Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 02:08 PM EST

PDB ID	:	4LY6
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 (i) symbol.

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

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

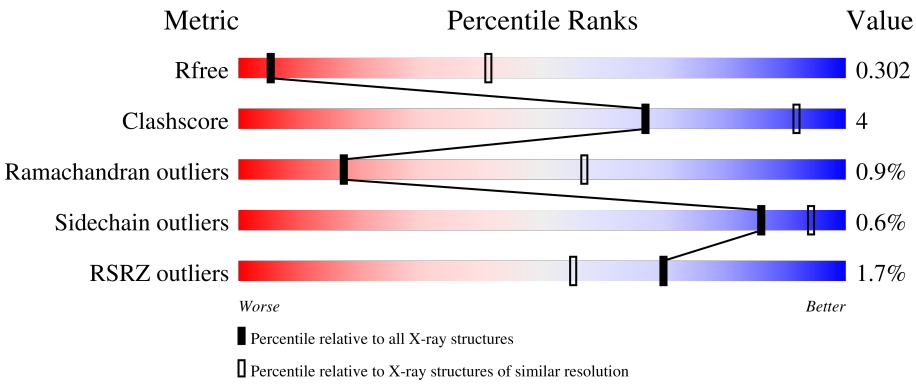
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 <=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	.% 84% 9% 8%
1	B	268	.% 85% 7% 8%
1	C	268	.% 84% 9% 8%
1	D	268	80% 11% • 8%
1	E	268	83% 9% 8%

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Mol	Chain	Length	Quality of chain
1	F	268	%, 81%, 10%, 8%
1	G	268	9%, 84%, 8%, 8%
1	H	268	85%, 7%, 8%
1	I	268	81%, 11%, 8%
1	J	268	%, 79%, 13%, 8%
1	K	268	83%, 9%, 8%
1	L	268	6%, 81%, 10%, 8%
1	M	268	%, 82%, 10%, 8%
1	N	268	%, 86%, 6%, 8%
1	O	268	79%, 12%, 8%
1	P	268	79%, 12%, 8%
1	Q	268	82%, 10%, 8%
1	R	268	2%, 76%, 15%, 8%
1	S	268	8%, 85%, 7%, 8%
1	T	268	82%, 9%, 8%
1	U	268	82%, 10%, 8%
1	V	268	%, 83%, 8%, 8%
1	W	268	84%, 8%, 8%
1	X	268	5%, 76%, 15%, 8%

2 Entry composition (i)

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
			Total	C	H	N	O	S			
1	A	247	4020	1278	2041	333	364	4	0	0	0
1	B	247	4021	1278	2042	333	364	4	0	0	0
1	C	247	4021	1278	2042	333	364	4	0	0	0
1	D	247	4021	1278	2042	333	364	4	0	0	0
1	E	247	4021	1278	2042	333	364	4	0	0	0
1	F	247	4021	1278	2042	333	364	4	0	0	0
1	G	247	4021	1278	2042	333	364	4	0	0	0
1	H	247	4021	1278	2042	333	364	4	0	0	0
1	I	247	4020	1278	2041	333	364	4	0	0	0
1	J	247	4021	1278	2042	333	364	4	0	0	0
1	K	247	4021	1278	2042	333	364	4	0	0	0
1	L	247	4021	1278	2042	333	364	4	0	0	0
1	M	247	4021	1278	2042	333	364	4	0	0	0
1	N	247	4021	1278	2042	333	364	4	0	0	0
1	O	247	4021	1278	2042	333	364	4	0	0	0
1	P	247	4021	1278	2042	333	364	4	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	Q	247	4021	1278	2042	333	364	4	0	0	0
1	R	247	4021	1278	2042	333	364	4	0	0	0
1	S	247	4021	1278	2042	333	364	4	0	0	0
1	T	247	4020	1278	2041	333	364	4	0	0	0
1	U	247	4021	1278	2042	333	364	4	0	0	0
1	V	247	4021	1278	2042	333	364	4	0	0	0
1	W	247	4021	1278	2042	333	364	4	0	0	0
1	X	247	4021	1278	2042	333	364	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

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

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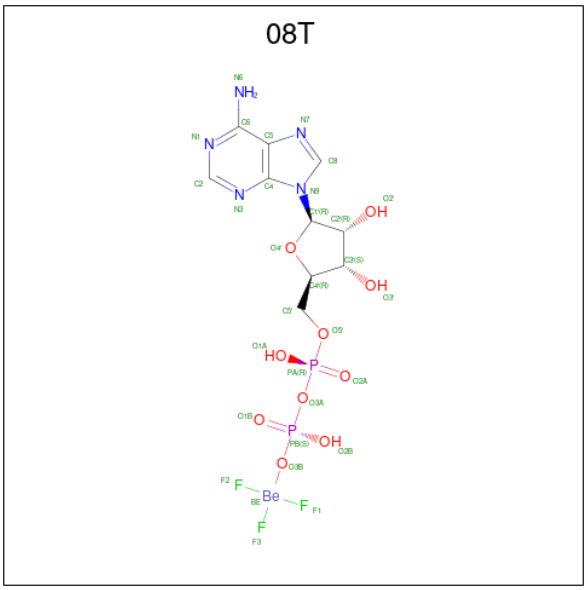
Chain	Residue	Modelled	Actual	Comment	Reference
X	120	MET	-	initiating methionine	UNP O67198

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



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

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

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

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

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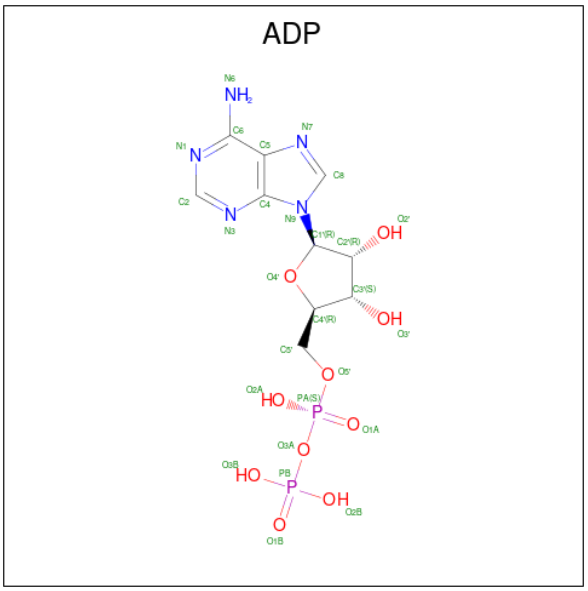
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	P	1	Total Mg 1 1	0	0
3	Q	1	Total Mg 1 1	0	0
3	S	1	Total Mg 1 1	0	0
3	T	1	Total Mg 1 1	0	0
3	U	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0
3	W	1	Total Mg 1 1	0	0

