0.45
1:S:318:ILE:N	1:S:319:PRO:CD	2.80	0.45
1:X:328:PHE:O	1:X:331:LYS:N	2.50	0.45
1:C:283:ILE:HD11	1:C:292:PHE:CE2	2.52	0.45
1:N:212:GLU:HG3	1:N:213:LYS:H	1.82	0.45
1:Q:260:PHE:CD1	1:Q:260:PHE:C	2.95	0.45
1:P:324:PHE:CD2	1:P:360:LYS:HA	2.52	0.45
1:V:253:ARG:NH2	1:V:268:GLU:OE2	2.50	0.45
1:X:314:LYS:HB3	1:X:348:LEU:HD22	1.98	0.45
1:E:192:VAL:HG12	1:E:194:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:PHE:CD1	1:H:260:PHE:C	2.95	0.44
1:P:223:LYS:HD3	1:Q:264:GLY:O	2.17	0.44
1:V:200:PRO:HG2	1:V:203:ILE:CG1	2.47	0.44
1:J:169:SER:O	1:J:355:ASN:ND2	2.49	0.44
1:E:365:ARG:NH1	1:E:383:LEU:HG	2.32	0.44
1:P:232:GLY:HA3	1:T:220:VAL:HG21	1.99	0.44
1:U:244:SER:O	1:U:247:ALA:N	2.50	0.44
1:O:174:GLU:N	2:O:400:08T:O1A	2.37	0.44
1:U:200:PRO:HG2	1:U:203:ILE:CG1	2.47	0.44
1:C:318:ILE:N	1:C:319:PRO:CD	2.80	0.44
1:P:283:ILE:HD11	1:P:292:PHE:CE2	2.53	0.44
1:K:194:LEU:HD21	1:K:226:PHE:CD2	2.53	0.44
1:M:205:GLU:OE1	1:M:250:LYS:NZ	2.50	0.44
1:X:196:VAL:HG11	1:X:240:ILE:HD13	1.98	0.44
1:X:205:GLU:N	1:X:205:GLU:OE1	2.50	0.44
1:X:317:ILE:HD12	1:X:348:LEU:HD23	2.00	0.44
1:H:318:ILE:N	1:H:319:PRO:CD	2.80	0.44
1:O:216:PHE:CG	1:P:217:THR:HG22	2.53	0.44
1:P:285:GLU:HA	1:P:288:LYS:HE3	2.00	0.44
1:X:261:TYR:CZ	1:X:268:GLU:HG3	2.53	0.44
1:B:186:ARG:NH2	1:B:272:ASN:OD1	2.43	0.44
1:B:260:PHE:CD1	1:B:260:PHE:C	2.96	0.44
1:F:159:ALA:O	1:F:274:ARG:NH1	2.50	0.44
1:M:260:PHE:CD1	1:M:260:PHE:C	2.95	0.44
1:T:174:GLU:OE1	1:T:178:ARG:NH1	2.51	0.44
1:W:357:ARG:NH2	2:W:400:08T:O3A	2.51	0.44
1:X:175:VAL:HG21	4:X:400:ADP:C5	2.53	0.44
1:A:354:GLY:HA2	1:B:298:TYR:CE2	2.53	0.44
1:O:283:ILE:HD11	1:O:292:PHE:CD2	2.53	0.44
1:D:318:ILE:N	1:D:319:PRO:CD	2.81	0.43
1:G:207:GLU:OE1	1:H:264:GLY:N	2.50	0.43
1:G:238:ASP:OD2	2:G:400:08T:F2	2.26	0.43
1:P:318:ILE:N	1:P:319:PRO:CD	2.81	0.43
1:R:199:ILE:HA	1:R:200:PRO:HD3	1.91	0.43
1:R:212:GLU:HG3	1:R:213:LYS:H	1.83	0.43
1:S:138:GLU:O	1:S:323:HIS:NE2	2.51	0.43
1:L:260:PHE:CD1	1:L:260:PHE:C	2.96	0.43
1:O:200:PRO:HG2	1:O:203:ILE:HG12	1.99	0.43
1:R:196:VAL:HG21	1:R:243:LEU:HD22	2.00	0.43
1:T:318:ILE:N	1:T:319:PRO:CD	2.82	0.43
1:X:216:PHE:HB3	1:X:218:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:PHE:CD1	1:E:260:PHE:C	2.96	0.43
1:F:216:PHE:HB3	1:F:218:GLY:N	2.34	0.43
1:G:318:ILE:N	1:G:319:PRO:CD	2.80	0.43
1:I:217:THR:C	1:I:219:ALA:H	2.27	0.43
1:R:265:GLY:O	1:R:266:ARG:HD3	2.19	0.43
1:V:216:PHE:C	1:V:218:GLY:N	2.76	0.43
1:X:145:LYS:O	1:X:148:GLU:HG2	2.19	0.43
1:D:365:ARG:NH2	1:E:301:GLY:O	2.50	0.43
1:M:184:SER:O	1:M:187:SER:OG	2.37	0.43
1:N:169:SER:O	1:N:355:ASN:ND2	2.46	0.43
1:N:173:LYS:NZ	2:N:400:08T:O1B	2.50	0.43
1:N:260:PHE:CD1	1:N:260:PHE:C	2.97	0.43
1:W:207:GLU:HA	1:X:266:ARG:HH22	1.83	0.43
1:M:318:ILE:N	1:M:319:PRO:CD	2.81	0.43
1:U:297:TYR:O	1:U:301:GLY:N	2.52	0.43
1:B:318:ILE:N	1:B:319:PRO:CD	2.82	0.43
1:H:207:GLU:OE1	1:I:264:GLY:N	2.50	0.43
1:J:361:ASN:ND2	1:K:298:TYR:O	2.51	0.43
1:K:215:ALA:O	1:K:216:PHE:HB2	2.19	0.43
1:O:212:GLU:HG3	1:O:213:LYS:H	1.83	0.43
1:P:198:SER:HA	1:Q:250:LYS:HD3	2.00	0.43
1:X:317:ILE:HG23	1:X:359:LEU:HD11	2.00	0.43
1:C:260:PHE:CD1	1:C:260:PHE:C	2.97	0.43
1:F:260:PHE:C	1:F:260:PHE:CD1	2.97	0.43
1:N:186:ARG:NH2	1:N:272:ASN:OD1	2.50	0.43
1:O:174:GLU:HB3	2:O:400:08T:O2A	2.19	0.43
1:E:328:PHE:CE2	1:E:364:GLU:HB2	2.54	0.42
1:J:168:GLU:HB2	1:J:355:ASN:HD21	1.84	0.42
1:J:318:ILE:N	1:J:319:PRO:CD	2.82	0.42
1:K:318:ILE:N	1:K:319:PRO:CD	2.82	0.42
1:L:318:ILE:N	1:L:319:PRO:CD	2.82	0.42
1:M:200:PRO:HD2	1:M:203:ILE:HD11	2.01	0.42
1:M:292:PHE:CE1	1:M:296:LEU:HD23	2.54	0.42
1:F:283:ILE:HG13	1:F:284:LYS:N	2.33	0.42
1:G:215:ALA:CB	1:G:264:GLY:HA3	2.49	0.42
1:G:366:ALA:O	1:G:370:SER:N	2.52	0.42
1:I:297:TYR:O	1:I:301:GLY:N	2.52	0.42
1:I:354:GLY:HA3	1:I:358:GLU:HB2	2.00	0.42
1:O:318:ILE:N	1:O:319:PRO:CD	2.82	0.42
1:S:239:GLU:N	1:S:278:ALA:O	2.52	0.42
1:U:196:VAL:HG13	1:U:196:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ASN:ND2	1:I:249:ALA:O	2.49	0.42
1:I:318:ILE:N	1:I:319:PRO:CD	2.82	0.42
1:O:283:ILE:HD11	1:O:292:PHE:CE2	2.54	0.42
1:X:314:LYS:HD3	1:X:348:LEU:HB3	2.01	0.42
1:F:194:LEU:HD22	1:F:226:PHE:CD2	2.54	0.42
1:L:283:ILE:HD11	1:L:292:PHE:CE2	2.55	0.42
1:N:173:LYS:H	2:N:400:08T:H9	1.66	0.42
1:H:253:ARG:HB2	1:H:253:ARG:NH1	2.34	0.42
1:O:174:GLU:H	2:O:400:08T:H9	1.59	0.42
1:Q:192:VAL:HG12	1:Q:194:LEU:CD1	2.50	0.42
1:X:339:PHE:HA	1:X:375:ILE:H	1.84	0.42
1:H:176:VAL:HG21	1:H:307:ILE:HD11	2.02	0.42
1:L:317:ILE:HD12	1:L:348:LEU:HD23	2.01	0.42
1:O:354:GLY:HA3	1:O:358:GLU:HB2	2.02	0.42
1:P:174:GLU:HB3	2:P:400:08T:O2A	2.19	0.42
1:S:356:VAL:CG1	2:S:400:08T:H8	2.50	0.42
1:A:318:ILE:N	1:A:319:PRO:CD	2.83	0.42
1:V:161:CYS:SG	1:V:303:ILE:HD11	2.59	0.42
1:A:143:SER:N	1:A:316:ASP:OD1	2.47	0.42
1:H:328:PHE:CE2	1:H:364:GLU:HB2	2.55	0.42
1:L:305:ILE:HG22	1:L:307:ILE:HG12	2.02	0.42
1:O:172:GLY:HA3	2:O:400:08T:H10	2.01	0.42
1:V:318:ILE:N	1:V:319:PRO:CD	2.82	0.42
1:B:217:THR:C	1:B:219:ALA:H	2.28	0.41
1:F:184:SER:OG	1:F:185:ASP:N	2.53	0.41
1:O:245:LEU:HD12	1:O:245:LEU:H	1.84	0.41
1:Q:328:PHE:CE2	1:Q:364:GLU:HB2	2.55	0.41
1:R:181:HIS:NE2	1:R:186:ARG:O	2.53	0.41
1:R:194:LEU:HD23	1:R:195:ASN:N	2.35	0.41
1:S:297:TYR:O	1:S:301:GLY:N	2.51	0.41
1:X:216:PHE:HB2	1:X:218:GLY:N	2.35	0.41
1:A:234:THR:HG23	1:A:276:LEU:HD13	2.02	0.41
1:D:195:ASN:ND2	1:D:198:SER:OG	2.47	0.41
1:S:260:PHE:C	1:S:260:PHE:HD1	2.28	0.41
1:D:280:ASN:ND2	2:D:400:08T:F3	2.40	0.41
1:R:227:PHE:CE2	1:R:254:VAL:HG11	2.55	0.41
1:V:351:PRO:O	1:V:352:TRP:C	2.64	0.41
1:X:170:GLY:N	4:X:400:ADP:O3B	2.53	0.41
1:U:260:PHE:CD1	1:U:260:PHE:C	2.98	0.41
1:X:194:LEU:HD21	1:X:199:ILE:HD11	2.02	0.41
1:X:352:TRP:CZ3	1:X:359:LEU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ILE:HD11	1:D:292:PHE:CE2	2.56	0.41
1:F:171:VAL:O	1:F:173:LYS:N	2.53	0.41
1:I:212:GLU:HG3	1:I:213:LYS:H	1.85	0.41
1:L:139:TYR:CE1	1:L:175:VAL:HG13	2.55	0.41
1:M:196:VAL:HG13	1:M:196:VAL:O	2.20	0.41
1:Q:216:PHE:O	1:Q:217:THR:CB	2.68	0.41
1:A:170:GLY:H	2:A:400:08T:PB	2.44	0.41
1:K:215:ALA:O	1:K:216:PHE:CB	2.68	0.41
1:R:354:GLY:HA3	1:R:358:GLU:HB2	2.03	0.41
1:S:186:ARG:NH2	1:S:272:ASN:OD1	2.47	0.41
1:W:260:PHE:CD1	1:W:260:PHE:C	2.99	0.41
1:C:212:GLU:HG3	1:C:213:LYS:H	1.85	0.41
1:E:207:GLU:OE1	1:F:264:GLY:N	2.48	0.41
1:L:260:PHE:C	1:L:260:PHE:HD1	2.29	0.41
1:L:356:VAL:HG12	1:L:356:VAL:O	2.20	0.41
1:O:200:PRO:HG2	1:O:203:ILE:CG1	2.50	0.41
1:P:232:GLY:HA3	1:T:220:VAL:CB	2.50	0.41
1:U:318:ILE:N	1:U:319:PRO:CD	2.83	0.41
1:D:260:PHE:C	1:D:260:PHE:HD1	2.29	0.41
1:I:260:PHE:CD1	1:I:260:PHE:C	2.99	0.41
1:J:198:SER:HA	1:K:250:LYS:HD3	2.02	0.41
1:K:313:ARG:O	1:K:315:GLU:N	2.54	0.41
1:M:186:ARG:NH1	1:M:233:GLY:O	2.53	0.41
1:O:297:TYR:O	1:O:301:GLY:N	2.54	0.41
1:U:198:SER:HA	1:V:250:LYS:HD3	2.03	0.41
1:A:283:ILE:HD11	1:A:292:PHE:CD2	2.55	0.40
1:F:216:PHE:CB	1:F:218:GLY:N	2.84	0.40
1:I:196:VAL:O	1:I:196:VAL:HG13	2.22	0.40
1:K:192:VAL:HG12	1:K:194:LEU:CD1	2.50	0.40
1:M:216:PHE:CZ	1:R:221:SER:HB3	2.55	0.40
1:Q:166:THR:HG22	1:Q:167:GLY:N	2.36	0.40
1:Q:365:ARG:NE	1:R:302:VAL:O	2.54	0.40
1:U:358:GLU:O	1:U:362:VAL:N	2.46	0.40
1:C:196:VAL:HG13	1:C:196:VAL:O	2.21	0.40
1:I:245:LEU:H	1:I:245:LEU:HD12	1.86	0.40
1:M:243:LEU:HD23	1:M:248:GLN:HG2	2.04	0.40
1:R:211:TYR:CZ	1:R:223:LYS:HB2	2.57	0.40
1:R:256:GLU:HB2	1:R:299:ARG:HE	1.85	0.40
1:S:212:GLU:HG3	1:S:213:LYS:H	1.86	0.40
1:T:175:VAL:O	1:T:179:LEU:N	2.53	0.40
1:U:143:SER:N	1:U:316:ASP:OD1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:260:PHE:C	1:V:260:PHE:HD1	2.29	0.40
1:W:173:LYS:NZ	2:W:400:08T:O1B	2.53	0.40
1:W:365:ARG:NE	1:X:302:VAL:O	2.55	0.40
1:G:168:GLU:O	1:G:173:LYS:NZ	2.54	0.40
1:J:204:PHE:HE2	1:J:247:ALA:HB1	1.86	0.40
1:J:351:PRO:O	1:J:352:TRP:C	2.63	0.40
1:L:216:PHE:HB3	1:L:217:THR:C	2.46	0.40
1:P:328:PHE:CE2	1:P:364:GLU:HB2	2.57	0.40
1:A:354:GLY:HA3	1:A:358:GLU:HB2	2.03	0.40
1:D:161:CYS:SG	1:D:303:ILE:HD11	2.61	0.40
1:D:283:ILE:HD11	1:D:292:PHE:CD2	2.57	0.40
1:E:260:PHE:CE1	1:E:269:ILE:HB	2.57	0.40
1:H:297:TYR:O	1:H:301:GLY:N	2.54	0.40
1:J:366:ALA:O	1:J:370:SER:N	2.55	0.40
1:K:260:PHE:C	1:K:260:PHE:HD1	2.29	0.40
1:O:196:VAL:O	1:O:196:VAL:HG13	2.22	0.40
1:O:244:SER:O	1:O:247:ALA:N	2.53	0.40
1:P:297:TYR:O	1:P:301:GLY:N	2.54	0.40
1:S:354:GLY:HA2	1:T:298:TYR:CE2	2.57	0.40
1:T:297:TYR:O	1:T:301:GLY:N	2.53	0.40
1:U:283:ILE:HD11	1:U:292:PHE:CE2	2.57	0.40
1:X:318:ILE:HB	1:X:319:PRO:HD3	2.02	0.40
1:J:365:ARG:NE	1:K:302:VAL:O	2.37	0.40
1:L:173:LYS:N	4:L:400:ADP:O2A	2.54	0.40
1:P:206:ALA:HB2	1:P:216:PHE:HE2	1.86	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%)	232 (95%)	12 (5%)	1 (0%)	30 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	30	61
1	C	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	30	61
1	D	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	10	41
1	E	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	16	49
1	F	245/268 (91%)	221 (90%)	20 (8%)	4 (2%)	7	36
1	G	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	30	61
1	H	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	16	49
1	I	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	30	61
1	J	245/268 (91%)	230 (94%)	12 (5%)	3 (1%)	10	41
1	K	245/268 (91%)	227 (93%)	15 (6%)	3 (1%)	10	41
1	L	245/268 (91%)	226 (92%)	17 (7%)	2 (1%)	16	49
1	M	245/268 (91%)	229 (94%)	15 (6%)	1 (0%)	30	61
1	N	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	16	49
1	O	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	30	61
1	P	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	16	49
1	Q	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	10	41
1	R	245/268 (91%)	235 (96%)	6 (2%)	4 (2%)	7	36
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	30	61
1	T	245/268 (91%)	229 (94%)	14 (6%)	2 (1%)	16	49
1	U	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	30	61
1	V	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	10	41
1	W	245/268 (91%)	229 (94%)	13 (5%)	3 (1%)	10	41
1	X	245/268 (91%)	234 (96%)	8 (3%)	3 (1%)	10	41
All	All	5880/6432 (91%)	5513 (94%)	317 (5%)	50 (1%)	14	46

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	H	196	VAL
1	J	216	PHE
1	N	196	VAL
1	P	216	PHE
1	R	217	THR

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Mol	Chain	Res	Type
1	R	307	ILE
1	T	196	VAL
1	V	217	THR
1	X	213	LYS
1	D	216	PHE
1	J	218	GLY
1	K	216	PHE
1	R	172	GLY
1	W	215	ALA
1	X	329	SER
1	F	215	ALA
1	F	283	ILE
1	K	314	LYS
1	E	352	TRP
1	G	352	TRP
1	I	352	TRP
1	J	352	TRP
1	L	352	TRP
1	M	352	TRP
1	N	314	LYS
1	Q	314	LYS
1	Q	352	TRP
1	S	352	TRP
1	V	352	TRP
1	W	314	LYS
1	W	352	TRP
1	A	352	TRP
1	C	352	TRP
1	D	352	TRP
1	E	314	LYS
1	H	352	TRP
1	K	352	TRP
1	O	352	TRP
1	P	352	TRP
1	Q	219	ALA
1	T	314	LYS
1	U	352	TRP
1	D	215	ALA
1	F	307	ILE
1	R	350	TYR
1	F	172	GLY
1	L	317	ILE

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Mol	Chain	Res	Type
1	X	220	VAL
1	V	220	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	B	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	C	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	D	212/233 (91%)	208 (98%)	4 (2%)	50	67
1	E	212/233 (91%)	208 (98%)	4 (2%)	50	67
1	F	212/233 (91%)	208 (98%)	4 (2%)	50	67
1	G	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	H	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	I	212/233 (91%)	212 (100%)	0	100	100
1	J	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	K	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	L	212/233 (91%)	209 (99%)	3 (1%)	59	71
1	M	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	N	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	O	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	P	212/233 (91%)	209 (99%)	3 (1%)	59	71
1	Q	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	R	212/233 (91%)	207 (98%)	5 (2%)	43	63
1	S	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	T	212/233 (91%)	211 (100%)	1 (0%)	81	80
1	U	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	V	212/233 (91%)	211 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	212/233 (91%)	210 (99%)	2 (1%)	70	76
1	X	212/233 (91%)	208 (98%)	4 (2%)	50	67
All	All	5088/5592 (91%)	5037 (99%)	51 (1%)	68	75

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	B	260	PHE
1	C	260	PHE
1	D	213	LYS
1	D	216	PHE
1	D	220	VAL
1	D	263	LEU
1	E	145	LYS
1	E	216	PHE
1	E	260	PHE
1	E	263	LEU
1	F	260	PHE
1	F	263	LEU
1	F	280	ASN
1	F	282	ASN
1	G	263	LEU
1	G	267	LYS
1	H	260	PHE
1	J	263	LEU
1	K	260	PHE
1	K	263	LEU
1	L	259	LYS
1	L	260	PHE
1	L	263	LEU
1	M	260	PHE
1	M	263	LEU
1	N	260	PHE
1	O	256	GLU
1	O	280	ASN
1	P	216	PHE
1	P	217	THR
1	P	263	LEU
1	Q	260	PHE
1	Q	263	LEU

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Mol	Chain	Res	Type
1	R	227	PHE
1	R	263	LEU
1	R	280	ASN
1	R	336	VAL
1	R	383	LEU
1	S	260	PHE
1	S	263	LEU
1	T	260	PHE
1	U	260	PHE
1	U	280	ASN
1	V	263	LEU
1	W	216	PHE
1	W	263	LEU
1	X	259	LYS
1	X	263	LEU
1	X	281	ARG
1	X	364	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	282	ASN
1	B	323	HIS
1	B	344	GLN
1	C	323	HIS
1	F	322	ASN
1	G	355	ASN
1	H	323	HIS
1	J	195	ASN
1	J	355	ASN
1	L	323	HIS
1	N	323	HIS
1	N	344	GLN
1	O	280	ASN
1	R	322	ASN
1	S	248	GLN
1	W	322	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 20 are monoatomic - leaving 22 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	M	400	3	31,33,33	3.21	12 (38%)	41,52,52	2.50	9 (21%)
2	08T	E	400	3	31,33,33	3.22	12 (38%)	41,52,52	2.49	10 (24%)
2	08T	C	400	3	31,33,33	3.21	12 (38%)	41,52,52	2.49	8 (19%)
2	08T	H	400	1,3	31,33,33	3.27	14 (45%)	41,52,52	2.56	9 (21%)
2	08T	S	400	3	31,33,33	3.22	12 (38%)	41,52,52	2.49	10 (24%)
2	08T	T	400	1,3	31,33,33	3.23	13 (41%)	41,52,52	2.55	9 (21%)
2	08T	K	400	-	31,33,33	3.21	12 (38%)	41,52,52	2.51	10 (24%)
2	08T	I	400	1,3	31,33,33	3.17	12 (38%)	41,52,52	2.48	9 (21%)
2	08T	N	400	1,3	31,33,33	3.23	13 (41%)	41,52,52	2.58	14 (34%)
2	08T	A	400	1,3	31,33,33	3.23	12 (38%)	41,52,52	2.43	10 (24%)
2	08T	Q	400	-	31,33,33	3.20	12 (38%)	41,52,52	2.56	10 (24%)
2	08T	W	400	3	31,33,33	3.21	12 (38%)	41,52,52	2.50	9 (21%)
2	08T	J	400	3	31,33,33	3.20	12 (38%)	41,52,52	2.48	11 (26%)
2	08T	D	400	3	31,33,33	3.22	12 (38%)	41,52,52	2.47	10 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	L	400	-	28,29,29	1.42	5 (17%)	43,45,45	1.88	11 (25%)
2	08T	O	400	3	31,33,33	3.26	13 (41%)	41,52,52	2.49	11 (26%)
2	08T	V	400	3	31,33,33	3.22	12 (38%)	41,52,52	2.48	9 (21%)
2	08T	B	400	3	31,33,33	3.25	13 (41%)	41,52,52	2.53	10 (24%)
2	08T	P	400	3	31,33,33	3.23	12 (38%)	41,52,52	2.51	9 (21%)
2	08T	U	400	1,3	31,33,33	3.21	12 (38%)	41,52,52	2.50	9 (21%)
4	ADP	X	400	-	28,29,29	1.40	5 (17%)	43,45,45	1.88	10 (23%)
2	08T	G	400	3	31,33,33	3.28	12 (38%)	41,52,52	2.56	11 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08T	M	400	3	-	4/16/38/38	0/3/3/3
2	08T	E	400	3	-	1/16/38/38	0/3/3/3
2	08T	C	400	3	-	4/16/38/38	0/3/3/3
2	08T	H	400	1,3	-	3/16/38/38	0/3/3/3
2	08T	S	400	3	-	6/16/38/38	0/3/3/3
2	08T	T	400	1,3	-	5/16/38/38	0/3/3/3
2	08T	K	400	-	-	5/16/38/38	0/3/3/3
2	08T	I	400	1,3	-	3/16/38/38	0/3/3/3
2	08T	N	400	1,3	-	3/16/38/38	0/3/3/3
2	08T	A	400	1,3	-	5/16/38/38	0/3/3/3
2	08T	Q	400	-	-	0/16/38/38	0/3/3/3
2	08T	W	400	3	-	3/16/38/38	0/3/3/3
2	08T	J	400	3	-	9/16/38/38	0/3/3/3
2	08T	D	400	3	-	0/16/38/38	0/3/3/3
4	ADP	L	400	-	-	2/16/32/32	0/3/3/3
2	08T	O	400	3	-	7/16/38/38	0/3/3/3
2	08T	V	400	3	-	4/16/38/38	0/3/3/3
2	08T	B	400	3	-	2/16/38/38	0/3/3/3
2	08T	P	400	3	-	5/16/38/38	0/3/3/3
2	08T	U	400	1,3	-	6/16/38/38	0/3/3/3
4	ADP	X	400	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	08T	G	400	3	-	4/16/38/38	0/3/3/3

All (256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	08T	F2-BE	-8.67	1.34	1.54
2	O	400	08T	F2-BE	-8.51	1.34	1.54
2	H	400	08T	F2-BE	-8.43	1.35	1.54
2	D	400	08T	F2-BE	-8.28	1.35	1.54
2	N	400	08T	F2-BE	-8.25	1.35	1.54
2	I	400	08T	F2-BE	-8.21	1.35	1.54
2	B	400	08T	F2-BE	-8.21	1.35	1.54
2	V	400	08T	F2-BE	-8.21	1.35	1.54
2	P	400	08T	F2-BE	-8.21	1.35	1.54
2	S	400	08T	F2-BE	-8.18	1.35	1.54
2	A	400	08T	F2-BE	-8.18	1.35	1.54
2	J	400	08T	F2-BE	-8.16	1.35	1.54
2	C	400	08T	F2-BE	-8.16	1.35	1.54
2	M	400	08T	F2-BE	-8.16	1.35	1.54
2	T	400	08T	F2-BE	-8.16	1.35	1.54
2	U	400	08T	F2-BE	-8.16	1.35	1.54
2	E	400	08T	F2-BE	-8.12	1.35	1.54
2	Q	400	08T	F2-BE	-8.00	1.36	1.54
2	G	400	08T	F1-BE	-7.95	1.36	1.54
2	K	400	08T	F2-BE	-7.92	1.36	1.54
2	W	400	08T	F2-BE	-7.88	1.36	1.54
2	B	400	08T	F1-BE	-7.73	1.36	1.54
2	A	400	08T	F3-BE	-7.71	1.36	1.54
2	T	400	08T	F1-BE	-7.68	1.36	1.54
2	K	400	08T	F1-BE	-7.64	1.36	1.54
2	O	400	08T	F1-BE	-7.64	1.36	1.54
2	V	400	08T	F1-BE	-7.58	1.36	1.54
2	W	400	08T	F1-BE	-7.57	1.36	1.54
2	D	400	08T	F1-BE	-7.55	1.37	1.54
2	C	400	08T	F1-BE	-7.55	1.37	1.54
2	M	400	08T	F1-BE	-7.55	1.37	1.54
2	Q	400	08T	F1-BE	-7.55	1.37	1.54
2	E	400	08T	F1-BE	-7.54	1.37	1.54
2	P	400	08T	F1-BE	-7.54	1.37	1.54
2	E	400	08T	F3-BE	-7.54	1.37	1.54
2	J	400	08T	F1-BE	-7.53	1.37	1.54
2	U	400	08T	F1-BE	-7.53	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	400	08T	F3-BE	-7.53	1.37	1.54
2	P	400	08T	F3-BE	-7.51	1.37	1.54
2	H	400	08T	F1-BE	-7.50	1.37	1.54
2	O	400	08T	F3-BE	-7.49	1.37	1.54
2	N	400	08T	F1-BE	-7.49	1.37	1.54
2	A	400	08T	F1-BE	-7.47	1.37	1.54
2	J	400	08T	F3-BE	-7.47	1.37	1.54
2	S	400	08T	F1-BE	-7.46	1.37	1.54
2	K	400	08T	F3-BE	-7.46	1.37	1.54
2	I	400	08T	F1-BE	-7.45	1.37	1.54
2	B	400	08T	F3-BE	-7.44	1.37	1.54
2	D	400	08T	F3-BE	-7.44	1.37	1.54
2	S	400	08T	F3-BE	-7.43	1.37	1.54
2	Q	400	08T	F3-BE	-7.42	1.37	1.54
2	M	400	08T	F3-BE	-7.41	1.37	1.54
2	V	400	08T	F3-BE	-7.41	1.37	1.54
2	H	400	08T	F3-BE	-7.41	1.37	1.54
2	C	400	08T	F3-BE	-7.40	1.37	1.54
2	U	400	08T	F3-BE	-7.40	1.37	1.54
2	G	400	08T	F3-BE	-7.39	1.37	1.54
2	N	400	08T	F3-BE	-7.39	1.37	1.54
2	T	400	08T	F3-BE	-7.30	1.37	1.54
2	I	400	08T	F3-BE	-6.99	1.38	1.54
2	N	400	08T	C5-N7	-6.22	1.27	1.39
2	B	400	08T	C5-N7	-6.21	1.27	1.39
2	O	400	08T	C5-N7	-6.21	1.27	1.39
2	W	400	08T	C5-N7	-6.21	1.27	1.39
2	T	400	08T	C5-N7	-6.19	1.27	1.39
2	I	400	08T	C5-N7	-6.18	1.27	1.39
2	C	400	08T	C5-N7	-6.17	1.27	1.39
2	H	400	08T	C5-N7	-6.17	1.27	1.39
2	V	400	08T	C5-N7	-6.14	1.27	1.39
2	K	400	08T	C5-N7	-6.13	1.27	1.39
2	M	400	08T	C5-N7	-6.13	1.27	1.39
2	U	400	08T	C5-N7	-6.13	1.27	1.39
2	P	400	08T	C5-N7	-6.11	1.27	1.39
2	Q	400	08T	C5-N7	-6.11	1.27	1.39
2	A	400	08T	C5-N7	-6.10	1.27	1.39
2	S	400	08T	C5-N7	-6.10	1.27	1.39
2	G	400	08T	C5-N7	-6.07	1.28	1.39
2	E	400	08T	C5-N7	-6.05	1.28	1.39
2	J	400	08T	C5-N7	-6.04	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	08T	C5-N7	-6.02	1.28	1.39
2	O	400	08T	C5-C4	-4.98	1.30	1.39
2	D	400	08T	C5-C4	-4.94	1.30	1.39
2	S	400	08T	C5-C4	-4.94	1.30	1.39
2	P	400	08T	C5-C4	-4.93	1.30	1.39
2	J	400	08T	C5-C4	-4.91	1.30	1.39
2	A	400	08T	C5-C4	-4.90	1.30	1.39
2	M	400	08T	C5-C4	-4.90	1.30	1.39
2	E	400	08T	C5-C4	-4.90	1.30	1.39
2	G	400	08T	C5-C4	-4.89	1.30	1.39
2	B	400	08T	C5-C4	-4.89	1.30	1.39
2	K	400	08T	C5-C4	-4.89	1.30	1.39
2	Q	400	08T	C5-C4	-4.88	1.30	1.39
2	C	400	08T	C5-C4	-4.88	1.30	1.39
2	U	400	08T	C5-C4	-4.88	1.30	1.39
2	T	400	08T	C5-C4	-4.85	1.30	1.39
2	W	400	08T	C5-C4	-4.85	1.30	1.39
2	V	400	08T	C5-C4	-4.83	1.30	1.39
2	H	400	08T	C5-C4	-4.83	1.30	1.39
2	N	400	08T	C5-C4	-4.78	1.30	1.39
2	I	400	08T	C5-C4	-4.77	1.30	1.39
4	L	400	ADP	C5-C4	4.60	1.47	1.39
4	X	400	ADP	C5-C4	4.56	1.47	1.39
2	H	400	08T	O4'-C1'	3.62	1.50	1.42
2	N	400	08T	O4'-C1'	3.58	1.50	1.42
2	P	400	08T	O4'-C1'	3.56	1.50	1.42
2	E	400	08T	O4'-C1'	3.54	1.50	1.42
2	Q	400	08T	O4'-C1'	3.52	1.50	1.42
2	S	400	08T	O4'-C1'	3.52	1.50	1.42
2	D	400	08T	O4'-C1'	3.51	1.50	1.42
2	T	400	08T	O4'-C1'	3.51	1.50	1.42
2	B	400	08T	O4'-C1'	3.50	1.50	1.42
2	N	400	08T	C6-N6	3.47	1.43	1.34
2	A	400	08T	O4'-C1'	3.46	1.50	1.42
2	V	400	08T	C6-N6	3.46	1.43	1.34
2	U	400	08T	O4'-C1'	3.46	1.50	1.42
2	K	400	08T	O4'-C1'	3.45	1.50	1.42
2	I	400	08T	O4'-C1'	3.44	1.50	1.42
2	U	400	08T	C6-N6	3.44	1.43	1.34
2	W	400	08T	O4'-C1'	3.44	1.49	1.42
2	B	400	08T	C6-N6	3.43	1.43	1.34
2	D	400	08T	C6-N6	3.42	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	08T	C6-N6	3.42	1.42	1.34
2	Q	400	08T	C6-N6	3.42	1.42	1.34
2	I	400	08T	C6-N6	3.42	1.42	1.34
2	P	400	08T	C6-N6	3.41	1.42	1.34
2	H	400	08T	C6-N6	3.41	1.42	1.34
2	V	400	08T	O4'-C1'	3.40	1.49	1.42
2	W	400	08T	C6-N6	3.40	1.42	1.34
2	T	400	08T	C6-N6	3.40	1.42	1.34
2	C	400	08T	C6-N6	3.39	1.42	1.34
2	K	400	08T	C6-N6	3.39	1.42	1.34
2	O	400	08T	O4'-C1'	3.39	1.49	1.42
2	G	400	08T	C6-N6	3.39	1.42	1.34
2	S	400	08T	C6-N6	3.38	1.42	1.34
2	M	400	08T	O4'-C1'	3.38	1.49	1.42
2	C	400	08T	O4'-C1'	3.38	1.49	1.42
2	M	400	08T	C6-N6	3.38	1.42	1.34
2	A	400	08T	C6-N6	3.37	1.42	1.34
2	J	400	08T	O4'-C1'	3.34	1.49	1.42
2	J	400	08T	C6-N6	3.33	1.42	1.34
2	I	400	08T	C2'-C3'	-3.32	1.44	1.53
2	G	400	08T	O4'-C1'	3.31	1.49	1.42
2	V	400	08T	C2'-C3'	-3.27	1.44	1.53
2	U	400	08T	C2'-C3'	-3.18	1.44	1.53
2	S	400	08T	C2'-C3'	-3.16	1.44	1.53
2	O	400	08T	C6-N6	3.15	1.42	1.34
2	P	400	08T	C2'-C3'	-3.15	1.44	1.53
2	M	400	08T	C2'-C3'	-3.14	1.44	1.53
2	A	400	08T	C2'-C3'	-3.14	1.44	1.53
2	C	400	08T	C2'-C3'	-3.12	1.44	1.53
2	W	400	08T	C2'-C3'	-3.12	1.44	1.53
2	D	400	08T	C2'-C3'	-3.11	1.44	1.53
2	O	400	08T	C2'-C3'	-3.08	1.45	1.53
2	J	400	08T	C2'-C3'	-3.04	1.45	1.53
2	K	400	08T	C2'-C3'	-3.01	1.45	1.53
2	T	400	08T	C2'-C3'	-3.01	1.45	1.53
2	B	400	08T	C2'-C3'	-2.97	1.45	1.53
2	H	400	08T	C2'-C3'	-2.97	1.45	1.53
2	E	400	08T	C2'-C3'	-2.94	1.45	1.53
2	N	400	08T	C2'-C3'	-2.94	1.45	1.53
2	Q	400	08T	C2'-C3'	-2.93	1.45	1.53
2	G	400	08T	C2'-C3'	-2.90	1.45	1.53
4	L	400	ADP	C5-C6	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	400	ADP	C5-C6	2.70	1.48	1.41
2	U	400	08T	C8-N9	2.53	1.41	1.37
2	K	400	08T	C8-N9	2.52	1.41	1.37
2	H	400	08T	PA-O3A	2.51	1.62	1.59
2	C	400	08T	C8-N9	2.51	1.41	1.37
2	P	400	08T	C8-N9	2.51	1.41	1.37
2	A	400	08T	C8-N9	2.50	1.41	1.37
2	H	400	08T	C2-N3	2.50	1.38	1.33
2	I	400	08T	C8-N9	2.50	1.41	1.37
2	W	400	08T	C8-N9	2.50	1.41	1.37
2	H	400	08T	PB-O3A	2.49	1.62	1.59
2	Q	400	08T	C8-N9	2.47	1.41	1.37
2	V	400	08T	C8-N9	2.46	1.41	1.37
2	T	400	08T	C8-N9	2.46	1.41	1.37
2	D	400	08T	C8-N7	2.45	1.36	1.31
2	M	400	08T	C8-N9	2.44	1.41	1.37
2	J	400	08T	C8-N7	2.43	1.36	1.31
2	H	400	08T	C8-N9	2.43	1.41	1.37
2	A	400	08T	C8-N7	2.43	1.36	1.31
2	I	400	08T	C2-N3	2.43	1.38	1.33
2	O	400	08T	C8-N7	2.42	1.36	1.31
2	U	400	08T	C2-N3	2.42	1.38	1.33
2	Q	400	08T	C8-N7	2.42	1.36	1.31
2	I	400	08T	C8-N7	2.42	1.36	1.31
2	E	400	08T	C8-N7	2.41	1.36	1.31
2	C	400	08T	C8-N7	2.41	1.36	1.31
2	G	400	08T	C8-N7	2.41	1.36	1.31
2	B	400	08T	C8-N7	2.40	1.36	1.31
2	M	400	08T	C8-N7	2.40	1.36	1.31
2	Q	400	08T	C2-N3	2.40	1.38	1.33
2	D	400	08T	C8-N9	2.39	1.41	1.37
2	S	400	08T	C8-N7	2.39	1.36	1.31
4	L	400	ADP	C8-N7	2.39	1.36	1.31
2	K	400	08T	C8-N7	2.38	1.36	1.31
2	T	400	08T	C8-N7	2.38	1.36	1.31
4	X	400	ADP	C8-N7	2.37	1.36	1.31
2	E	400	08T	C8-N9	2.37	1.41	1.37
2	G	400	08T	C8-N9	2.37	1.41	1.37
2	P	400	08T	C2-N3	2.37	1.38	1.33
2	U	400	08T	C8-N7	2.37	1.36	1.31
2	W	400	08T	C2-N3	2.37	1.38	1.33
2	P	400	08T	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	400	08T	C8-N7	2.36	1.36	1.31
2	W	400	08T	C8-N7	2.36	1.36	1.31
2	B	400	08T	C8-N9	2.36	1.41	1.37
2	V	400	08T	C8-N7	2.35	1.36	1.31
2	J	400	08T	C1'-N9	-2.35	1.39	1.46
2	E	400	08T	C2-N3	2.35	1.38	1.33
2	T	400	08T	C2-N3	2.35	1.38	1.33
2	O	400	08T	C1'-N9	-2.34	1.39	1.46
2	N	400	08T	C2-N3	2.34	1.38	1.33
2	K	400	08T	C1'-N9	-2.33	1.39	1.46
2	V	400	08T	C2-N3	2.33	1.38	1.33
2	N	400	08T	C1'-N9	-2.33	1.39	1.46
2	G	400	08T	C2-N3	2.32	1.38	1.33
4	X	400	ADP	C5-N7	-2.32	1.34	1.39
2	K	400	08T	C2-N3	2.32	1.38	1.33
2	B	400	08T	C2-N3	2.31	1.38	1.33
2	N	400	08T	C8-N7	2.31	1.36	1.31
2	S	400	08T	C2-N3	2.31	1.38	1.33
2	G	400	08T	C1'-N9	-2.30	1.40	1.46
2	J	400	08T	C2-N3	2.30	1.38	1.33
2	M	400	08T	C2-N3	2.29	1.38	1.33
4	L	400	ADP	C5-N7	-2.28	1.34	1.39
2	S	400	08T	C8-N9	2.26	1.41	1.37
2	A	400	08T	C1'-N9	-2.26	1.40	1.46
2	C	400	08T	C1'-N9	-2.25	1.40	1.46
2	C	400	08T	C2-N3	2.24	1.37	1.33
2	W	400	08T	C1'-N9	-2.24	1.40	1.46
2	N	400	08T	PB-O3A	2.24	1.61	1.59
2	E	400	08T	C1'-N9	-2.24	1.40	1.46
2	J	400	08T	C8-N9	2.23	1.41	1.37
2	O	400	08T	C2-N3	2.23	1.37	1.33
4	L	400	ADP	PA-O3A	2.23	1.61	1.59
2	A	400	08T	C2-N3	2.23	1.37	1.33
2	S	400	08T	C1'-N9	-2.22	1.40	1.46
2	N	400	08T	PA-O3A	2.21	1.61	1.59
2	B	400	08T	C1'-N9	-2.21	1.40	1.46
2	V	400	08T	C1'-N9	-2.20	1.40	1.46
2	M	400	08T	C1'-N9	-2.19	1.40	1.46
2	D	400	08T	C1'-N9	-2.19	1.40	1.46
2	P	400	08T	C1'-N9	-2.18	1.40	1.46
2	U	400	08T	C1'-N9	-2.17	1.40	1.46
2	D	400	08T	C2-N3	2.17	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	400	08T	C1'-N9	-2.16	1.40	1.46
2	B	400	08T	PB-O3A	2.16	1.61	1.59
2	T	400	08T	PB-O3A	2.15	1.61	1.59
2	I	400	08T	C1'-N9	-2.12	1.40	1.46
2	O	400	08T	C8-N9	2.12	1.41	1.37
2	Q	400	08T	C1'-N9	-2.11	1.40	1.46
2	H	400	08T	C1'-N9	-2.08	1.40	1.46
2	O	400	08T	PB-O3A	2.08	1.61	1.59
4	X	400	ADP	PA-O3A	2.04	1.61	1.59