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



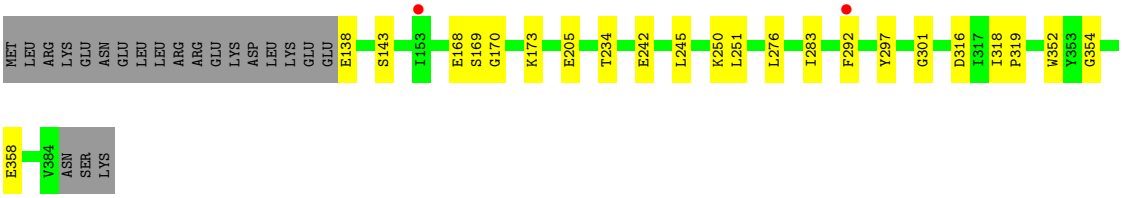
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	L	1	39	10	12	5	10	2	0	0
			Total	C	H	N	O	P		
4	X	1	39	10	12	5	10	2	0	0

3 Residue-property plots (i)

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

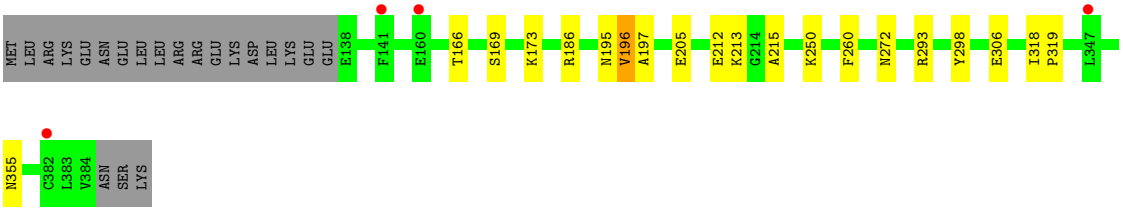
• Molecule 1: Transcriptional regulator (NtrC family)

Chain A:



• Molecule 1: Transcriptional regulator (NtrC family)

Chain B:

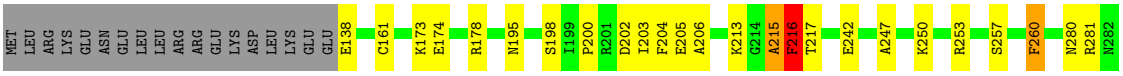


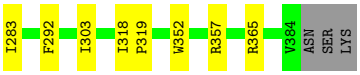
• Molecule 1: Transcriptional regulator (NtrC family)

Chain C:

• Molecule 1: Transcriptional regulator (NtrC family)

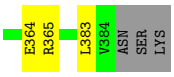
Chain D:





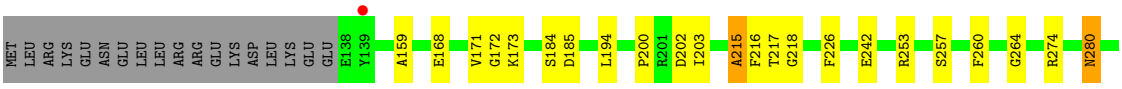
• Molecule 1: Transcriptional regulator (NtrC family)

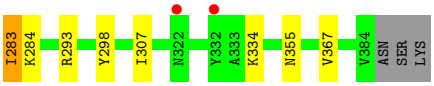
Chain E:



• Molecule 1: Transcriptional regulator (NtrC family)

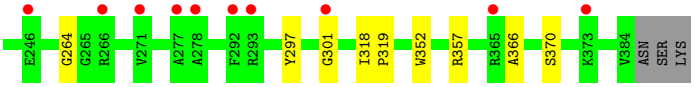
Chain F:





• Molecule 1: Transcriptional regulator (NtrC family)

Chain G:



• Molecule 1: Transcriptional regulator (NtrC family)

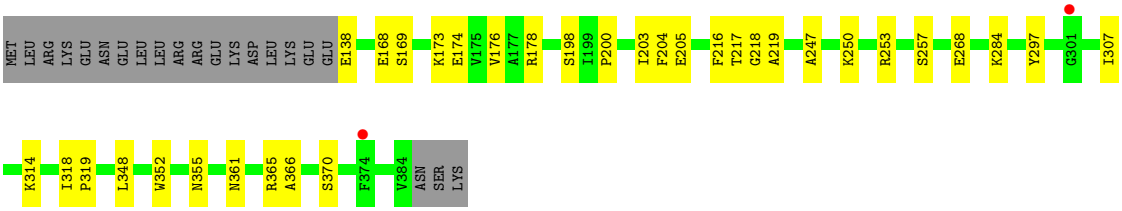
Chain H:

• Molecule 1: Transcriptional regulator (NtrC family)

Chain I:

• Molecule 1: Transcriptional regulator (NtrC family)

Chain J:

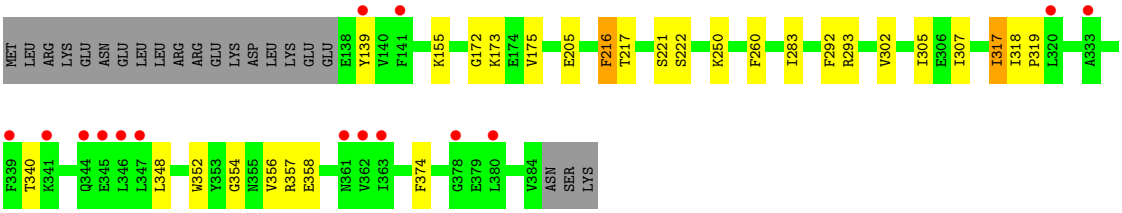


• Molecule 1: Transcriptional regulator (NtrC family)

Chain K:

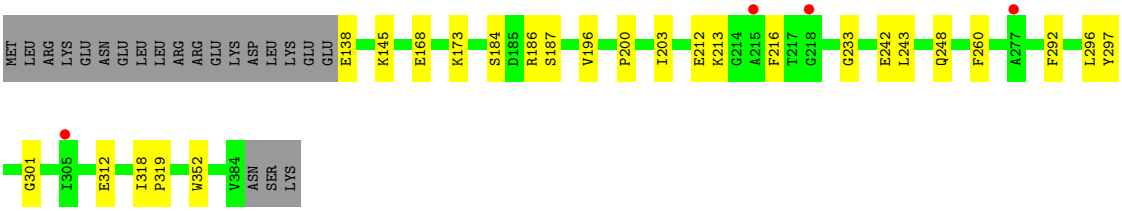
• Molecule 1: Transcriptional regulator (NtrC family)