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	400	08T	C6-C5-N7	-6.99	118.62	132.09
2	H	400	08T	C6-C5-N7	-6.90	118.79	132.09
2	W	400	08T	C6-C5-N7	-6.85	118.89	132.09
2	T	400	08T	C6-C5-N7	-6.83	118.93	132.09
2	U	400	08T	C6-C5-N7	-6.79	119.00	132.09
2	P	400	08T	C6-C5-N7	-6.78	119.01	132.09
2	I	400	08T	C6-C5-N7	-6.75	119.07	132.09
2	O	400	08T	C6-C5-N7	-6.73	119.11	132.09
2	B	400	08T	C6-C5-N7	-6.72	119.13	132.09
2	Q	400	08T	C6-C5-N7	-6.72	119.13	132.09
2	K	400	08T	C6-C5-N7	-6.72	119.14	132.09
2	V	400	08T	C6-C5-N7	-6.71	119.15	132.09
2	C	400	08T	C6-C5-N7	-6.70	119.18	132.09
2	M	400	08T	C6-C5-N7	-6.68	119.22	132.09
2	S	400	08T	C6-C5-N7	-6.64	119.28	132.09
2	G	400	08T	C6-C5-N7	-6.61	119.34	132.09
2	E	400	08T	C6-C5-N7	-6.58	119.41	132.09
2	N	400	08T	C6-C5-C4	6.56	126.13	117.18
2	A	400	08T	C6-C5-N7	-6.55	119.46	132.09
2	D	400	08T	C6-C5-N7	-6.55	119.47	132.09
2	H	400	08T	C6-C5-C4	6.50	126.05	117.18
2	T	400	08T	C6-C5-C4	6.46	126.00	117.18
2	Q	400	08T	C6-C5-C4	6.41	125.92	117.18
2	J	400	08T	C6-C5-N7	-6.40	119.75	132.09
2	H	400	08T	C5-C4-N3	-6.40	117.91	126.72
2	U	400	08T	C6-C5-C4	6.38	125.89	117.18
2	P	400	08T	C6-C5-C4	6.37	125.88	117.18
2	I	400	08T	C6-C5-C4	6.33	125.82	117.18
2	W	400	08T	C6-C5-C4	6.31	125.80	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	400	08T	C6-C5-C4	6.29	125.77	117.18
2	B	400	08T	C6-C5-C4	6.28	125.76	117.18
2	V	400	08T	C6-C5-C4	6.28	125.75	117.18
2	Q	400	08T	C5-C4-N3	-6.27	118.09	126.72
2	C	400	08T	C6-C5-C4	6.25	125.71	117.18
2	K	400	08T	C6-C5-C4	6.24	125.70	117.18
2	T	400	08T	C5-C4-N3	-6.22	118.15	126.72
2	M	400	08T	C6-C5-C4	6.21	125.66	117.18
2	E	400	08T	C6-C5-C4	6.20	125.65	117.18
2	S	400	08T	C6-C5-C4	6.18	125.62	117.18
2	O	400	08T	C5-C4-N3	-6.16	118.24	126.72
2	P	400	08T	C5-C4-N3	-6.14	118.26	126.72
2	G	400	08T	C6-C5-C4	6.14	125.56	117.18
2	U	400	08T	C5-C4-N3	-6.13	118.28	126.72
2	D	400	08T	C6-C5-C4	6.13	125.55	117.18
2	N	400	08T	C5-C4-N3	-6.09	118.33	126.72
2	I	400	08T	C5-C4-N3	-6.07	118.36	126.72
2	A	400	08T	C6-C5-C4	6.07	125.47	117.18
2	E	400	08T	C5-C4-N3	-6.03	118.42	126.72
2	J	400	08T	C6-C5-C4	6.02	125.39	117.18
2	B	400	08T	C5-C4-N3	-6.01	118.44	126.72
2	W	400	08T	C5-C4-N3	-5.97	118.49	126.72
2	C	400	08T	C5-C4-N3	-5.97	118.50	126.72
2	K	400	08T	C5-C4-N3	-5.95	118.52	126.72
2	V	400	08T	C5-C4-N3	-5.95	118.52	126.72
2	S	400	08T	C5-C4-N3	-5.92	118.56	126.72
2	M	400	08T	C5-C4-N3	-5.86	118.64	126.72
4	X	400	ADP	C5-C4-N3	-5.86	118.65	126.72
2	G	400	08T	C5-C4-N3	-5.83	118.69	126.72
2	D	400	08T	C5-C4-N3	-5.78	118.77	126.72
2	A	400	08T	C5-C4-N3	-5.77	118.77	126.72
4	L	400	ADP	C5-C4-N3	-5.75	118.80	126.72
2	B	400	08T	N3-C2-N1	-5.71	119.94	128.58
2	D	400	08T	N3-C2-N1	-5.71	119.95	128.58
2	A	400	08T	N3-C2-N1	-5.70	119.95	128.58
2	G	400	08T	N3-C2-N1	-5.69	119.96	128.58
2	H	400	08T	N3-C2-N1	-5.66	120.01	128.58
2	P	400	08T	N3-C2-N1	-5.66	120.01	128.58
2	J	400	08T	N3-C2-N1	-5.66	120.02	128.58
2	J	400	08T	C5-C4-N3	-5.65	118.94	126.72
2	E	400	08T	N3-C2-N1	-5.65	120.03	128.58
2	S	400	08T	N3-C2-N1	-5.64	120.04	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	400	08T	N3-C2-N1	-5.63	120.06	128.58
2	M	400	08T	N3-C2-N1	-5.62	120.07	128.58
2	W	400	08T	N3-C2-N1	-5.61	120.08	128.58
2	C	400	08T	N3-C2-N1	-5.61	120.09	128.58
2	T	400	08T	N3-C2-N1	-5.61	120.09	128.58
2	K	400	08T	N3-C2-N1	-5.60	120.11	128.58
2	I	400	08T	N3-C2-N1	-5.59	120.12	128.58
2	V	400	08T	N3-C2-N1	-5.59	120.12	128.58
2	Q	400	08T	N3-C2-N1	-5.52	120.23	128.58
2	N	400	08T	N3-C2-N1	-5.52	120.23	128.58
2	O	400	08T	N3-C2-N1	-5.33	120.52	128.58
2	H	400	08T	N3-C4-N9	5.10	135.84	127.17
2	N	400	08T	N3-C4-N9	4.97	135.63	127.17
2	T	400	08T	N3-C4-N9	4.93	135.55	127.17
2	G	400	08T	N9-C8-N7	-4.91	106.97	113.94
2	O	400	08T	N3-C4-N9	4.89	135.48	127.17
2	P	400	08T	N3-C4-N9	4.89	135.48	127.17
2	Q	400	08T	N3-C4-N9	4.88	135.46	127.17
2	J	400	08T	N9-C8-N7	-4.88	107.02	113.94
2	C	400	08T	N9-C8-N7	-4.85	107.06	113.94
2	U	400	08T	N3-C4-N9	4.84	135.40	127.17
2	W	400	08T	N3-C4-N9	4.84	135.39	127.17
2	A	400	08T	N9-C8-N7	-4.83	107.08	113.94
2	I	400	08T	N3-C4-N9	4.83	135.38	127.17
2	D	400	08T	N9-C8-N7	-4.83	107.09	113.94
2	K	400	08T	N9-C8-N7	-4.81	107.12	113.94
2	P	400	08T	N9-C8-N7	-4.79	107.14	113.94
2	V	400	08T	N9-C8-N7	-4.77	107.16	113.94
2	E	400	08T	N9-C8-N7	-4.76	107.18	113.94
2	M	400	08T	N9-C8-N7	-4.76	107.18	113.94
2	V	400	08T	N3-C4-N9	4.75	135.24	127.17
2	W	400	08T	N9-C8-N7	-4.75	107.20	113.94
2	I	400	08T	N9-C8-N7	-4.74	107.21	113.94
2	T	400	08T	N9-C8-N7	-4.74	107.22	113.94
2	B	400	08T	N3-C4-N9	4.73	135.22	127.17
2	C	400	08T	N3-C4-N9	4.73	135.22	127.17
2	K	400	08T	N3-C4-N9	4.73	135.21	127.17
2	Q	400	08T	N9-C8-N7	-4.72	107.24	113.94
2	E	400	08T	N3-C4-N9	4.72	135.19	127.17
2	U	400	08T	N9-C8-N7	-4.71	107.25	113.94
2	G	400	08T	N3-C4-N9	4.71	135.17	127.17
2	B	400	08T	N9-C8-N7	-4.69	107.29	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	400	08T	N9-C8-N7	-4.67	107.32	113.94
4	X	400	ADP	N3-C4-N9	4.65	135.08	127.17
2	M	400	08T	N3-C4-N9	4.64	135.06	127.17
2	S	400	08T	N3-C4-N9	4.61	135.01	127.17
2	H	400	08T	N9-C8-N7	-4.59	107.43	113.94
2	S	400	08T	N9-C8-N7	-4.55	107.48	113.94
2	A	400	08T	N3-C4-N9	4.53	134.88	127.17
2	D	400	08T	N3-C4-N9	4.51	134.83	127.17
4	L	400	ADP	N3-C4-N9	4.48	134.78	127.17
2	J	400	08T	N3-C4-N9	4.44	134.71	127.17
2	N	400	08T	N9-C8-N7	-4.34	107.77	113.94
2	W	400	08T	C4-C5-N7	4.14	115.31	110.58
2	N	400	08T	C4-C5-N7	4.08	115.25	110.58
2	K	400	08T	C4-C5-N7	4.01	115.16	110.58
2	H	400	08T	C4-C5-N7	4.00	115.16	110.58
2	O	400	08T	C4-C5-N7	3.98	115.13	110.58
2	M	400	08T	C4-C5-N7	3.97	115.12	110.58
2	B	400	08T	C4-C5-N7	3.96	115.11	110.58
2	I	400	08T	C4-C5-N7	3.96	115.11	110.58
2	P	400	08T	C4-C5-N7	3.96	115.11	110.58
2	U	400	08T	C4-C5-N7	3.96	115.11	110.58
2	C	400	08T	C4-C5-N7	3.96	115.11	110.58
2	V	400	08T	C4-C5-N7	3.95	115.10	110.58
2	G	400	08T	C4-C5-N7	3.95	115.09	110.58
2	S	400	08T	C4-C5-N7	3.95	115.09	110.58
2	A	400	08T	C4-C5-N7	3.93	115.07	110.58
2	T	400	08T	C4-C5-N7	3.92	115.07	110.58
4	X	400	ADP	C2-N3-C4	3.86	121.26	111.83
2	D	400	08T	C4-C5-N7	3.85	114.99	110.58
4	L	400	ADP	C2-N3-C4	3.82	121.15	111.83
2	Q	400	08T	C4-C5-N7	3.81	114.94	110.58
2	E	400	08T	C4-C5-N7	3.81	114.94	110.58
2	J	400	08T	C4-C5-N7	3.74	114.86	110.58
4	X	400	ADP	N3-C2-N1	-3.65	123.05	128.58
4	L	400	ADP	N3-C2-N1	-3.64	123.07	128.58
4	L	400	ADP	C4-C5-N7	-3.63	106.44	110.58
4	X	400	ADP	C4-C5-N7	-3.45	106.64	110.58
2	Q	400	08T	C3'-C2'-C1'	3.38	107.86	101.46
2	G	400	08T	C3'-C2'-C1'	3.27	107.65	101.46
2	H	400	08T	C2-N3-C4	3.19	119.63	111.83
2	Q	400	08T	C2-N3-C4	3.18	119.60	111.83
2	P	400	08T	C2-N3-C4	3.13	119.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	400	08T	C2-N3-C4	3.13	119.47	111.83
2	E	400	08T	C2-N3-C4	3.11	119.43	111.83
2	U	400	08T	C2-N3-C4	3.11	119.43	111.83
2	B	400	08T	C2-N3-C4	3.11	119.42	111.83
2	I	400	08T	C2-N3-C4	3.07	119.34	111.83
2	K	400	08T	C2-N3-C4	3.07	119.33	111.83
2	S	400	08T	C2-N3-C4	3.07	119.32	111.83
2	A	400	08T	C2-N3-C4	3.05	119.29	111.83
2	D	400	08T	C2-N3-C4	3.05	119.28	111.83
2	W	400	08T	C2-N3-C4	3.05	119.28	111.83
2	C	400	08T	C2-N3-C4	3.05	119.27	111.83
2	V	400	08T	C2-N3-C4	3.04	119.25	111.83
2	N	400	08T	C2-N3-C4	3.03	119.23	111.83
2	G	400	08T	C2-N3-C4	3.03	119.22	111.83
2	M	400	08T	C2-N3-C4	3.02	119.22	111.83
2	O	400	08T	C2-N3-C4	3.02	119.21	111.83
2	J	400	08T	C2-N3-C4	3.00	119.15	111.83
2	J	400	08T	C3'-C2'-C1'	2.78	106.73	101.46
4	L	400	ADP	C5-N7-C8	2.78	107.81	103.45
4	X	400	ADP	C4-N9-C8	2.76	108.64	105.74
2	B	400	08T	C3'-C2'-C1'	2.75	106.67	101.46
4	X	400	ADP	C5-N7-C8	2.75	107.77	103.45
2	M	400	08T	C3'-C2'-C1'	2.73	106.63	101.46
4	L	400	ADP	C4-N9-C8	2.69	108.57	105.74
2	T	400	08T	C3'-C2'-C1'	2.65	106.47	101.46
2	G	400	08T	C2'-C3'-C4'	2.58	107.59	102.61
2	N	400	08T	C3'-C2'-C1'	2.58	106.33	101.46
4	X	400	ADP	C3'-C2'-C1'	2.56	106.31	101.46
2	S	400	08T	C3'-C2'-C1'	2.56	106.30	101.46
2	J	400	08T	C4'-O4'-C1'	-2.55	103.84	109.47
2	E	400	08T	C3'-C2'-C1'	2.53	106.25	101.46
2	D	400	08T	C4'-O4'-C1'	-2.46	104.02	109.47
4	L	400	ADP	C3'-C2'-C1'	2.46	106.12	101.46
2	E	400	08T	C4'-O4'-C1'	-2.46	104.04	109.47
2	D	400	08T	C3'-C2'-C1'	2.44	106.08	101.46
2	O	400	08T	C4'-O4'-C1'	-2.42	104.11	109.47
2	K	400	08T	C3'-C2'-C1'	2.42	106.03	101.46
2	N	400	08T	C4'-O4'-C1'	-2.41	104.15	109.47
2	N	400	08T	C4-N9-C1'	2.40	132.26	126.63
2	Q	400	08T	C2'-C3'-C4'	2.39	107.22	102.61
2	G	400	08T	C4'-O4'-C1'	-2.34	104.30	109.47
4	X	400	ADP	N9-C8-N7	-2.29	110.69	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	400	08T	C4'-O4'-C1'	-2.28	104.44	109.47
2	O	400	08T	C3'-C2'-C1'	2.27	105.76	101.46
4	L	400	ADP	N9-C8-N7	-2.24	110.76	113.94
2	J	400	08T	C2'-C3'-C4'	2.19	106.84	102.61
4	L	400	ADP	C6-C5-N7	2.17	136.28	132.09
2	P	400	08T	C4'-O4'-C1'	-2.16	104.69	109.47
2	S	400	08T	C4'-O4'-C1'	-2.12	104.78	109.47
2	B	400	08T	C4'-O4'-C1'	-2.11	104.80	109.47
4	X	400	ADP	C6-C5-N7	2.11	136.15	132.09
2	V	400	08T	C4'-O4'-C1'	-2.10	104.83	109.47
4	L	400	ADP	C2-N1-C6	2.09	122.17	118.73
2	H	400	08T	C3'-C2'-C1'	2.09	105.42	101.46
2	N	400	08T	C2'-C1'-N9	-2.09	108.12	113.30
2	A	400	08T	C4'-O4'-C1'	-2.08	104.88	109.47
2	K	400	08T	N6-C6-N1	2.08	123.00	118.38
2	W	400	08T	N6-C6-N1	2.05	122.94	118.38
2	O	400	08T	C2'-C1'-N9	-2.02	108.28	113.30
2	N	400	08T	C1'-N9-C8	-2.02	122.61	127.09
2	N	400	08T	N6-C6-N1	2.01	122.86	118.38
2	A	400	08T	C3'-C2'-C1'	2.01	105.27	101.46
2	U	400	08T	N6-C6-N1	2.00	122.83	118.38

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	08T	O4'-C4'-C5'-O5'
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	J	400	08T	C5'-O5'-PA-O2A
2	J	400	08T	C5'-O5'-PA-O3A
2	M	400	08T	C5'-O5'-PA-O1A
2	M	400	08T	C5'-O5'-PA-O3A
2	O	400	08T	C5'-O5'-PA-O2A
2	O	400	08T	C5'-O5'-PA-O3A
2	O	400	08T	O4'-C4'-C5'-O5'
2	S	400	08T	C5'-O5'-PA-O1A
2	S	400	08T	C5'-O5'-PA-O2A
2	S	400	08T	C5'-O5'-PA-O3A
2	T	400	08T	C5'-O5'-PA-O1A
2	T	400	08T	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	T	400	08T	C5'-O5'-PA-O3A
4	L	400	ADP	C5'-O5'-PA-O1A
2	C	400	08T	C3'-C4'-C5'-O5'
2	S	400	08T	C3'-C4'-C5'-O5'
2	A	400	08T	C3'-C4'-C5'-O5'
2	C	400	08T	O4'-C4'-C5'-O5'
2	I	400	08T	O4'-C4'-C5'-O5'
2	I	400	08T	C3'-C4'-C5'-O5'
2	O	400	08T	C3'-C4'-C5'-O5'
2	P	400	08T	C3'-C4'-C5'-O5'
2	S	400	08T	O4'-C4'-C5'-O5'
2	U	400	08T	O4'-C4'-C5'-O5'
2	U	400	08T	C3'-C4'-C5'-O5'
2	W	400	08T	O4'-C4'-C5'-O5'
2	W	400	08T	C3'-C4'-C5'-O5'
2	M	400	08T	O4'-C4'-C5'-O5'
2	M	400	08T	C3'-C4'-C5'-O5'
2	P	400	08T	O4'-C4'-C5'-O5'
2	K	400	08T	O4'-C4'-C5'-O5'
2	V	400	08T	O4'-C4'-C5'-O5'
2	J	400	08T	O4'-C4'-C5'-O5'
2	V	400	08T	C3'-C4'-C5'-O5'
2	K	400	08T	C3'-C4'-C5'-O5'
2	J	400	08T	PA-O3A-PB-O1B
2	U	400	08T	PB-O3A-PA-O2A
2	J	400	08T	C4'-C5'-O5'-PA
2	J	400	08T	PB-O3A-PA-O5'
2	H	400	08T	O4'-C4'-C5'-O5'
2	J	400	08T	C3'-C4'-C5'-O5'
4	X	400	ADP	PA-O3A-PB-O1B
2	P	400	08T	PB-O3A-PA-O1A
2	A	400	08T	C5'-O5'-PA-O1A
2	A	400	08T	C5'-O5'-PA-O2A
2	A	400	08T	C5'-O5'-PA-O3A
2	J	400	08T	C5'-O5'-PA-O1A
2	U	400	08T	C5'-O5'-PA-O2A
2	N	400	08T	PB-O3A-PA-O1A
2	O	400	08T	PB-O3A-PA-O1A
2	H	400	08T	C3'-C4'-C5'-O5'
2	U	400	08T	C4'-C5'-O5'-PA
4	X	400	ADP	O4'-C4'-C5'-O5'
2	I	400	08T	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	O	400	08T	C4'-C5'-O5'-PA
2	B	400	08T	C4'-C5'-O5'-PA
2	N	400	08T	C4'-C5'-O5'-PA
2	P	400	08T	C4'-C5'-O5'-PA
2	C	400	08T	C4'-C5'-O5'-PA
2	H	400	08T	C4'-C5'-O5'-PA
2	K	400	08T	C4'-C5'-O5'-PA
4	X	400	ADP	PA-O3A-PB-O2B
4	X	400	ADP	PA-O3A-PB-O3B
2	C	400	08T	PB-O3A-PA-O2A
2	E	400	08T	PB-O3A-PA-O1A
2	J	400	08T	PB-O3A-PA-O2A
2	K	400	08T	PB-O3A-PA-O1A
2	N	400	08T	PB-O3A-PA-O2A
2	O	400	08T	PB-O3A-PA-O2A
2	P	400	08T	PB-O3A-PA-O2A
2	U	400	08T	PB-O3A-PA-O1A
2	V	400	08T	PB-O3A-PA-O1A
2	V	400	08T	PA-O3A-PB-O2B
4	L	400	ADP	C3'-C4'-C5'-O5'
2	B	400	08T	O4'-C4'-C5'-O5'
2	G	400	08T	PA-O3A-PB-O3B
2	T	400	08T	PA-O3A-PB-O3B
2	T	400	08T	C4'-C5'-O5'-PA
2	W	400	08T	C4'-C5'-O5'-PA
2	K	400	08T	PB-O3A-PA-O2A
2	S	400	08T	PA-O3A-PB-O2B

There are no ring outliers.

17 monomers are involved in 41 short contacts:

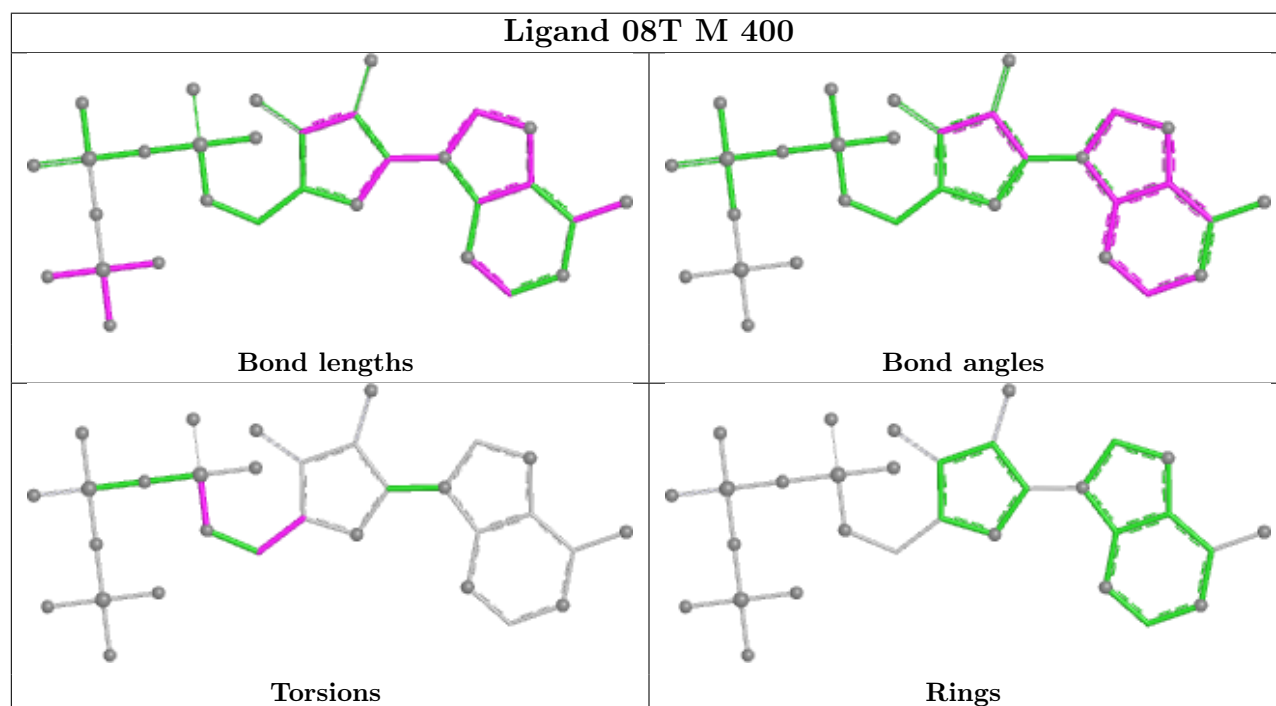
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	400	08T	2	0
2	E	400	08T	2	0
2	H	400	08T	1	0
2	S	400	08T	2	0
2	T	400	08T	1	0
2	K	400	08T	1	0
2	N	400	08T	4	0
2	A	400	08T	2	0
2	W	400	08T	2	0
2	J	400	08T	2	0

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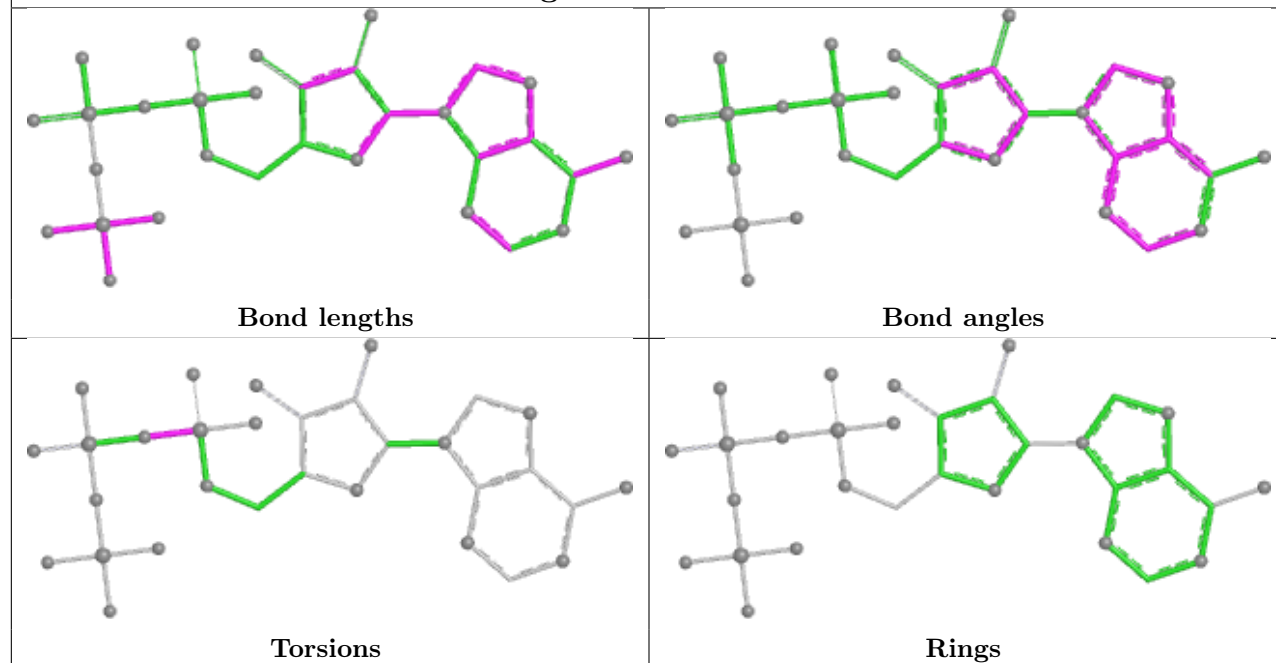
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	08T	3	0
4	L	400	ADP	3	0
2	O	400	08T	7	0
2	B	400	08T	1	0
2	P	400	08T	2	0
4	X	400	ADP	2	0
2	G	400	08T	4	0

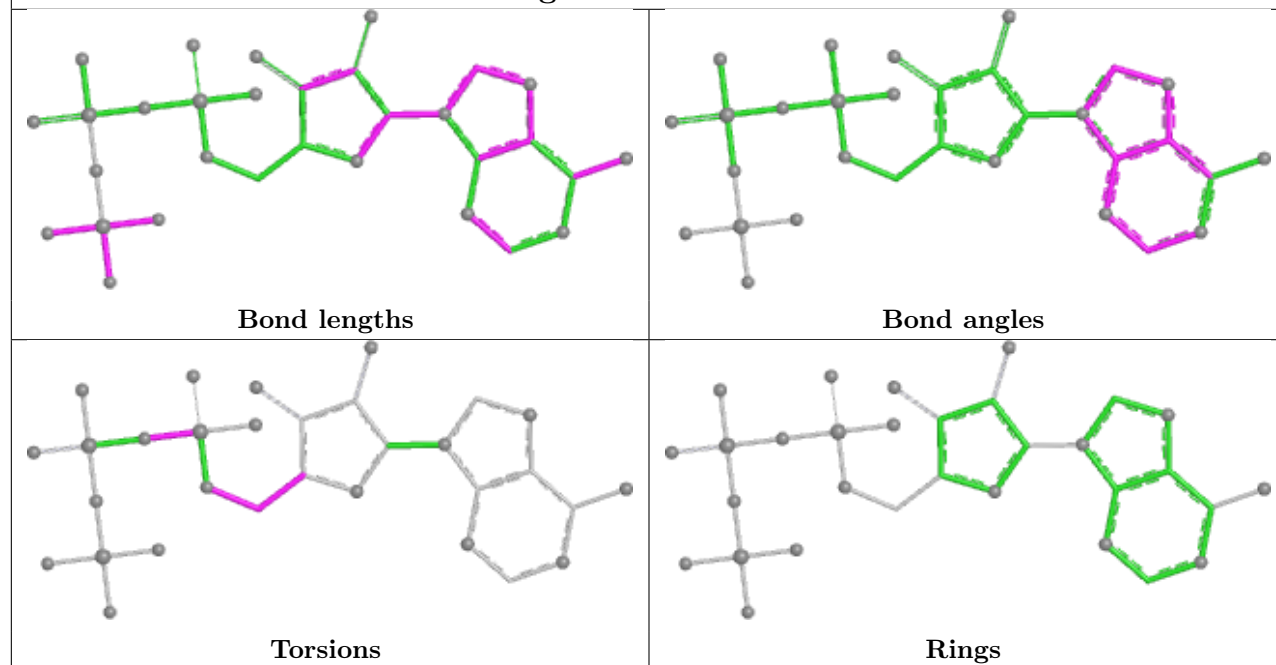
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