Chain L:



• Molecule 1: Transcriptional regulator (NtrC family)

Chain M:

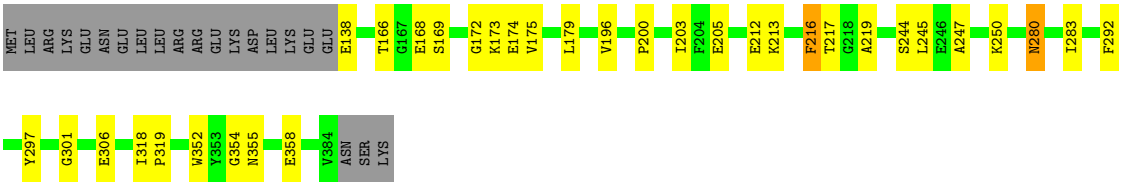


• Molecule 1: Transcriptional regulator (NtrC family)

Chain N:

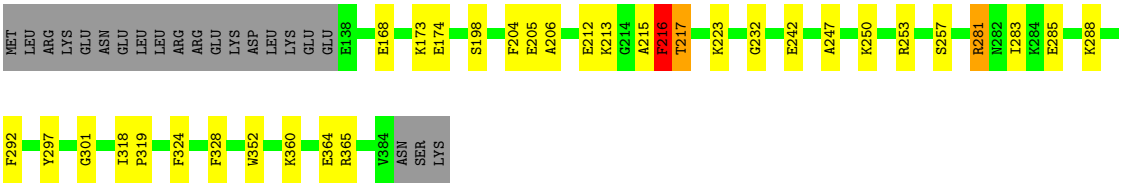
• Molecule 1: Transcriptional regulator (NtrC family)

Chain O:



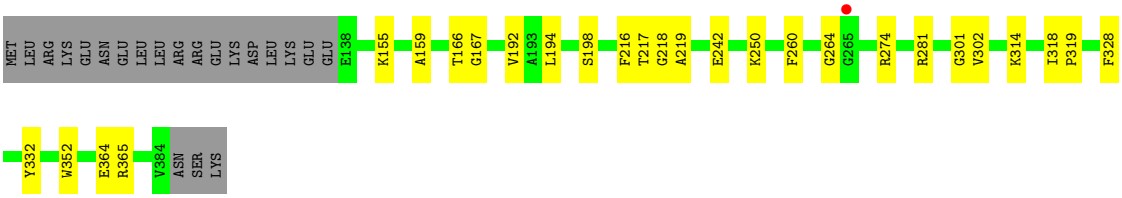
• Molecule 1: Transcriptional regulator (NtrC family)

Chain P:



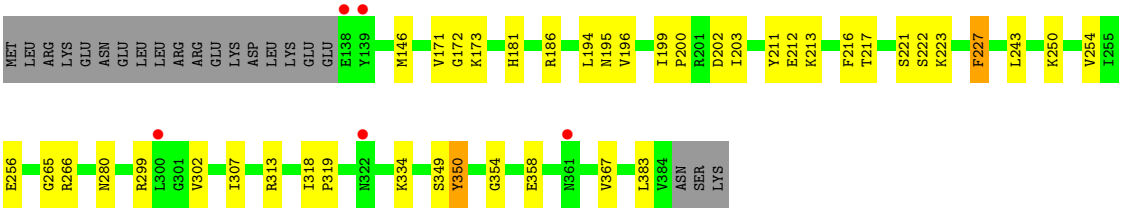
• Molecule 1: Transcriptional regulator (NtrC family)

Chain Q:



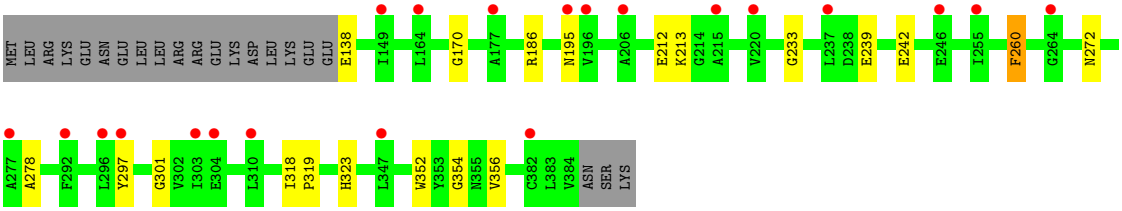
• Molecule 1: Transcriptional regulator (NtrC family)

Chain R:



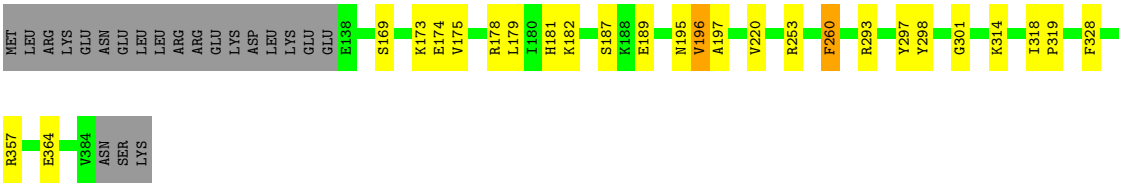
• Molecule 1: Transcriptional regulator (NtrC family)

Chain S:



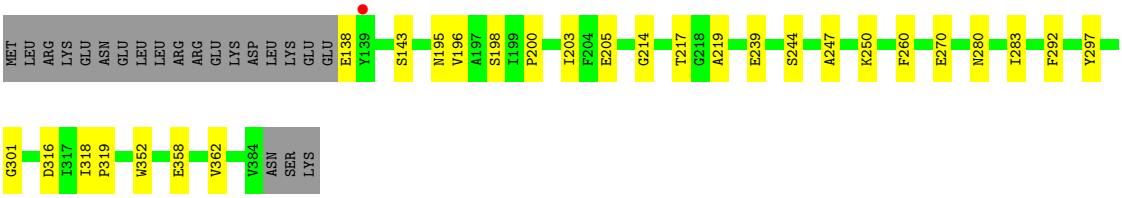
• Molecule 1: Transcriptional regulator (NtrC family)

Chain T:



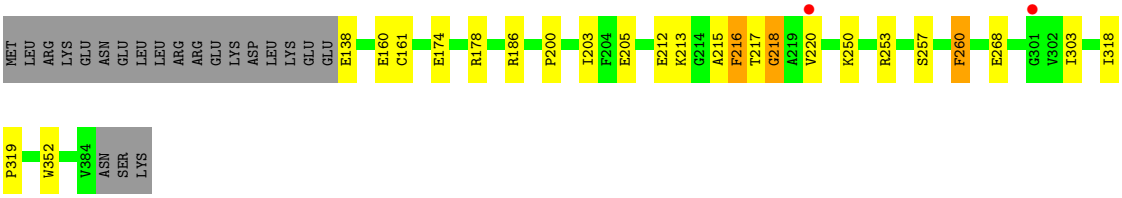
• Molecule 1: Transcriptional regulator (NtrC family)

Chain U:



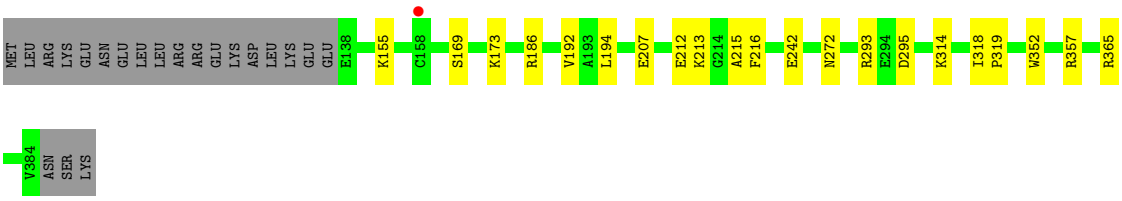
• Molecule 1: Transcriptional regulator (NtrC family)

Chain V:



• Molecule 1: Transcriptional regulator (NtrC family)

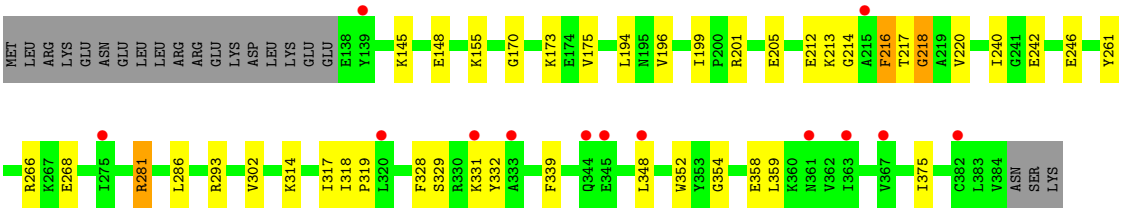
Chain W:



• Molecule 1: Transcriptional regulator (NtrC family)

Chain X:

5%
76%
15%
8%


MET LEU ARG LYS GLU ASN GLU LEU LEU ARG ARG GLU LYS ASP LEU LYS GLU GLU E138 Y139 K145 E148 K155 G170 K173 E174 V175 L194 N195 V196 I199 P200 R201 E205 E212 K213 G214 A215 F216 T217 G218 A219 V220 I240 G241 E242 E246 Y261
R266 K267 E268 I275 R281 L286 R293 V302 K314 I317 I318 P319 L320 F328 S329 R330 K331 Y332 A333 F339 Q344 E345 L348 W352 Y353 G354 E358 L359 K360 N361 V362 I363 V367 I375 C382 L383 V384 ASN SER LYS

4 Data and refinement statistics (i)

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 37.86 – 3.60	Depositor EDS
% Data completeness (in resolution range)	76.2 (37.85-3.60) 69.7 (37.86-3.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.258 , 0.308 0.255 , 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)	0.32 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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	0.92	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.24	0/2013	0.45	0/2700
1	B	0.25	0/2013	0.48	0/2700
1	C	0.26	0/2013	0.50	0/2700
1	D	0.27	0/2013	0.50	0/2700
1	E	0.26	0/2013	0.50	0/2700
1	F	0.27	0/2013	0.52	0/2700
1	G	0.24	0/2013	0.46	0/2700
1	H	0.26	0/2013	0.49	0/2700
1	I	0.26	0/2013	0.51	0/2700
1	J	0.27	0/2013	0.49	0/2700
1	K	0.26	0/2013	0.51	0/2700
1	L	0.25	0/2013	0.51	0/2700
1	M	0.25	0/2013	0.48	0/2700
1	N	0.26	0/2013	0.48	0/2700
1	O	0.26	0/2013	0.53	0/2700
1	P	0.27	0/2013	0.52	0/2700
1	Q	0.26	0/2013	0.50	0/2700
1	R	0.27	0/2013	0.65	0/2700
1	S	0.24	0/2013	0.47	0/2700
1	T	0.26	0/2013	0.50	0/2700
1	U	0.26	0/2013	0.51	0/2700
1	V	0.26	0/2013	0.51	0/2700
1	W	0.26	0/2013	0.50	0/2700
1	X	0.28	0/2013	0.62	1/2700 (0.0%)
All	All	0.26	0/48312	0.51	1/64800 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	218	GLY	N-CA-C	5.07	125.78	113.10

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	11	0
1	C	1979	2042	2040	13	0
1	D	1979	2042	2040	22	0
1	E	1979	2042	2040	18	0
1	F	1979	2042	2040	23	0
1	G	1979	2042	2040	14	0
1	H	1979	2042	2040	13	0
1	I	1979	2041	2039	17	0
1	J	1979	2042	2040	21	0
1	K	1979	2042	2040	17	0
1	L	1979	2042	2040	18	0
1	M	1979	2042	2040	16	0
1	N	1979	2042	2040	9	0
1	O	1979	2042	2040	27	0
1	P	1979	2042	2040	26	0
1	Q	1979	2042	2040	16	0
1	R	1979	2042	2040	22	0
1	S	1979	2042	2040	14	0
1	T	1979	2041	2039	17	0
1	U	1979	2042	2040	14	0
1	V	1979	2042	2040	16	0
1	W	1979	2042	2040	11	0
1	X	1979	2042	2040	30	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	3	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	2	0
2	O	31	11	13	7	0
2	P	31	11	13	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	31	11	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	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	3	0
All	All	48190	49249	49241	383	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 (383) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:W:242:GLU:OE2	1:X:293:ARG:NH2	2.21	0.73
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:E:173:LYS:NZ	2:E:400:08T:O2B	2.23	0.68
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:G:173:LYS:NZ	2:G:400:08T:O2B	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:P:217:THR:O	1:P:217:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:173:LYS:H	2:E:400:08T:H9	1.55	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:168:GLU:O	1:O:173:LYS:NZ	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:F:216:PHE:HB3	1:F:217:THR:C	2.31	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:174:GLU:OE2	1:D:178:ARG:NH1	2.48	0.46
1:R:200:PRO:HD2	1:R:203:ILE:HD11	1.97	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
1:D:204:PHE:HE2	1:D:247:ALA:HB1	1.81	0.46
1:K:216:PHE:C	1:K:218:GLY:H	2.18	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:H:205:GLU:OE1	1:H:205:GLU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:200:PRO:HG2	1:D:203:ILE:HG12	1.97	0.45
1:G:184:SER:O	1:G:187:SER:OG	2.33	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: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:E:318:ILE:N	1:E:319:PRO:CD	2.80	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: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
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:B:195:ASN:C	1:B:197:ALA:H	2.20	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