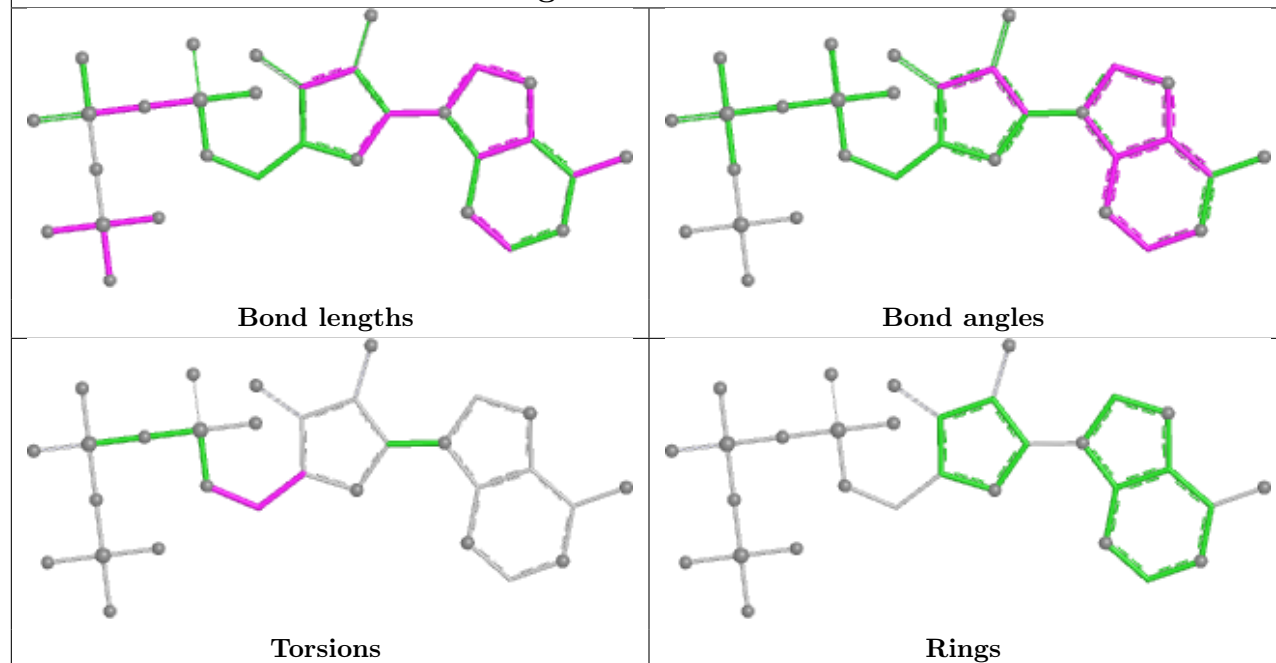
Ligand 08T E 400



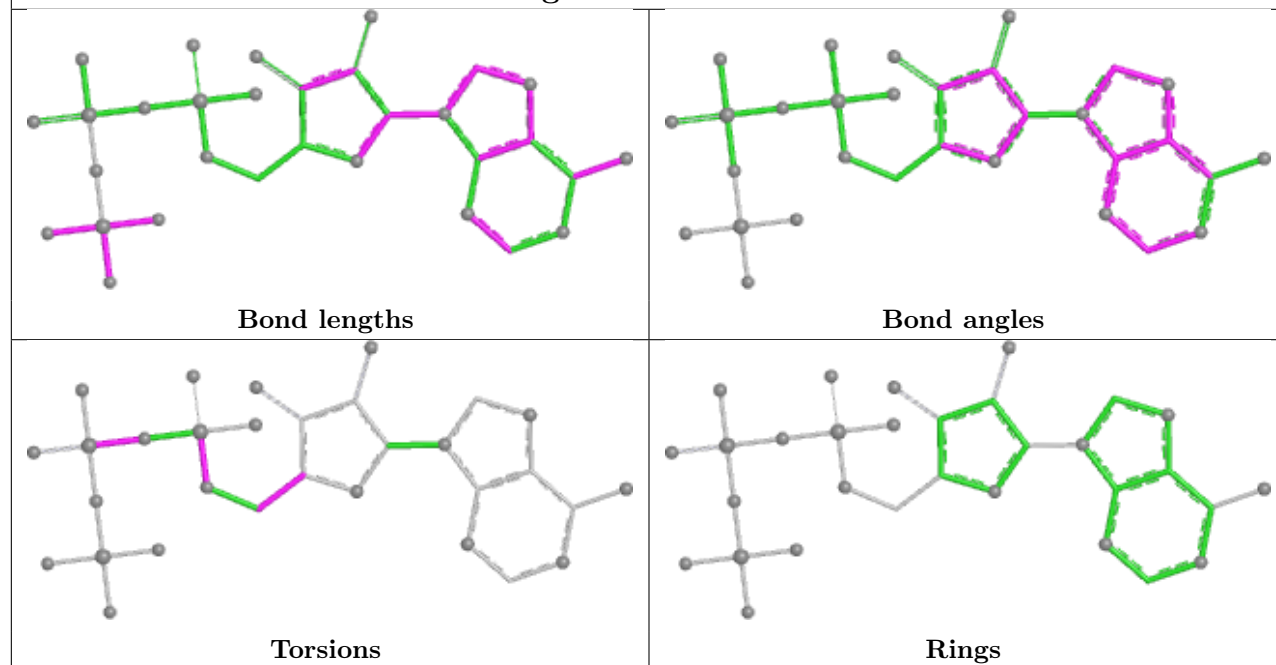
Ligand 08T C 400



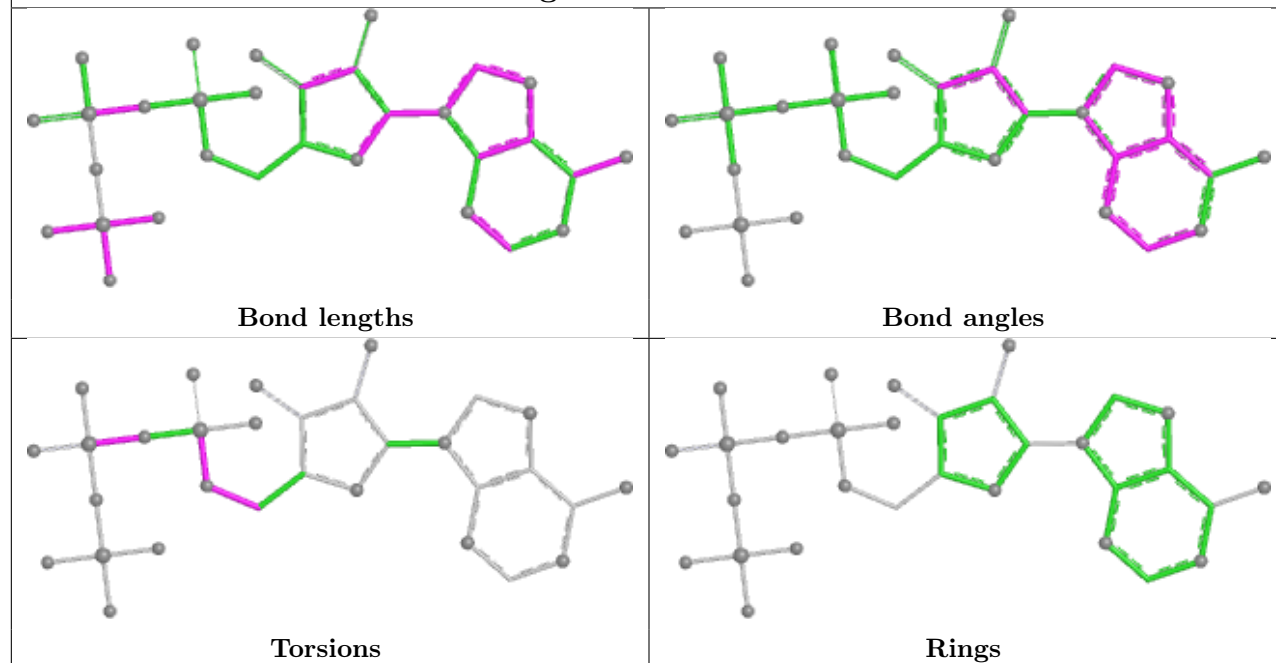
Ligand 08T H 400



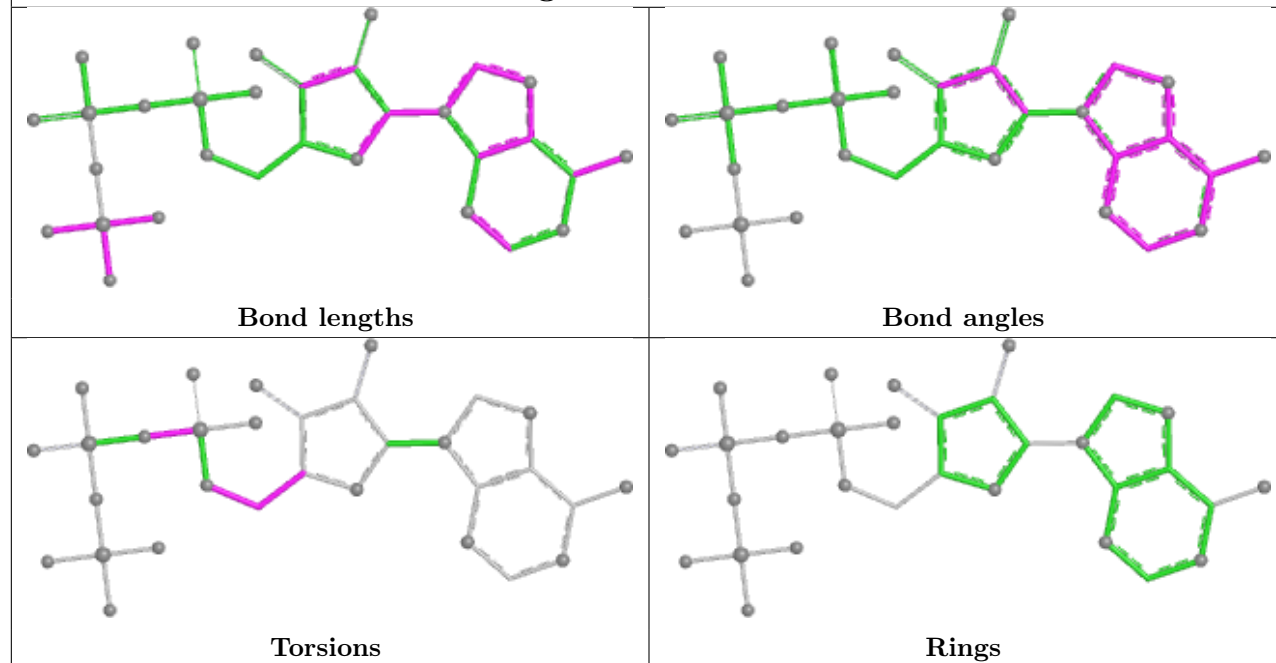
Ligand 08T S 400



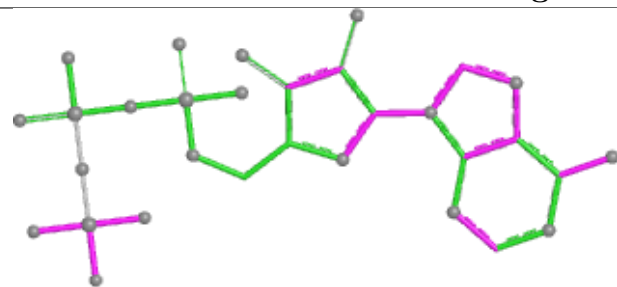
Ligand 08T T 400



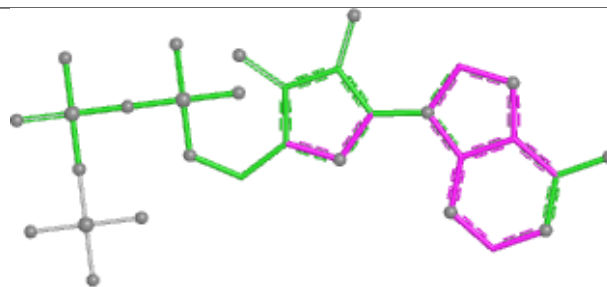
Ligand 08T K 400



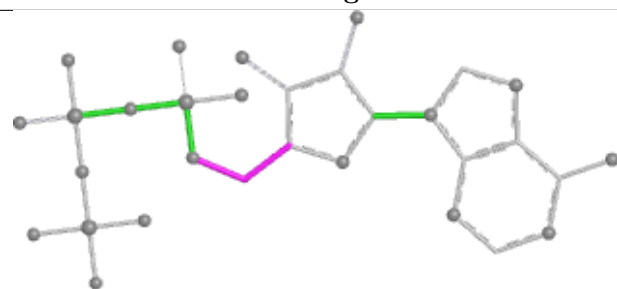
Ligand 08T I 400



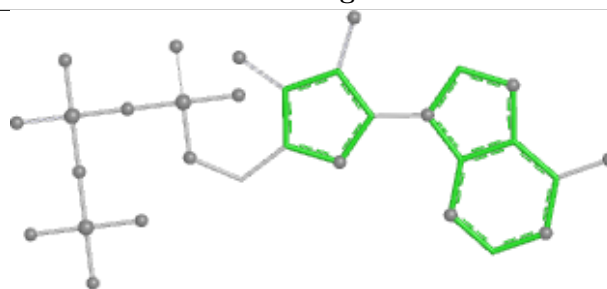
Bond lengths



Bond angles

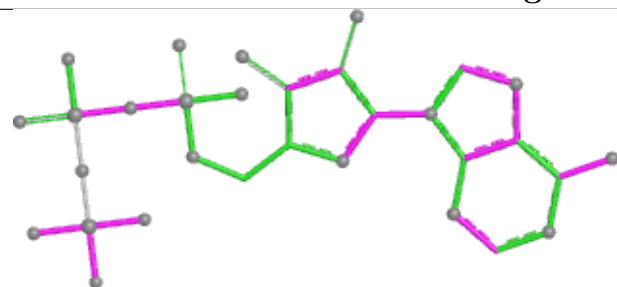


Torsions

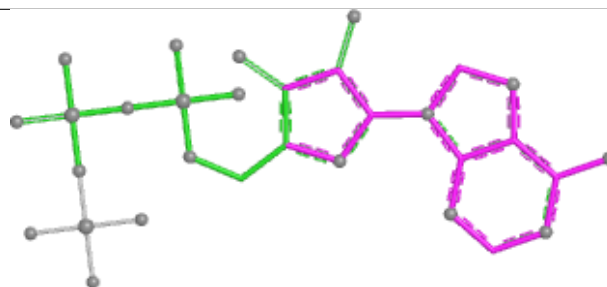


Rings

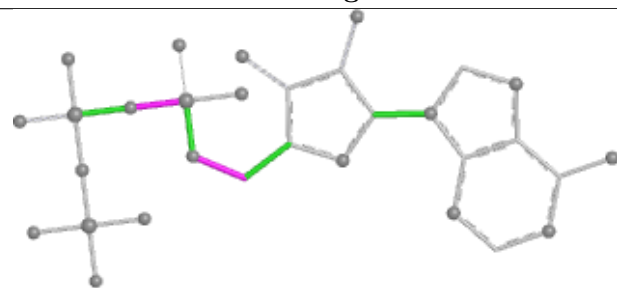
Ligand 08T N 400



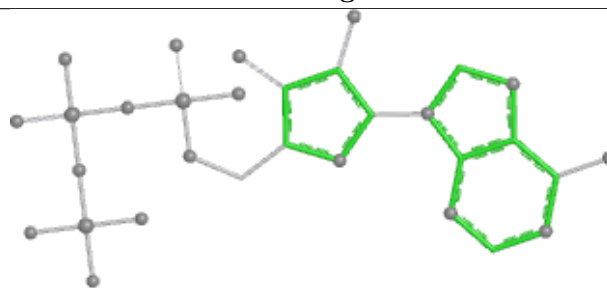
Bond lengths



Bond angles

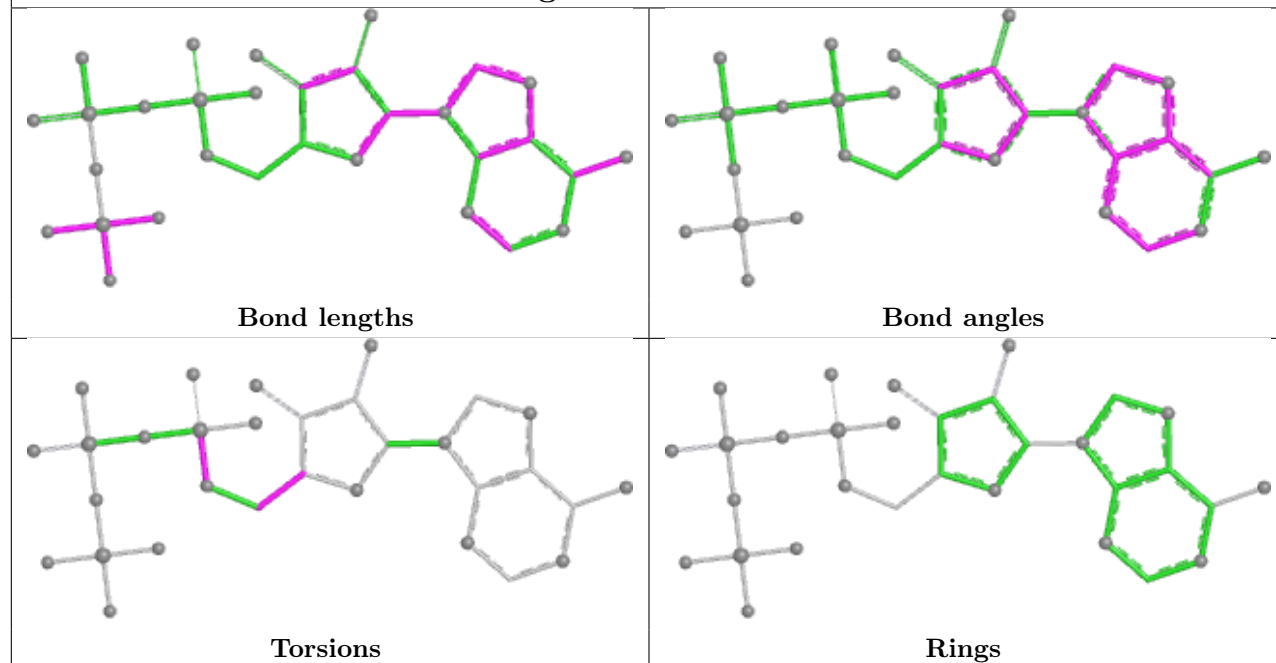


Torsions

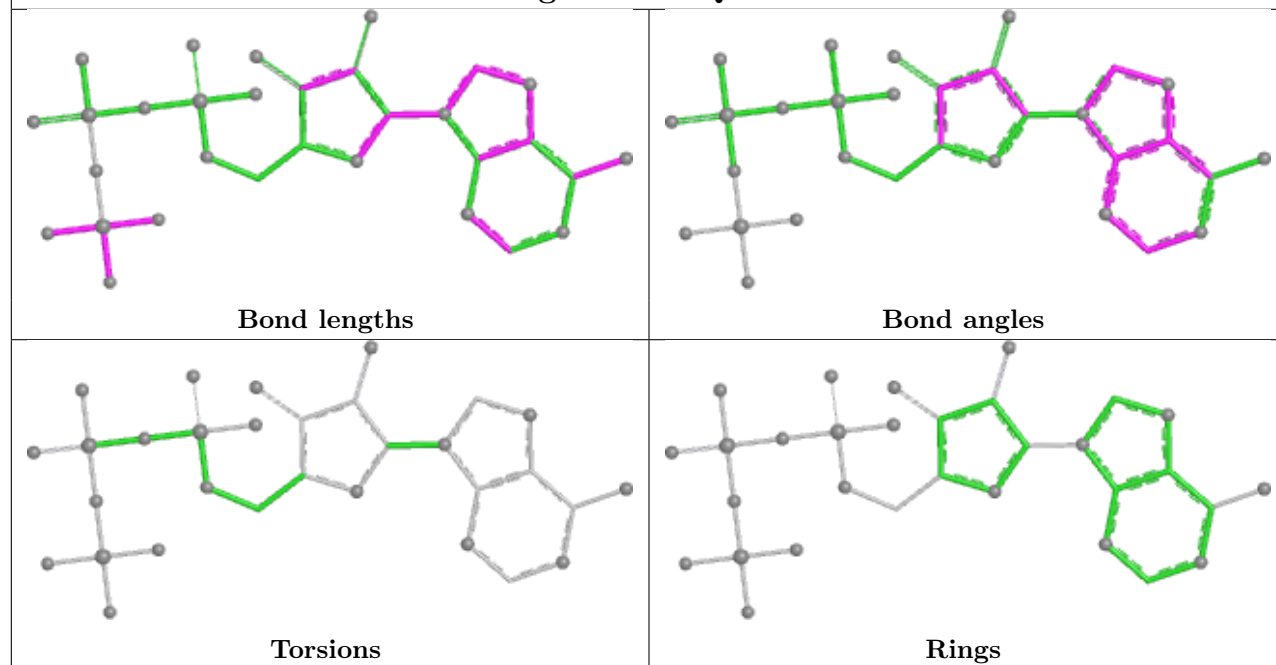


Rings

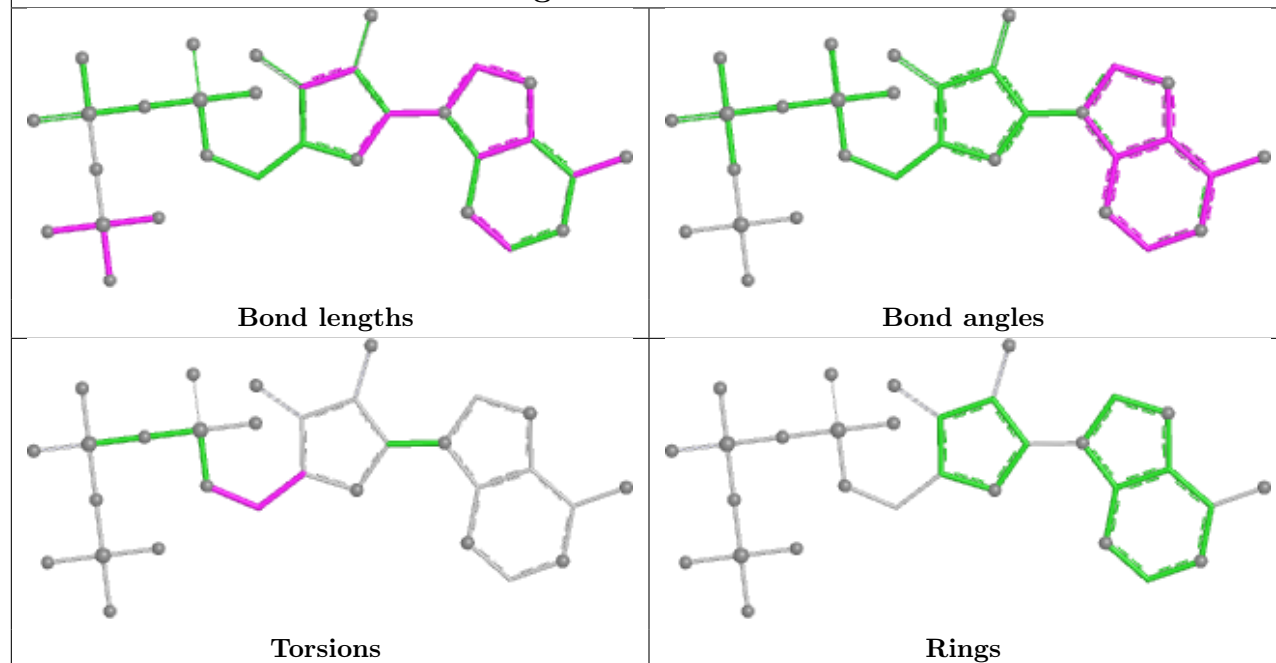
Ligand 08T A 400



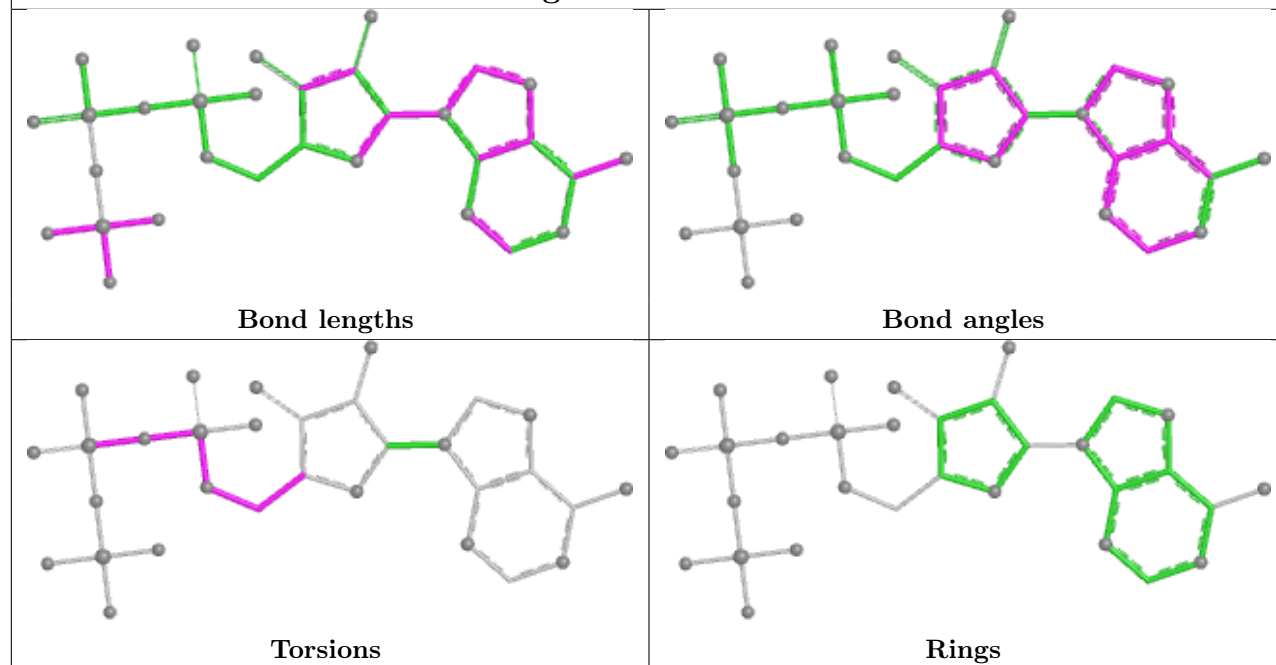
Ligand 08T Q 400



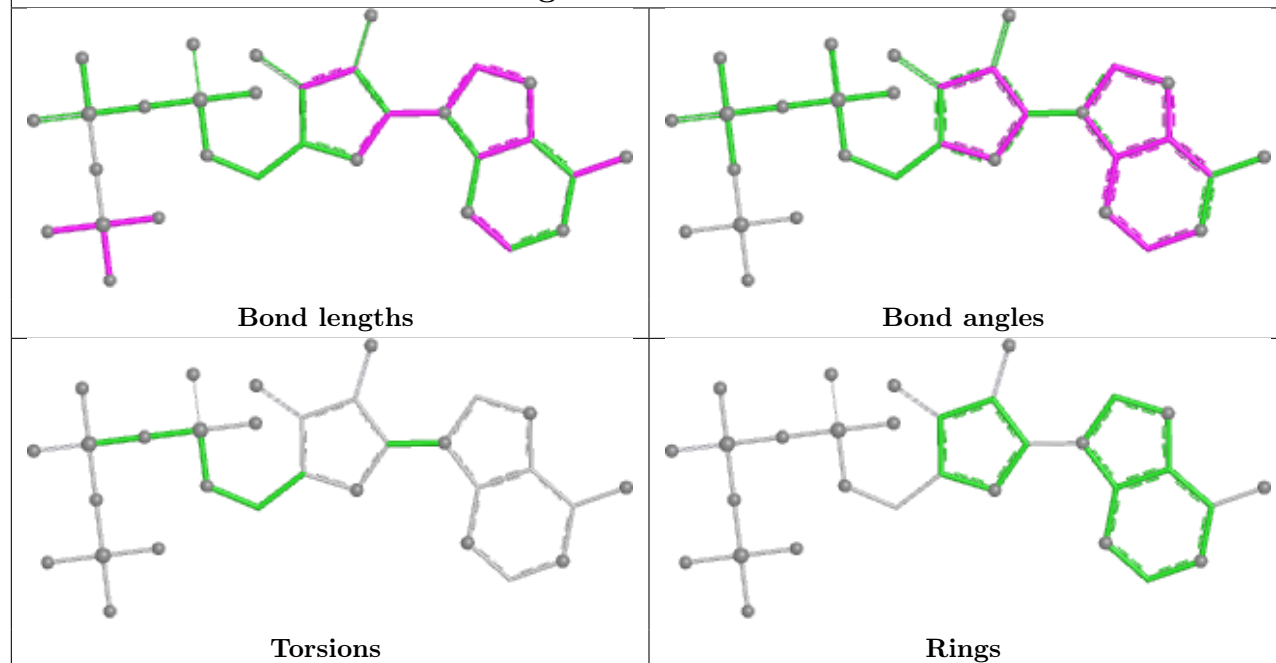
Ligand 08T W 400



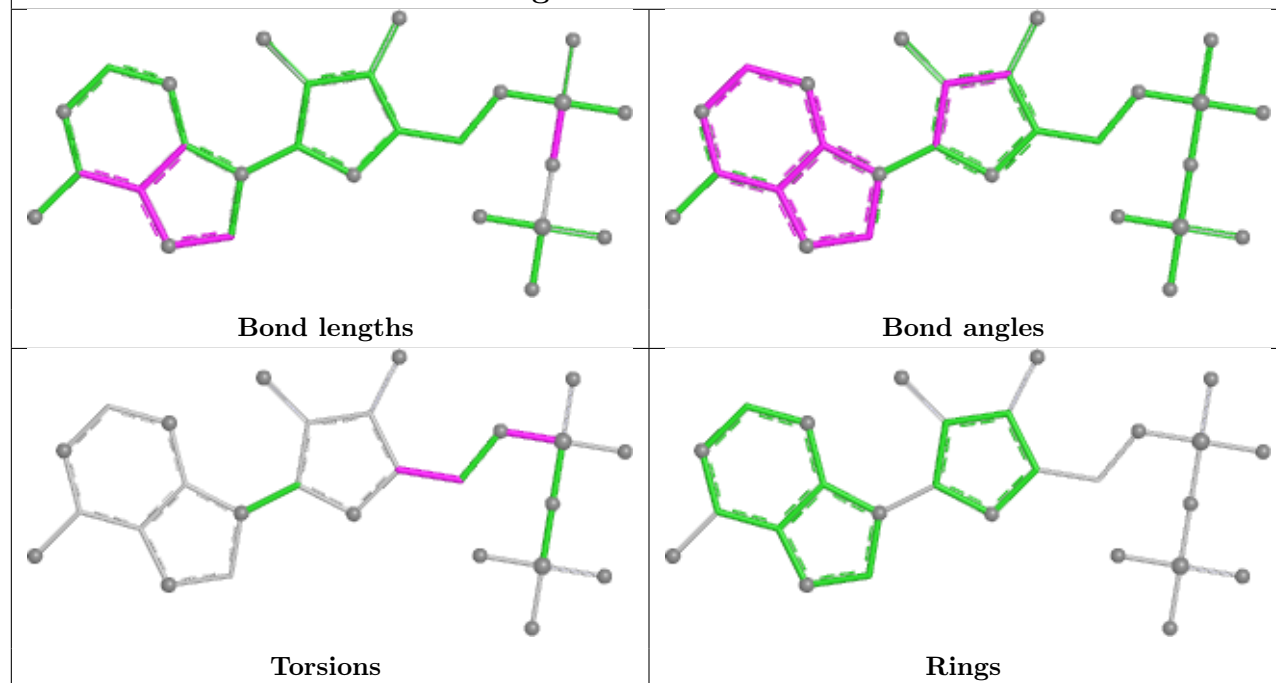
Ligand 08T J 400



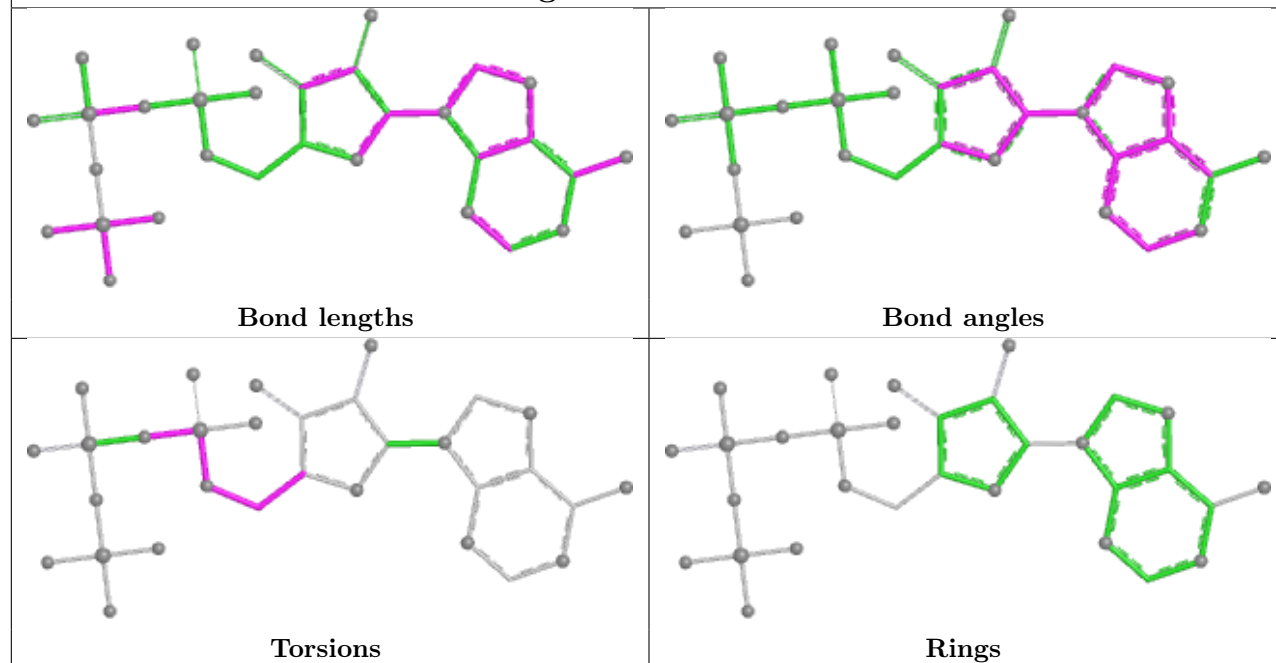
Ligand 08T D 400



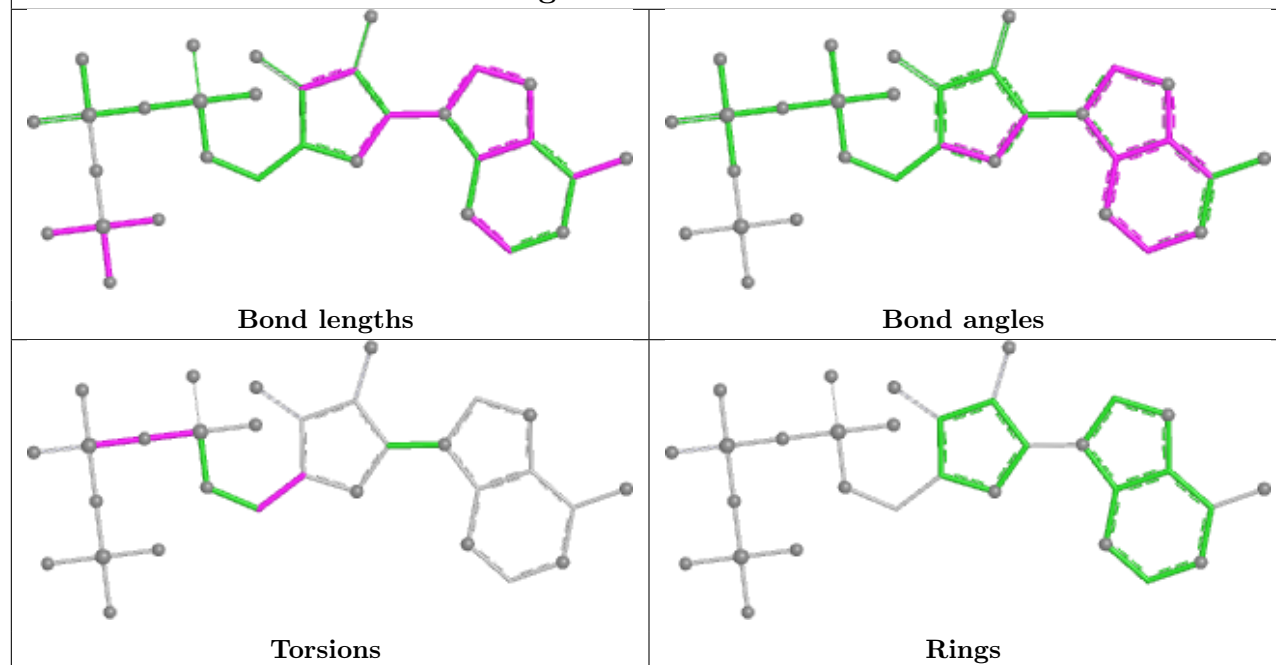
Ligand ADP L 400



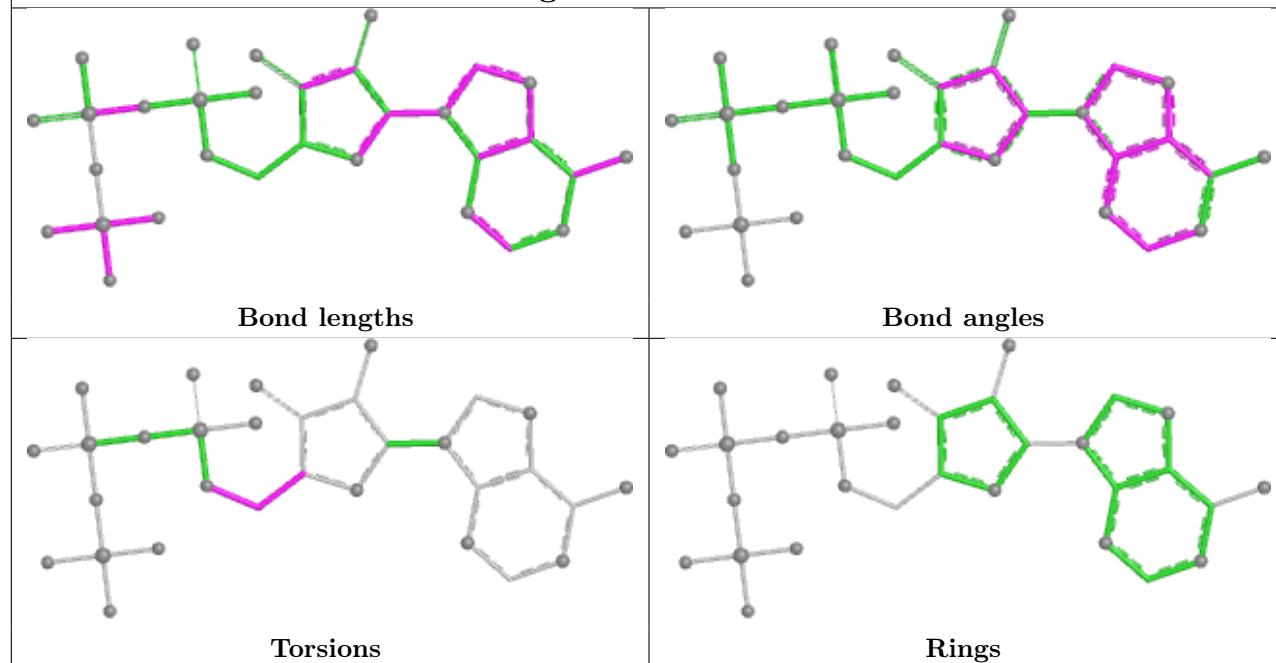
Ligand 08T O 400



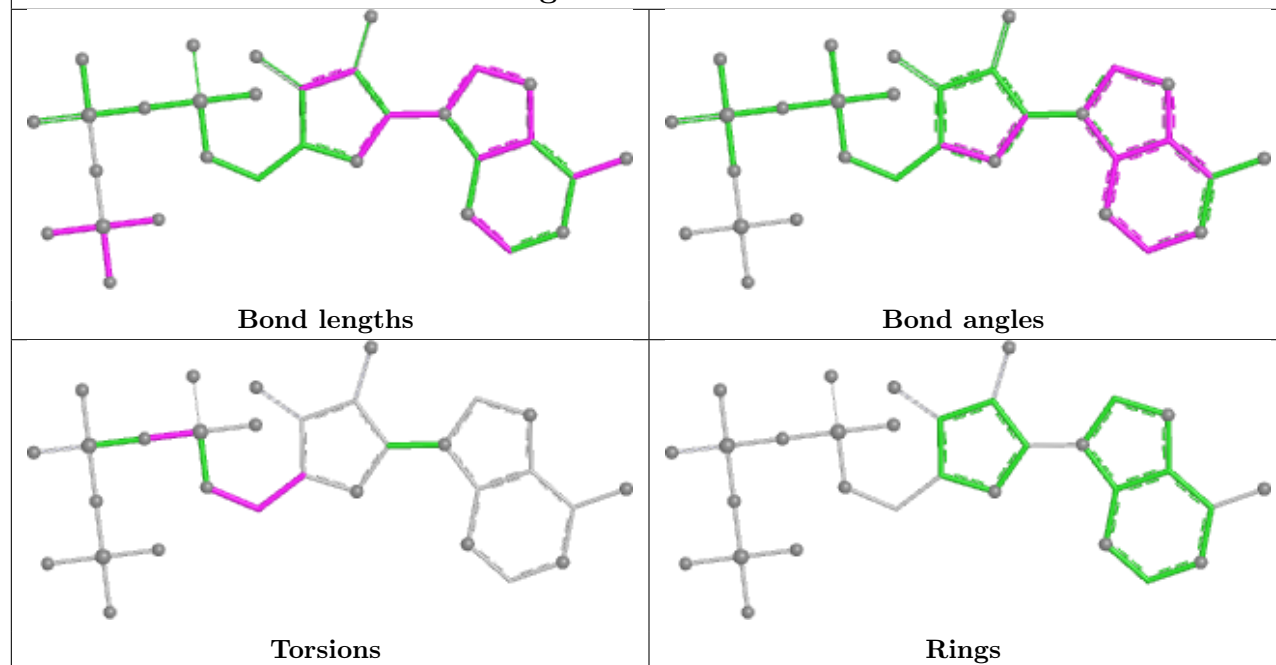
Ligand 08T V 400



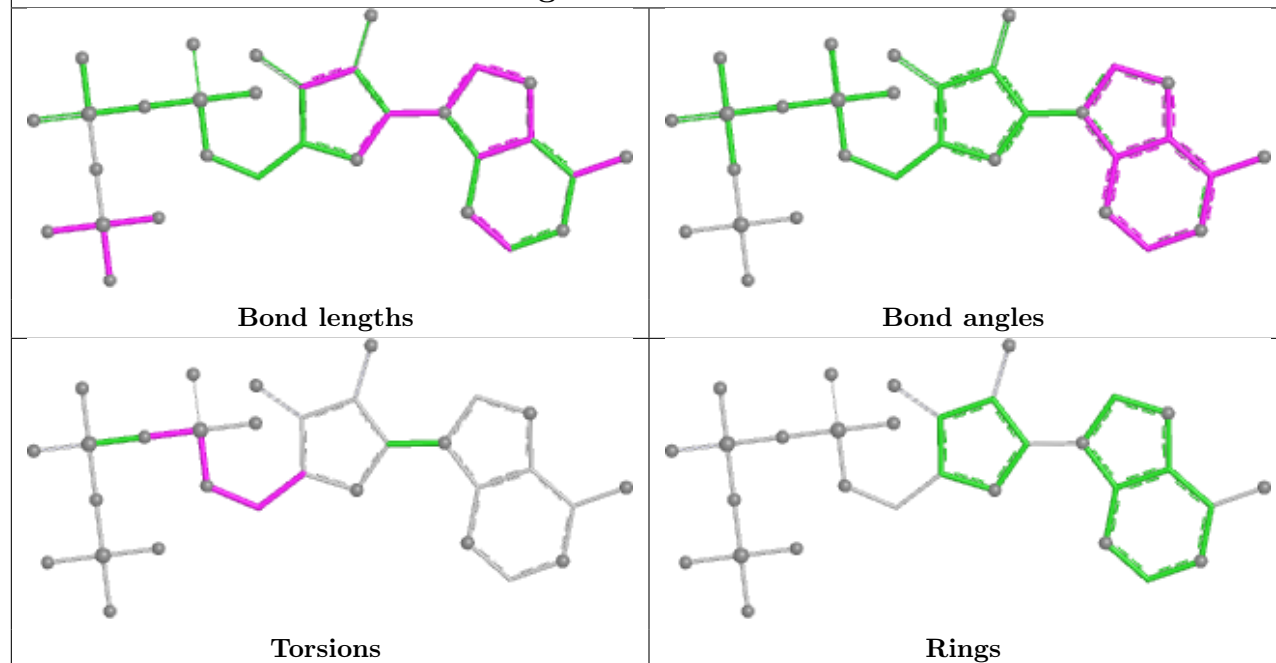
Ligand 08T B 400



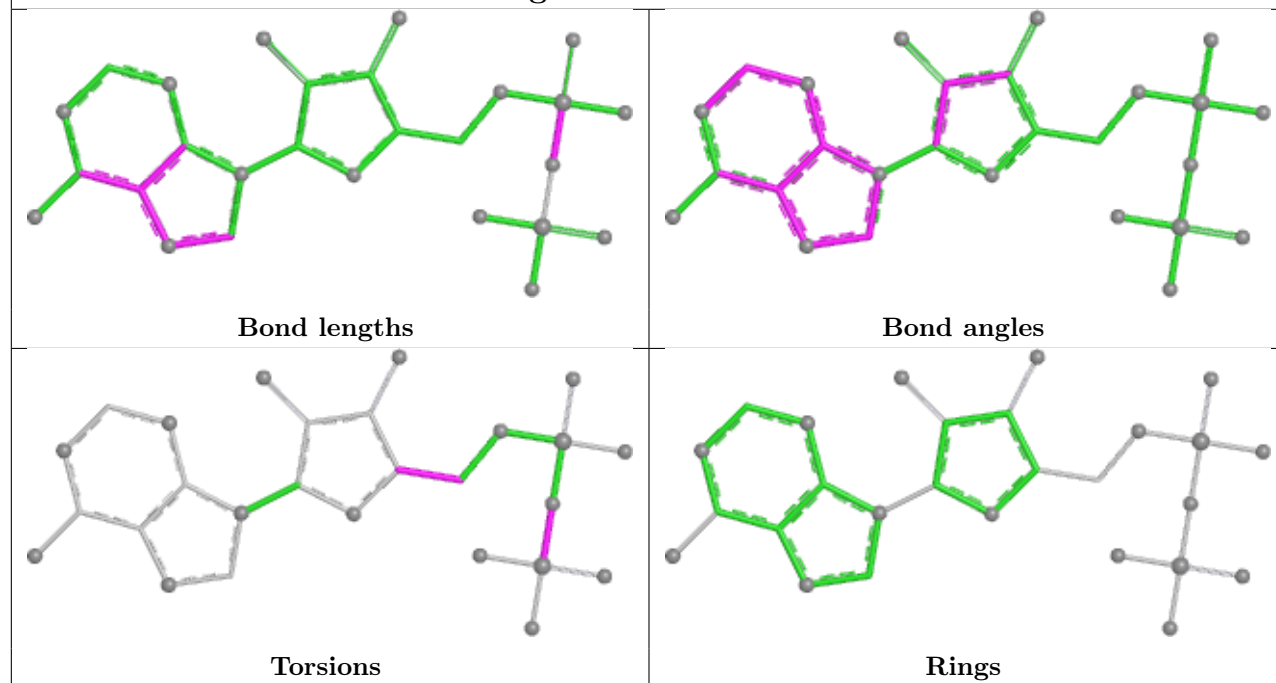
Ligand 08T P 400

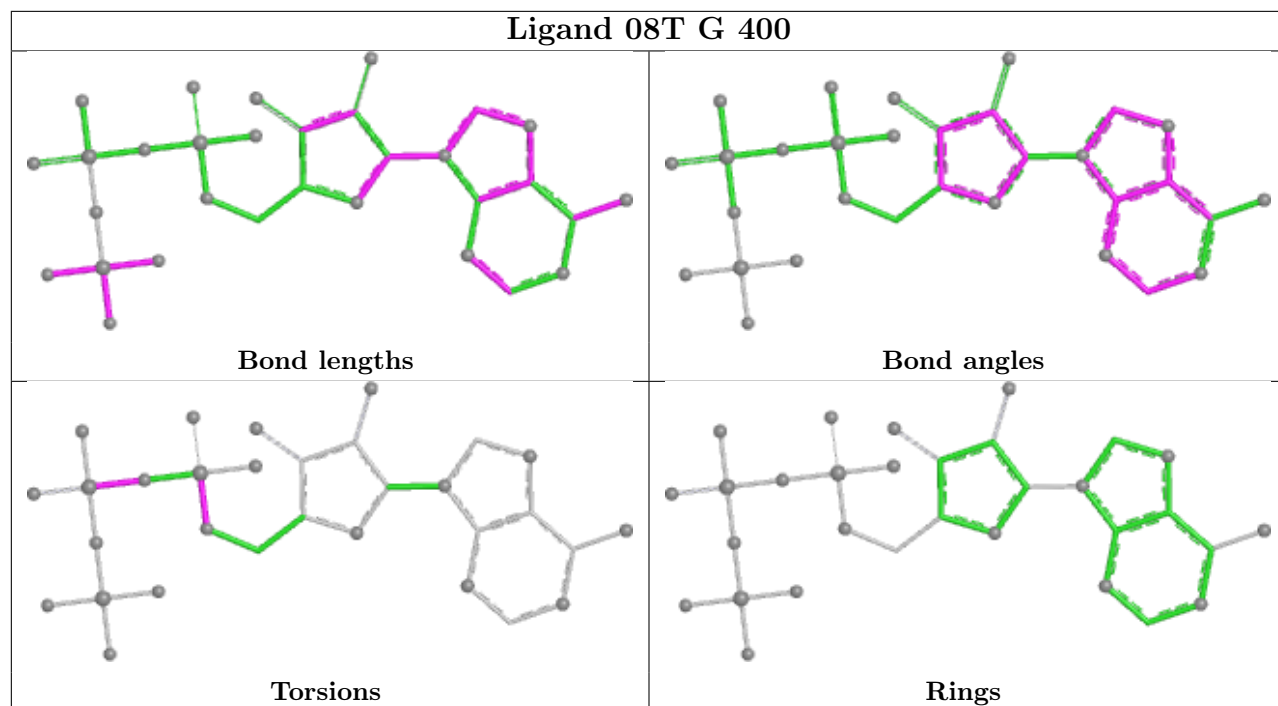


Ligand 08T U 400



Ligand ADP X 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	247/268 (92%)	-0.94	0	100	100	155, 197, 232, 255	0
1	B	247/268 (92%)	-1.01	0	100	100	93, 160, 198, 214	0
1	C	247/268 (92%)	-1.03	0	100	100	96, 149, 199, 220	0
1	D	247/268 (92%)	-1.11	0	100	100	84, 133, 171, 196	0
1	E	247/268 (92%)	-1.09	0	100	100	87, 135, 172, 215	0
1	F	247/268 (92%)	-1.02	0	100	100	93, 168, 238, 269	0
1	G	247/268 (92%)	-0.87	1 (0%)	88	70	171, 206, 248, 265	0
1	H	247/268 (92%)	-1.11	0	100	100	97, 156, 199, 214	0
1	I	247/268 (92%)	-1.04	0	100	100	95, 141, 203, 233	0
1	J	247/268 (92%)	-1.12	0	100	100	91, 139, 180, 197	0
1	K	247/268 (92%)	-1.09	0	100	100	94, 137, 175, 206	0
1	L	247/268 (92%)	-0.98	2 (0%)	82	58	99, 182, 278, 298	0
1	M	247/268 (92%)	-0.97	1 (0%)	88	70	136, 190, 223, 241	0
1	N	247/268 (92%)	-1.08	1 (0%)	88	70	95, 155, 193, 231	0