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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	0.44
1:K:194:LEU:HD21	1:K:226:PHE:CD2	2.53	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:F:159:ALA:O	1:F:274:ARG:NH1	2.50	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:173:LYS:NZ	4:X:400:ADP:O1B	2.48	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:J:217:THR:C	1:J:219:ALA:H	2.20	0.43
1:T:195:ASN:C	1:T:197:ALA:H	2.21	0.43
1:V:260:PHE:CD1	1:V:260:PHE:C	2.91	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: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
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:R:265:GLY:O	1:R:266:ARG:HD3	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:217:THR:C	1:O:219:ALA:H	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:S:260:PHE:CD1	1:S:260:PHE:C	2.93	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: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:X:170:GLY:N	4:X:400:ADP:O3B	2.53	0.41
1:C:217:THR:C	1:C:219:ALA:H	2.24	0.41
1:U:217:THR:C	1:U:219:ALA:H	2.24	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
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:169:SER:HA	1:W:173:LYS:HZ1	1.85	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: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:T:260:PHE:CD1	1:T:260:PHE:C	2.94	0.41
1:U:318:ILE:N	1:U:319:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:216:PHE:C	1:P:217:THR:HG23	2.42	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:X:216:PHE:HB3	1:X:217:THR:C	2.42	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:K:260:PHE:C	1:K:260:PHE:CD1	2.95	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
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:H:195:ASN:C	1:H:197:ALA:H	2.24	0.40
1:J:204:PHE:HE2	1:J:247:ALA:HB1	1.86	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: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

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

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	34	71
1	B	245/268 (91%)	231 (94%)	13 (5%)	1 (0%)	34	71
1	C	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	34	71
1	D	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	13	51
1	E	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	19	59
1	F	245/268 (91%)	221 (90%)	20 (8%)	4 (2%)	9	46
1	G	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	34	71
1	H	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	19	59
1	I	245/268 (91%)	233 (95%)	11 (4%)	1 (0%)	34	71
1	J	245/268 (91%)	230 (94%)	12 (5%)	3 (1%)	13	51
1	K	245/268 (91%)	227 (93%)	15 (6%)	3 (1%)	13	51
1	L	245/268 (91%)	226 (92%)	17 (7%)	2 (1%)	19	59
1	M	245/268 (91%)	229 (94%)	15 (6%)	1 (0%)	34	71
1	N	245/268 (91%)	231 (94%)	12 (5%)	2 (1%)	19	59
1	O	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	34	71
1	P	245/268 (91%)	230 (94%)	13 (5%)	2 (1%)	19	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	13	51
1	R	245/268 (91%)	235 (96%)	6 (2%)	4 (2%)	9	46
1	S	245/268 (91%)	232 (95%)	12 (5%)	1 (0%)	34	71
1	T	245/268 (91%)	229 (94%)	14 (6%)	2 (1%)	19	59
1	U	245/268 (91%)	230 (94%)	14 (6%)	1 (0%)	34	71
1	V	245/268 (91%)	228 (93%)	14 (6%)	3 (1%)	13	51
1	W	245/268 (91%)	229 (94%)	13 (5%)	3 (1%)	13	51
1	X	245/268 (91%)	234 (96%)	8 (3%)	3 (1%)	13	51
All	All	5880/6432 (91%)	5513 (94%)	317 (5%)	50 (1%)	17	57

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
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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/233 (91%)	212 (100%)	0	100	100
1	B	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	C	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	D	212/233 (91%)	209 (99%)	3 (1%)	67	85
1	E	212/233 (91%)	209 (99%)	3 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	212/233 (91%)	210 (99%)	2 (1%)	78	90
1	G	212/233 (91%)	212 (100%)	0	100	100
1	H	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	I	212/233 (91%)	212 (100%)	0	100	100
1	J	212/233 (91%)	212 (100%)	0	100	100
1	K	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	L	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	M	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	N	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	O	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	P	212/233 (91%)	209 (99%)	3 (1%)	67	85
1	Q	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	R	212/233 (91%)	208 (98%)	4 (2%)	57	80
1	S	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	T	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	U	212/233 (91%)	210 (99%)	2 (1%)	78	90
1	V	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	W	212/233 (91%)	211 (100%)	1 (0%)	88	95
1	X	212/233 (91%)	210 (99%)	2 (1%)	78	90
All	All	5088/5592 (91%)	5056 (99%)	32 (1%)	86	94

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	260	PHE
1	C	260	PHE
1	D	213	LYS
1	D	216	PHE
1	D	260	PHE
1	E	145	LYS
1	E	216	PHE
1	E	260	PHE
1	F	260	PHE
1	F	280	ASN
1	H	260	PHE

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Mol	Chain	Res	Type
1	K	260	PHE
1	L	260	PHE
1	M	260	PHE
1	N	260	PHE
1	O	280	ASN
1	P	216	PHE
1	P	217	THR
1	P	281	ARG
1	Q	260	PHE
1	R	216	PHE
1	R	227	PHE
1	R	280	ASN
1	R	383	LEU
1	S	260	PHE
1	T	260	PHE
1	U	260	PHE
1	U	280	ASN
1	V	260	PHE
1	W	216	PHE
1	X	281	ARG
1	X	332	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	J	400	3	26,33,33	3.31	10 (38%)	25,52,52	2.01	6 (24%)
4	ADP	X	400	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
4	ADP	L	400	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
2	08T	C	400	3	26,33,33	3.31	10 (38%)	25,52,52	2.01	6 (24%)
2	08T	Q	400	-	26,33,33	3.30	10 (38%)	25,52,52	2.17	6 (24%)
2	08T	N	400	1,3	26,33,33	3.32	10 (38%)	25,52,52	2.12	7 (28%)
2	08T	V	400	3	26,33,33	3.32	10 (38%)	25,52,52	1.90	6 (24%)
2	08T	O	400	3	26,33,33	3.35	10 (38%)	25,52,52	1.93	4 (16%)
2	08T	I	400	1,3	26,33,33	3.30	10 (38%)	25,52,52	1.93	4 (16%)
2	08T	D	400	3	26,33,33	3.33	10 (38%)	25,52,52	2.00	5 (20%)
2	08T	U	400	1,3	26,33,33	3.33	10 (38%)	25,52,52	1.98	6 (24%)
2	08T	G	400	3	26,33,33	3.37	10 (38%)	25,52,52	2.13	6 (24%)
2	08T	A	400	1,3	26,33,33	3.34	10 (38%)	25,52,52	2.00	5 (20%)
2	08T	P	400	3	26,33,33	3.35	10 (38%)	25,52,52	1.93	5 (20%)
2	08T	E	400	3	26,33,33	3.32	10 (38%)	25,52,52	2.03	5 (20%)
2	08T	K	400	-	26,33,33	3.30	10 (38%)	25,52,52	2.03	6 (24%)
2	08T	B	400	3	26,33,33	3.33	10 (38%)	25,52,52	2.05	5 (20%)
2	08T	W	400	3	26,33,33	3.31	10 (38%)	25,52,52	1.98	6 (24%)
2	08T	H	400	1,3	26,33,33	3.36	10 (38%)	25,52,52	2.00	7 (28%)
2	08T	S	400	3	26,33,33	3.33	10 (38%)	25,52,52	2.05	5 (20%)
2	08T	M	400	3	26,33,33	3.31	10 (38%)	25,52,52	2.10	5 (20%)
2	08T	T	400	1,3	26,33,33	3.32	10 (38%)	25,52,52	2.00	5 (20%)

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	J	400	3	-	9/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	X	400	-	-	4/12/32/32	0/3/3/3
4	ADP	L	400	-	-	2/12/32/32	0/3/3/3
2	08T	C	400	3	-	4/12/38/38	0/3/3/3
2	08T	Q	400	-	-	0/12/38/38	0/3/3/3
2	08T	N	400	1,3	-	3/12/38/38	0/3/3/3
2	08T	V	400	3	-	4/12/38/38	0/3/3/3
2	08T	O	400	3	-	7/12/38/38	0/3/3/3
2	08T	I	400	1,3	-	3/12/38/38	0/3/3/3
2	08T	D	400	3	-	0/12/38/38	0/3/3/3
2	08T	U	400	1,3	-	6/12/38/38	0/3/3/3
2	08T	G	400	3	-	4/12/38/38	0/3/3/3
2	08T	A	400	1,3	-	5/12/38/38	0/3/3/3
2	08T	P	400	3	-	5/12/38/38	0/3/3/3
2	08T	E	400	3	-	1/12/38/38	0/3/3/3
2	08T	K	400	-	-	4/12/38/38	0/3/3/3
2	08T	B	400	3	-	2/12/38/38	0/3/3/3
2	08T	W	400	3	-	3/12/38/38	0/3/3/3
2	08T	H	400	1,3	-	3/12/38/38	0/3/3/3
2	08T	S	400	3	-	5/12/38/38	0/3/3/3
2	08T	M	400	3	-	4/12/38/38	0/3/3/3
2	08T	T	400	1,3	-	5/12/38/38	0/3/3/3