1	O	247/268 (92%)	-1.07	0	100	100	95, 146, 204, 239	0
1	P	247/268 (92%)	-1.08	1 (0%)	88	70	88, 139, 173, 204	0
1	Q	247/268 (92%)	-1.15	0	100	100	78, 135, 171, 215	0
1	R	247/268 (92%)	-0.96	0	100	100	108, 180, 245, 264	0
1	S	247/268 (92%)	-0.82	0	100	100	170, 206, 244, 259	0
1	T	247/268 (92%)	-1.04	0	100	100	106, 160, 203, 223	0
1	U	247/268 (92%)	-1.05	0	100	100	90, 147, 204, 230	0
1	V	247/268 (92%)	-1.14	0	100	100	88, 138, 175, 219	0
1	W	247/268 (92%)	-1.14	0	100	100	85, 137, 176, 212	0
1	X	247/268 (92%)	-0.95	3 (1%)	76	50	109, 181, 274, 298	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5928/6432 (92%)	-1.04	9 (0%) 91 80	78, 157, 229, 298	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	344	GLN	4.5
1	L	344	GLN	3.1
1	L	363	ILE	2.8
1	X	229	LEU	2.3
1	P	158	CYS	2.2
1	N	213	LYS	2.1
1	M	221	SER	2.1
1	G	220	VAL	2.1
1	X	361	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	401	1/1	0.94	0.06	105,105,105,105	0
3	MG	Q	401	1/1	0.95	0.13	125,125,125,125	1
3	MG	M	401	1/1	0.97	0.08	133,133,133,133	1
3	MG	K	401	1/1	0.98	0.08	118,118,118,118	1
3	MG	C	401	1/1	0.98	0.05	82,82,82,82	0
3	MG	N	401	1/1	0.98	0.08	96,96,96,96	1
3	MG	H	401	1/1	0.98	0.06	111,111,111,111	1
3	MG	S	401	1/1	0.98	0.04	153,153,153,153	0

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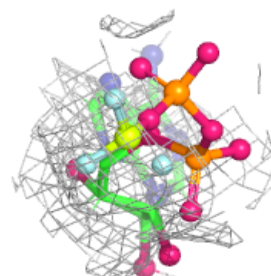
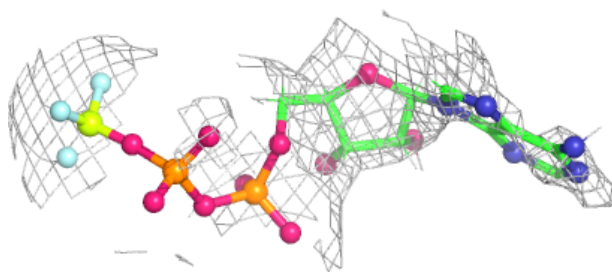
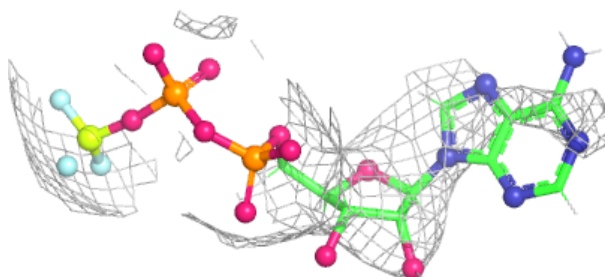
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	08T	J	400	31/31	0.99	0.04	93,118,134,159	42
2	08T	K	400	31/31	0.99	0.04	83,110,130,143	42
2	08T	M	400	31/31	0.99	0.05	129,155,180,188	42
2	08T	N	400	31/31	0.99	0.04	95,118,141,155	42
2	08T	O	400	31/31	0.99	0.04	72,118,139,159	42
2	08T	P	400	31/31	0.99	0.04	80,102,124,131	42
2	08T	Q	400	31/31	0.99	0.04	64,105,127,134	0
2	08T	S	400	31/31	0.99	0.05	127,163,203,237	42
2	08T	U	400	31/31	0.99	0.04	85,112,140,153	42
2	08T	V	400	31/31	0.99	0.03	84,112,126,143	42
2	08T	W	400	31/31	0.99	0.04	72,105,127,133	42
3	MG	A	401	1/1	0.99	0.03	140,140,140,140	1
3	MG	B	401	1/1	0.99	0.04	112,112,112,112	0
2	08T	A	400	31/31	0.99	0.04	124,147,166,181	42
2	08T	B	400	31/31	0.99	0.04	79,125,156,158	42
3	MG	G	401	1/1	0.99	0.09	155,155,155,155	1
2	08T	C	400	31/31	0.99	0.04	97,123,139,149	42
3	MG	I	401	1/1	0.99	0.05	109,109,109,109	0
2	08T	D	400	31/31	0.99	0.04	54,97,124,136	42
2	08T	E	400	31/31	0.99	0.05	86,115,137,160	42