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	08T	F2-BE	-8.09	1.34	1.54
2	O	400	08T	F2-BE	-7.94	1.34	1.54
2	H	400	08T	F2-BE	-7.86	1.35	1.54
2	D	400	08T	F2-BE	-7.72	1.35	1.54
2	N	400	08T	F2-BE	-7.70	1.35	1.54
2	I	400	08T	F2-BE	-7.66	1.35	1.54
2	B	400	08T	F2-BE	-7.66	1.35	1.54
2	V	400	08T	F2-BE	-7.66	1.35	1.54
2	P	400	08T	F2-BE	-7.66	1.35	1.54
2	S	400	08T	F2-BE	-7.64	1.35	1.54
2	A	400	08T	F2-BE	-7.63	1.35	1.54
2	J	400	08T	F2-BE	-7.62	1.35	1.54
2	C	400	08T	F2-BE	-7.62	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	400	08T	F2-BE	-7.62	1.35	1.54
2	T	400	08T	F2-BE	-7.62	1.35	1.54
2	U	400	08T	F2-BE	-7.61	1.35	1.54
2	E	400	08T	F2-BE	-7.58	1.35	1.54
2	Q	400	08T	F2-BE	-7.46	1.36	1.54
2	G	400	08T	F1-BE	-7.42	1.36	1.54
2	K	400	08T	F2-BE	-7.39	1.36	1.54
2	W	400	08T	F2-BE	-7.36	1.36	1.54
2	B	400	08T	F1-BE	-7.22	1.36	1.54
2	A	400	08T	F3-BE	-7.20	1.36	1.54
2	T	400	08T	F1-BE	-7.17	1.36	1.54
2	K	400	08T	F1-BE	-7.13	1.36	1.54
2	O	400	08T	F1-BE	-7.13	1.36	1.54
2	V	400	08T	F1-BE	-7.07	1.36	1.54
2	W	400	08T	F1-BE	-7.07	1.36	1.54
2	D	400	08T	F1-BE	-7.05	1.37	1.54
2	C	400	08T	F1-BE	-7.05	1.37	1.54
2	M	400	08T	F1-BE	-7.05	1.37	1.54
2	Q	400	08T	F1-BE	-7.05	1.37	1.54
2	E	400	08T	F1-BE	-7.04	1.37	1.54
2	P	400	08T	F1-BE	-7.04	1.37	1.54
2	E	400	08T	F3-BE	-7.04	1.37	1.54
2	J	400	08T	F1-BE	-7.04	1.37	1.54
2	U	400	08T	F1-BE	-7.03	1.37	1.54
2	W	400	08T	F3-BE	-7.03	1.37	1.54
2	P	400	08T	F3-BE	-7.01	1.37	1.54
2	H	400	08T	F1-BE	-7.00	1.37	1.54
2	O	400	08T	F3-BE	-6.99	1.37	1.54
2	N	400	08T	F1-BE	-6.99	1.37	1.54
2	A	400	08T	F1-BE	-6.98	1.37	1.54
2	J	400	08T	F3-BE	-6.97	1.37	1.54
2	S	400	08T	F1-BE	-6.97	1.37	1.54
2	K	400	08T	F3-BE	-6.96	1.37	1.54
2	I	400	08T	F1-BE	-6.96	1.37	1.54
2	B	400	08T	F3-BE	-6.95	1.37	1.54
2	D	400	08T	F3-BE	-6.95	1.37	1.54
2	S	400	08T	F3-BE	-6.94	1.37	1.54
2	Q	400	08T	F3-BE	-6.93	1.37	1.54
2	M	400	08T	F3-BE	-6.92	1.37	1.54
2	V	400	08T	F3-BE	-6.92	1.37	1.54
2	H	400	08T	F3-BE	-6.92	1.37	1.54
2	C	400	08T	F3-BE	-6.92	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	400	08T	F3-BE	-6.91	1.37	1.54
2	G	400	08T	F3-BE	-6.90	1.37	1.54
2	N	400	08T	F3-BE	-6.90	1.37	1.54
2	T	400	08T	F3-BE	-6.82	1.37	1.54
2	H	400	08T	O4'-C1'	6.66	1.50	1.41
2	N	400	08T	O4'-C1'	6.59	1.50	1.41
2	P	400	08T	O4'-C1'	6.56	1.50	1.41
2	I	400	08T	F3-BE	-6.53	1.38	1.54
2	E	400	08T	O4'-C1'	6.53	1.50	1.41
2	Q	400	08T	O4'-C1'	6.49	1.50	1.41
2	S	400	08T	O4'-C1'	6.49	1.50	1.41
2	D	400	08T	O4'-C1'	6.47	1.50	1.41
2	T	400	08T	O4'-C1'	6.47	1.50	1.41
2	B	400	08T	O4'-C1'	6.45	1.50	1.41
2	A	400	08T	O4'-C1'	6.40	1.50	1.41
2	U	400	08T	O4'-C1'	6.39	1.50	1.41
2	K	400	08T	O4'-C1'	6.37	1.50	1.41
2	I	400	08T	O4'-C1'	6.36	1.50	1.41
2	W	400	08T	O4'-C1'	6.35	1.49	1.41
2	V	400	08T	O4'-C1'	6.30	1.49	1.41
2	O	400	08T	O4'-C1'	6.27	1.49	1.41
2	M	400	08T	O4'-C1'	6.27	1.49	1.41
2	C	400	08T	O4'-C1'	6.26	1.49	1.41
2	J	400	08T	O4'-C1'	6.19	1.49	1.41
2	G	400	08T	O4'-C1'	6.14	1.49	1.41
2	I	400	08T	C2'-C1'	-4.19	1.47	1.53
2	O	400	08T	C5-C4	-4.06	1.30	1.40
2	U	400	08T	C2'-C1'	-4.05	1.47	1.53
2	J	400	08T	C2'-C1'	-4.05	1.47	1.53
2	C	400	08T	C2'-C1'	-4.04	1.47	1.53
2	D	400	08T	C5-C4	-4.03	1.30	1.40
2	S	400	08T	C5-C4	-4.03	1.30	1.40
2	P	400	08T	C5-C4	-4.02	1.30	1.40
2	J	400	08T	C5-C4	-4.01	1.30	1.40
2	A	400	08T	C5-C4	-4.00	1.30	1.40
2	M	400	08T	C5-C4	-4.00	1.30	1.40
2	E	400	08T	C5-C4	-4.00	1.30	1.40
2	G	400	08T	C5-C4	-4.00	1.30	1.40
2	B	400	08T	C5-C4	-4.00	1.30	1.40
2	K	400	08T	C5-C4	-3.99	1.30	1.40
2	Q	400	08T	C5-C4	-3.99	1.30	1.40
2	C	400	08T	C5-C4	-3.98	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	400	08T	C5-C4	-3.98	1.30	1.40
2	W	400	08T	C2'-C1'	-3.98	1.47	1.53
2	T	400	08T	C5-C4	-3.97	1.30	1.40
2	W	400	08T	C5-C4	-3.97	1.30	1.40
2	V	400	08T	C5-C4	-3.96	1.30	1.40
2	H	400	08T	C5-C4	-3.95	1.30	1.40
2	H	400	08T	C2'-C1'	-3.95	1.47	1.53
2	A	400	08T	C2'-C1'	-3.95	1.47	1.53
2	P	400	08T	C2'-C1'	-3.93	1.47	1.53
2	V	400	08T	C2'-C1'	-3.93	1.47	1.53
2	S	400	08T	C2'-C1'	-3.93	1.47	1.53
2	O	400	08T	C2'-C1'	-3.92	1.47	1.53
2	N	400	08T	C5-C4	-3.92	1.30	1.40
2	I	400	08T	C5-C4	-3.92	1.30	1.40
2	G	400	08T	C2'-C1'	-3.91	1.47	1.53
2	M	400	08T	C2'-C1'	-3.89	1.47	1.53
2	H	400	08T	C2-N3	3.89	1.38	1.32
2	K	400	08T	C2'-C1'	-3.82	1.48	1.53
2	I	400	08T	C2-N3	3.81	1.38	1.32
2	U	400	08T	C2-N3	3.81	1.38	1.32
2	D	400	08T	C2'-C1'	-3.80	1.48	1.53
2	Q	400	08T	C2-N3	3.78	1.38	1.32
2	T	400	08T	C2'-C1'	-3.76	1.48	1.53
2	P	400	08T	C2-N3	3.75	1.38	1.32
2	W	400	08T	C2-N3	3.75	1.38	1.32
2	E	400	08T	C2-N3	3.73	1.38	1.32
2	T	400	08T	C2-N3	3.72	1.38	1.32
2	N	400	08T	C2-N3	3.71	1.38	1.32
2	V	400	08T	C2-N3	3.71	1.38	1.32
2	G	400	08T	C2-N3	3.70	1.38	1.32
2	K	400	08T	C2-N3	3.70	1.38	1.32
2	B	400	08T	C2-N3	3.69	1.38	1.32
2	S	400	08T	C2-N3	3.69	1.38	1.32
2	Q	400	08T	C2'-C1'	-3.68	1.48	1.53
2	B	400	08T	C2'-C1'	-3.68	1.48	1.53
2	J	400	08T	C2-N3	3.67	1.38	1.32
2	E	400	08T	C2'-C1'	-3.67	1.48	1.53
2	M	400	08T	C2-N3	3.67	1.38	1.32
2	C	400	08T	C2-N3	3.61	1.37	1.32
2	O	400	08T	C2-N3	3.60	1.37	1.32
2	A	400	08T	C2-N3	3.59	1.37	1.32
2	D	400	08T	C2-N3	3.53	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	400	08T	C2'-C1'	-3.53	1.48	1.53
2	N	400	08T	C5-N7	-3.31	1.27	1.39
2	B	400	08T	C5-N7	-3.30	1.27	1.39
2	O	400	08T	C5-N7	-3.30	1.27	1.39
2	W	400	08T	C5-N7	-3.30	1.27	1.39
2	T	400	08T	C5-N7	-3.29	1.27	1.39
2	I	400	08T	C5-N7	-3.29	1.27	1.39
2	C	400	08T	C5-N7	-3.28	1.27	1.39
2	H	400	08T	C5-N7	-3.28	1.27	1.39
2	I	400	08T	C2'-C3'	-3.27	1.44	1.53
2	V	400	08T	C5-N7	-3.27	1.27	1.39
2	K	400	08T	C5-N7	-3.26	1.27	1.39
2	M	400	08T	C5-N7	-3.26	1.27	1.39
2	U	400	08T	C5-N7	-3.26	1.27	1.39
2	P	400	08T	C5-N7	-3.25	1.27	1.39
2	Q	400	08T	C5-N7	-3.25	1.27	1.39
2	A	400	08T	C5-N7	-3.25	1.27	1.39
2	S	400	08T	C5-N7	-3.25	1.27	1.39
2	G	400	08T	C5-N7	-3.23	1.28	1.39
2	V	400	08T	C2'-C3'	-3.22	1.44	1.53
2	E	400	08T	C5-N7	-3.22	1.28	1.39
2	J	400	08T	C5-N7	-3.22	1.28	1.39
2	D	400	08T	C5-N7	-3.21	1.28	1.39
2	U	400	08T	C2'-C3'	-3.14	1.44	1.53
2	S	400	08T	C2'-C3'	-3.11	1.44	1.53
2	P	400	08T	C2'-C3'	-3.11	1.44	1.53
2	M	400	08T	C2'-C3'	-3.10	1.44	1.53
2	A	400	08T	C2'-C3'	-3.10	1.44	1.53
2	C	400	08T	C2'-C3'	-3.08	1.44	1.53
2	W	400	08T	C2'-C3'	-3.08	1.44	1.53
2	D	400	08T	C2'-C3'	-3.07	1.44	1.53
2	O	400	08T	C2'-C3'	-3.03	1.45	1.53
2	J	400	08T	C2'-C3'	-3.00	1.45	1.53
2	K	400	08T	C2'-C3'	-2.97	1.45	1.53
2	T	400	08T	C2'-C3'	-2.97	1.45	1.53
2	B	400	08T	C2'-C3'	-2.93	1.45	1.53
2	H	400	08T	C2'-C3'	-2.93	1.45	1.53
2	E	400	08T	C2'-C3'	-2.90	1.45	1.53
2	N	400	08T	C2'-C3'	-2.90	1.45	1.53
2	Q	400	08T	C2'-C3'	-2.89	1.45	1.53
2	G	400	08T	C2'-C3'	-2.86	1.45	1.53
2	N	400	08T	C6-N6	2.48	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	400	08T	C6-N6	2.47	1.43	1.34
2	U	400	08T	C6-N6	2.46	1.43	1.34
2	B	400	08T	C6-N6	2.45	1.43	1.34
2	D	400	08T	C6-N6	2.45	1.43	1.34
2	E	400	08T	C6-N6	2.44	1.42	1.34
2	Q	400	08T	C6-N6	2.44	1.42	1.34
2	I	400	08T	C6-N6	2.44	1.42	1.34
2	P	400	08T	C6-N6	2.44	1.42	1.34
2	H	400	08T	C6-N6	2.43	1.42	1.34
2	W	400	08T	C6-N6	2.43	1.42	1.34
2	T	400	08T	C6-N6	2.43	1.42	1.34
2	C	400	08T	C6-N6	2.43	1.42	1.34
2	K	400	08T	C6-N6	2.43	1.42	1.34
2	G	400	08T	C6-N6	2.42	1.42	1.34
2	S	400	08T	C6-N6	2.42	1.42	1.34
2	M	400	08T	C6-N6	2.42	1.42	1.34
2	A	400	08T	C6-N6	2.41	1.42	1.34
4	L	400	ADP	C5-C4	2.41	1.47	1.40
2	J	400	08T	C6-N6	2.38	1.42	1.34
4	X	400	ADP	C5-C4	2.38	1.47	1.40
2	O	400	08T	C6-N6	2.26	1.42	1.34