2	08T	G	400	31/31	0.99	0.05	117,149,177,182	42
3	MG	O	401	1/1	0.99	0.05	110,110,110,110	0
3	MG	P	401	1/1	0.99	0.08	113,113,113,113	0
2	08T	H	400	31/31	0.99	0.04	77,111,128,146	42
2	08T	I	400	31/31	0.99	0.06	75,109,129,136	42
3	MG	T	401	1/1	0.99	0.07	129,129,129,129	0
3	MG	U	401	1/1	0.99	0.07	125,125,125,125	0
4	ADP	L	400	27/27	0.99	0.05	148,178,213,214	39
4	ADP	X	400	27/27	0.99	0.03	153,178,207,214	0
3	MG	J	401	1/1	1.00	0.04	85,85,85,85	0
3	MG	V	401	1/1	1.00	0.04	113,113,113,113	0
3	MG	W	401	1/1	1.00	0.05	109,109,109,109	0
3	MG	E	401	1/1	1.00	0.06	95,95,95,95	0
2	08T	T	400	31/31	1.00	0.04	97,122,150,150	42

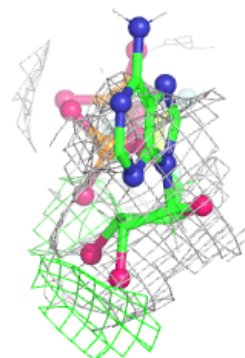
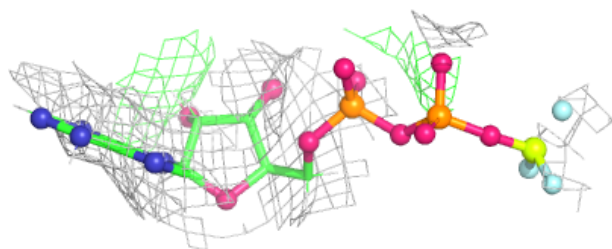
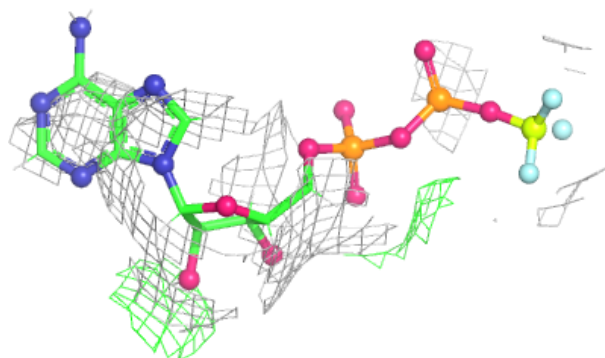
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 08T J 400:

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

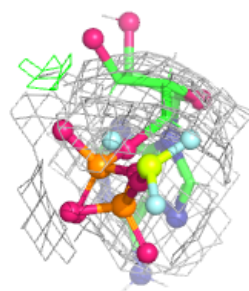
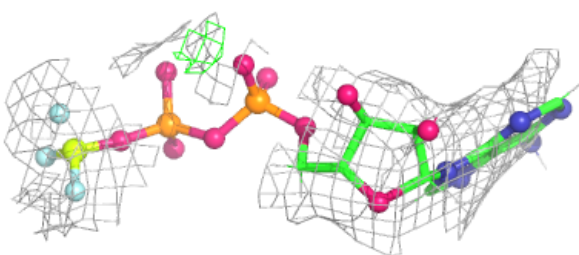
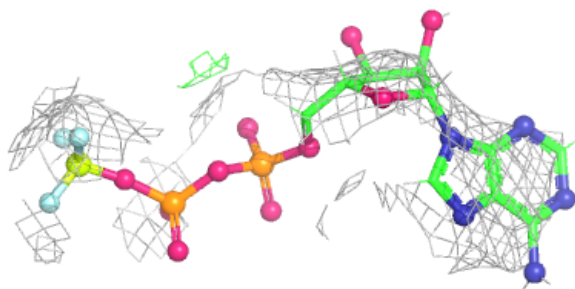
**Electron density around 08T K 400:**

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

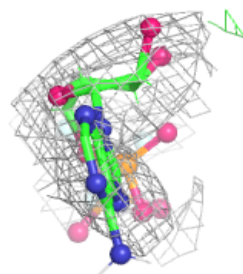
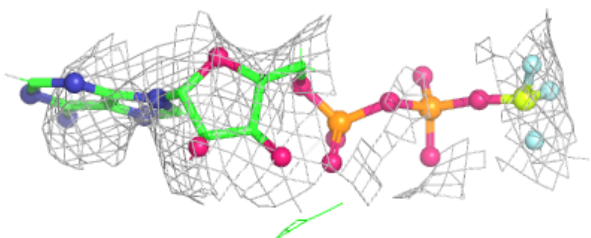
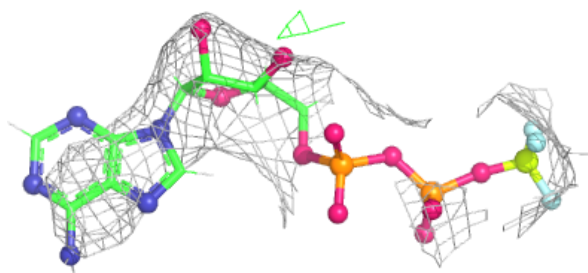


Electron density around 08T M 400:

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

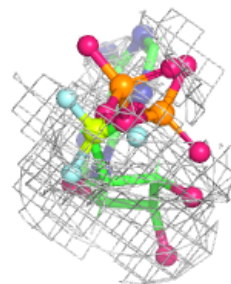
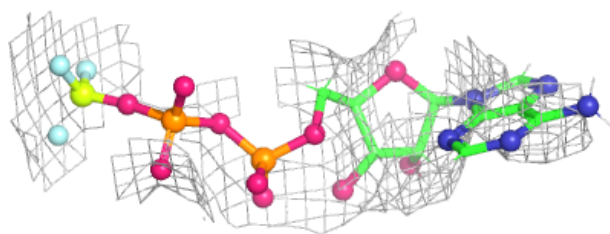
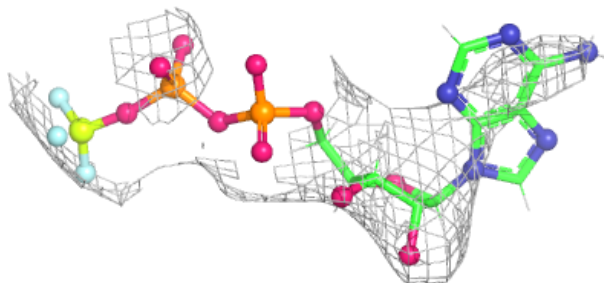
**Electron density around 08T N 400:**

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

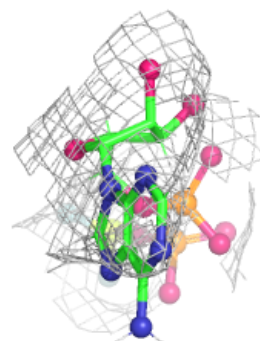
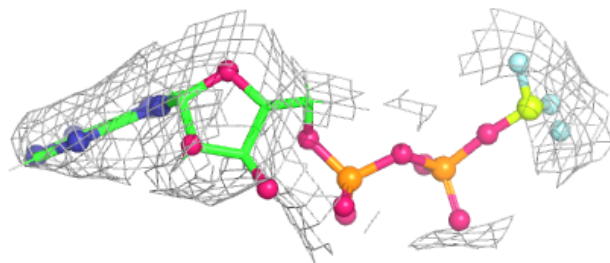
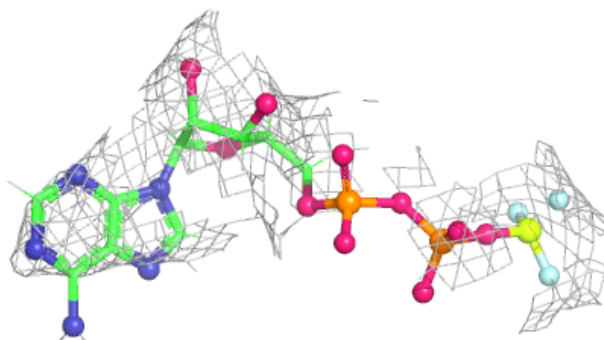


Electron density around 08T O 400:

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and green (positive)

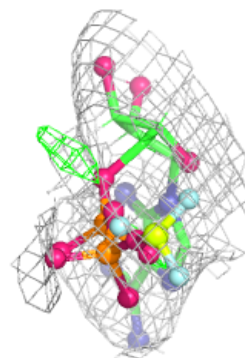
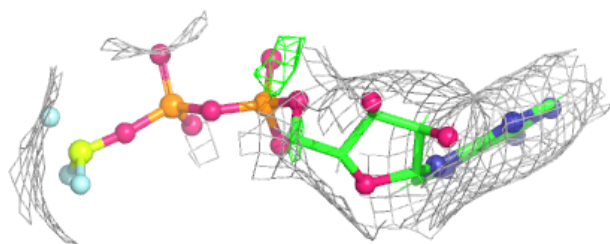
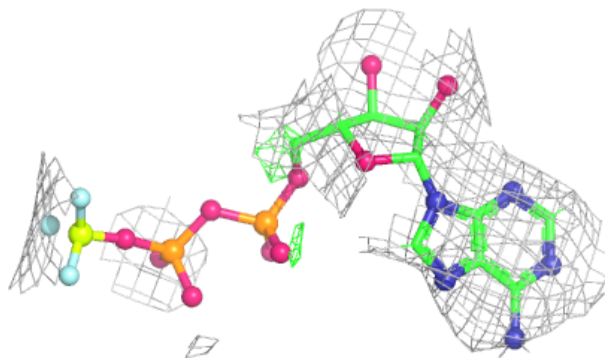
**Electron density around 08T P 400:**

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

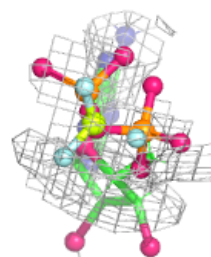
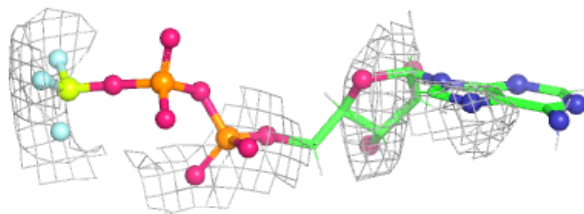
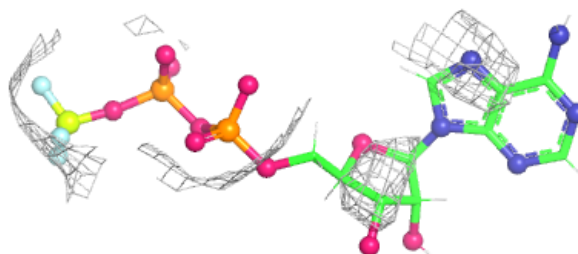


Electron density around 08T Q 400:

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

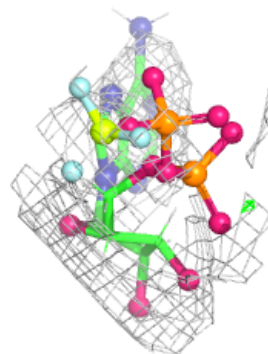
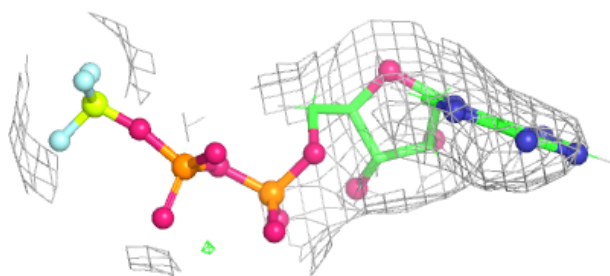
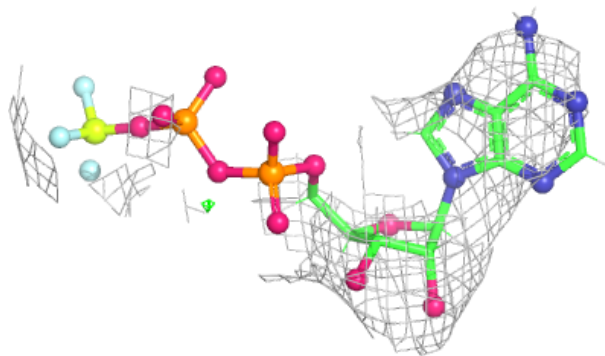
**Electron density around 08T S 400:**

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

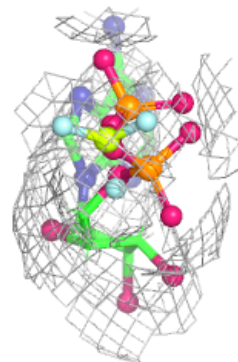
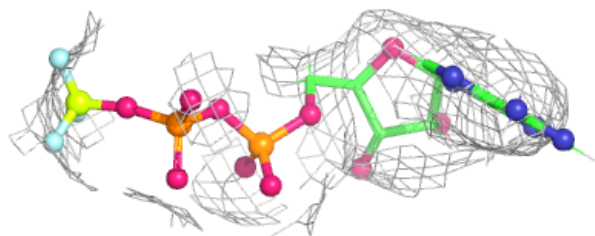
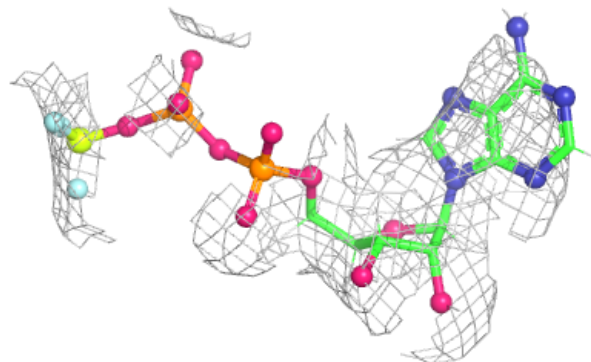


Electron density around 08T U 400:

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

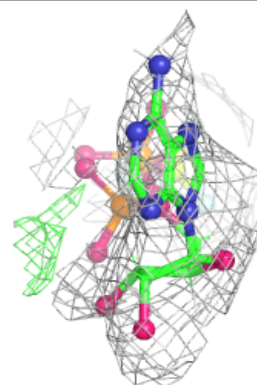
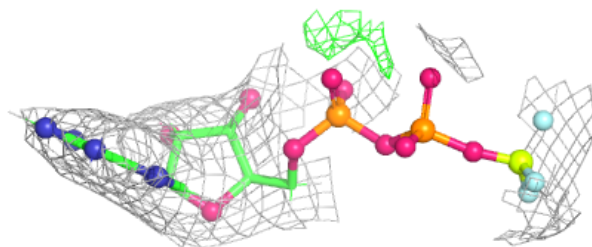
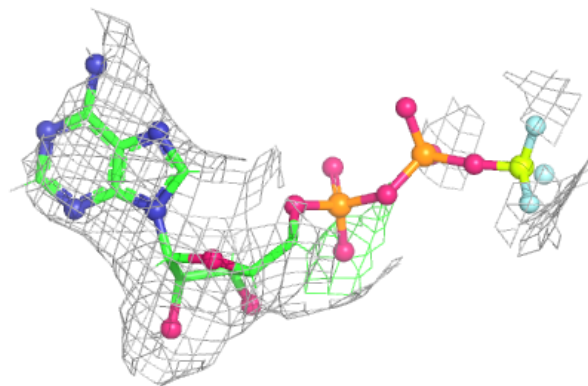
**Electron density around 08T V 400:**

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

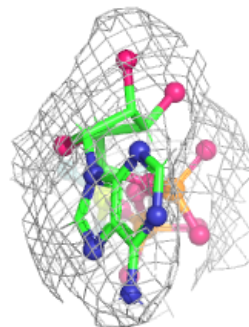
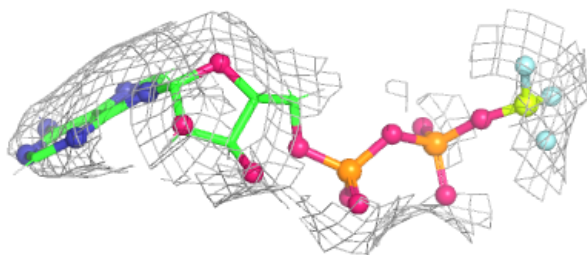
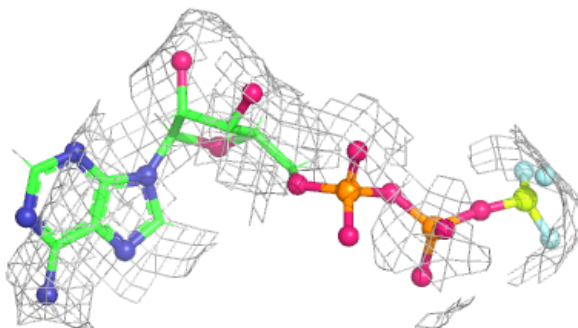


Electron density around 08T W 400:

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

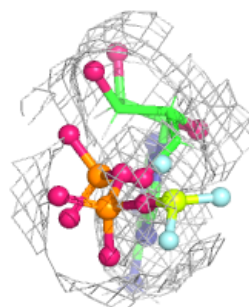
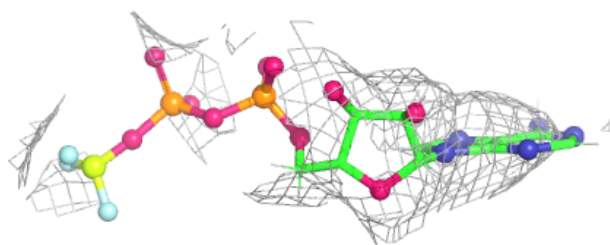
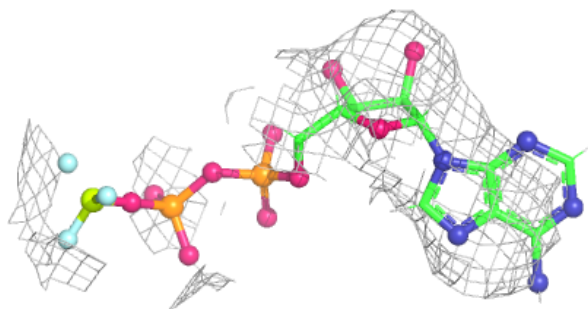
**Electron density around 08T A 400:**

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

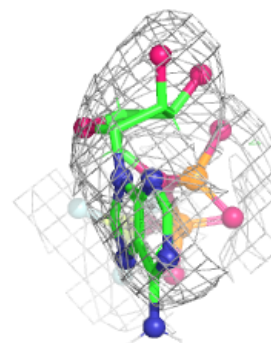
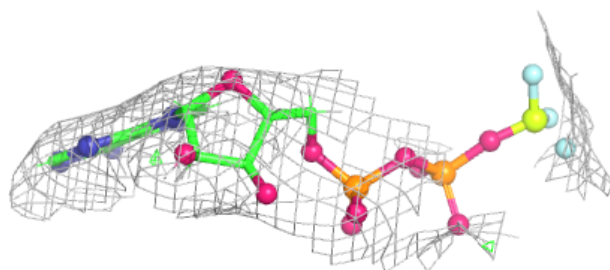
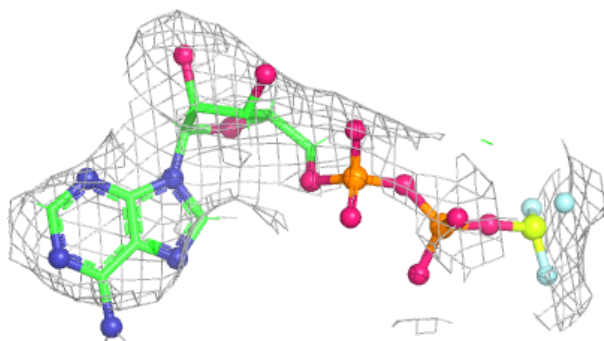


Electron density around 08T B 400:

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

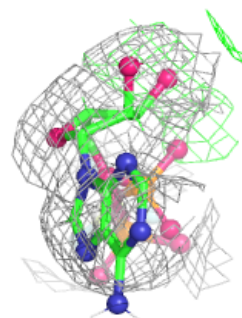
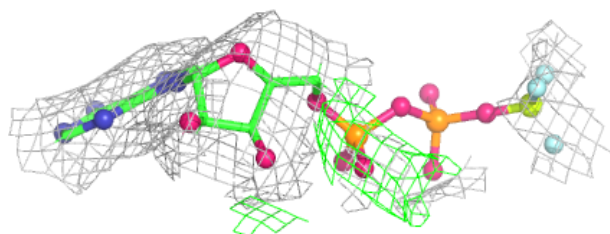
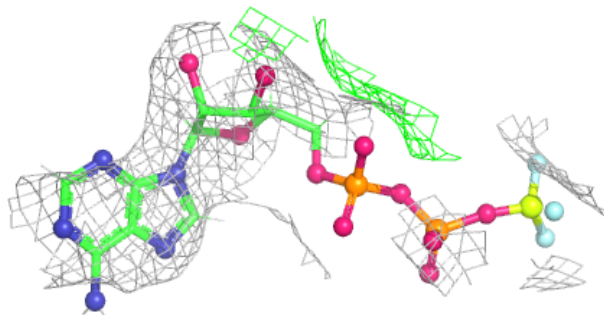
**Electron density around 08T C 400:**

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

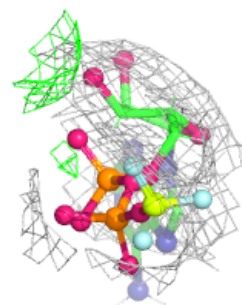
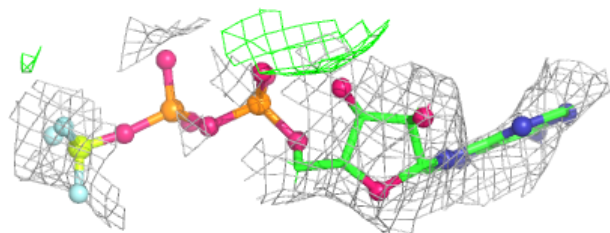
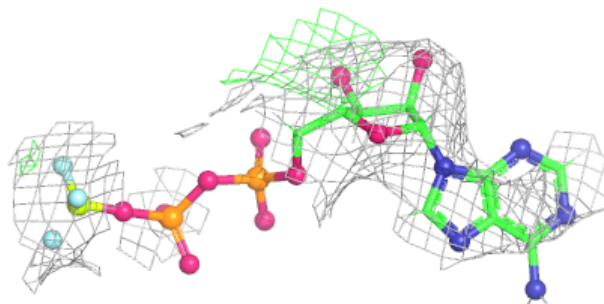


Electron density around 08T D 400:

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

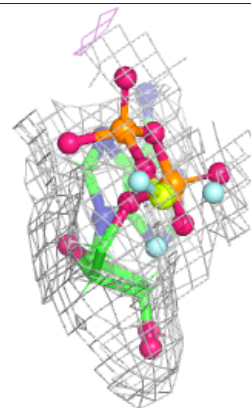
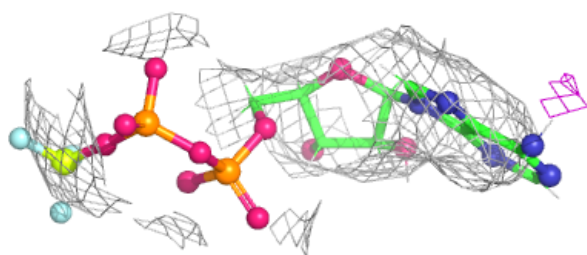
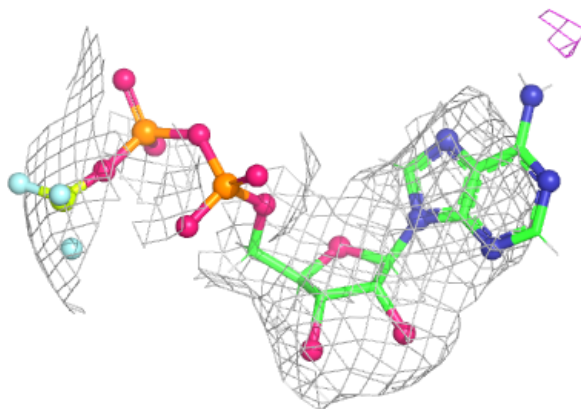
**Electron density around 08T E 400:**

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

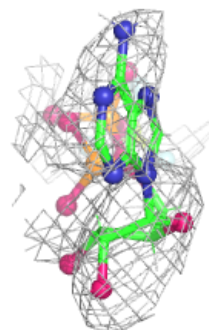
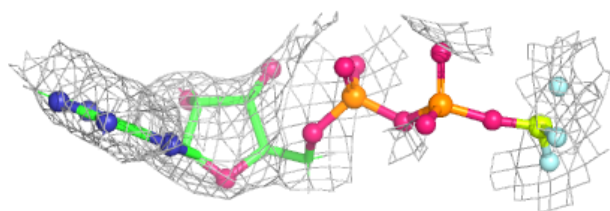
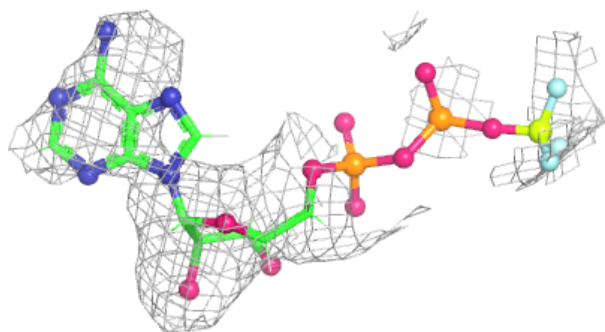


Electron density around 08T G 400:

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

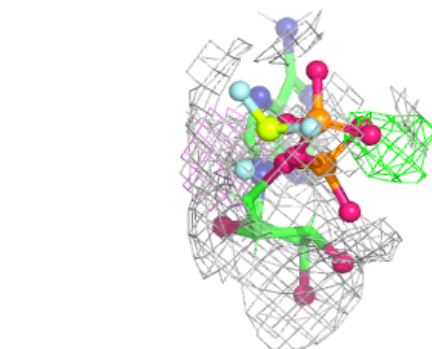
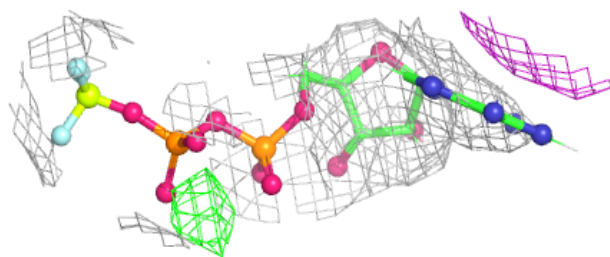
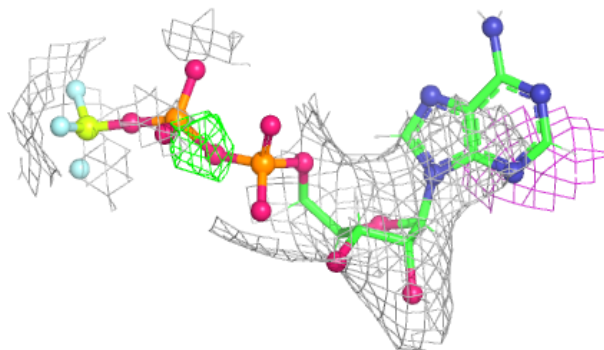
**Electron density around 08T H 400:**

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

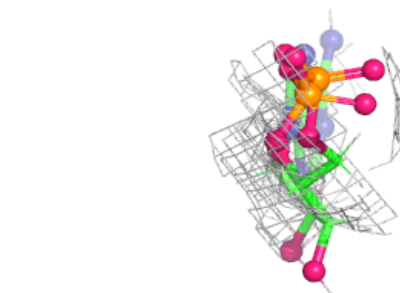
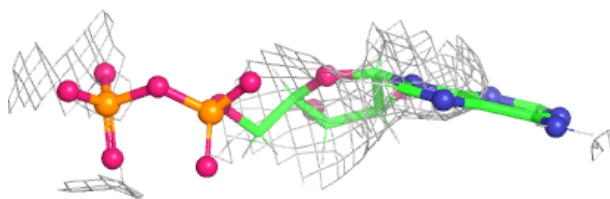
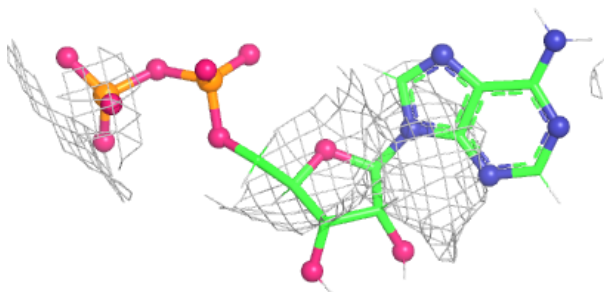


Electron density around 08T I 400:

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

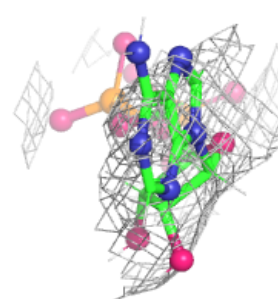
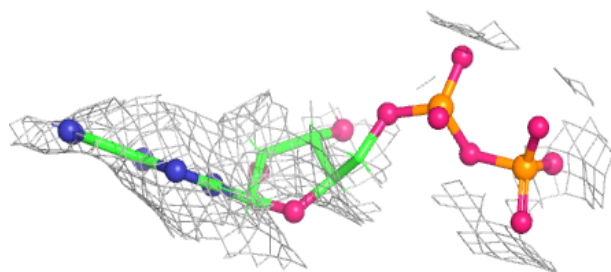
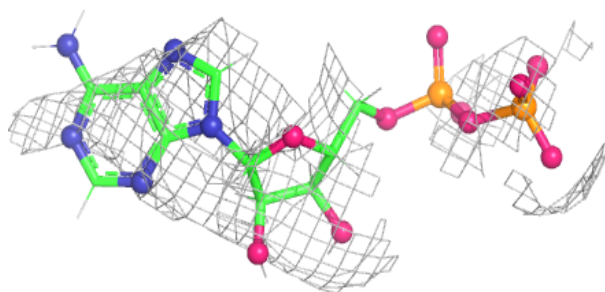
**Electron density around ADP L 400:**

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

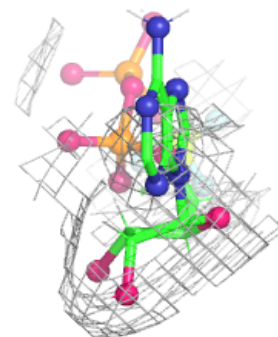
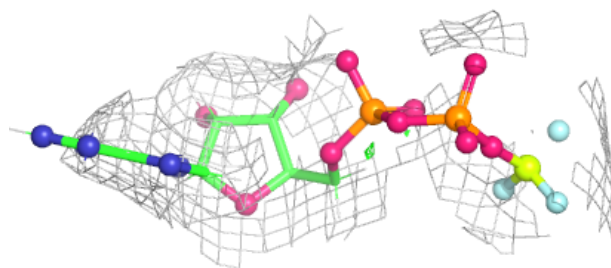
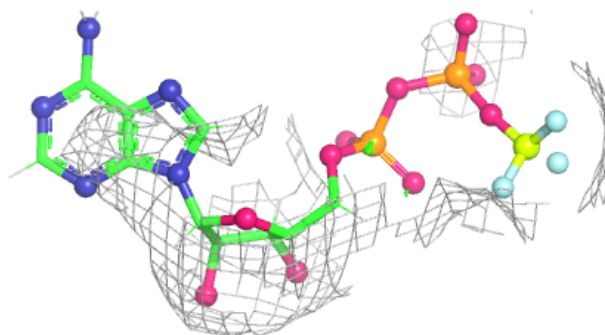


Electron density around ADP X 400:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.