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	400	08T	C4-C5-N7	5.67	115.31	109.40
2	N	400	08T	C4-C5-N7	5.61	115.25	109.40
2	B	400	08T	N3-C2-N1	-5.59	119.94	128.68
2	D	400	08T	N3-C2-N1	-5.59	119.95	128.68
2	A	400	08T	N3-C2-N1	-5.58	119.95	128.68
2	G	400	08T	N3-C2-N1	-5.58	119.96	128.68
2	H	400	08T	N3-C2-N1	-5.55	120.01	128.68
2	P	400	08T	N3-C2-N1	-5.55	120.01	128.68
2	J	400	08T	N3-C2-N1	-5.54	120.02	128.68
2	K	400	08T	C4-C5-N7	5.53	115.16	109.40
2	E	400	08T	N3-C2-N1	-5.53	120.03	128.68
2	H	400	08T	C4-C5-N7	5.53	115.16	109.40
2	S	400	08T	N3-C2-N1	-5.52	120.04	128.68
2	U	400	08T	N3-C2-N1	-5.51	120.06	128.68
2	M	400	08T	N3-C2-N1	-5.50	120.07	128.68
2	W	400	08T	N3-C2-N1	-5.50	120.08	128.68
2	O	400	08T	C4-C5-N7	5.50	115.13	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	08T	N3-C2-N1	-5.50	120.09	128.68
2	T	400	08T	N3-C2-N1	-5.50	120.09	128.68
2	M	400	08T	C4-C5-N7	5.49	115.12	109.40
2	K	400	08T	N3-C2-N1	-5.48	120.11	128.68
2	B	400	08T	C4-C5-N7	5.48	115.11	109.40
2	I	400	08T	C4-C5-N7	5.48	115.11	109.40
2	P	400	08T	C4-C5-N7	5.48	115.11	109.40
2	U	400	08T	C4-C5-N7	5.48	115.11	109.40
2	C	400	08T	C4-C5-N7	5.48	115.11	109.40
2	I	400	08T	N3-C2-N1	-5.47	120.12	128.68
2	V	400	08T	N3-C2-N1	-5.47	120.12	128.68
2	V	400	08T	C4-C5-N7	5.47	115.10	109.40
2	G	400	08T	C4-C5-N7	5.47	115.09	109.40
2	S	400	08T	C4-C5-N7	5.47	115.09	109.40
2	A	400	08T	C4-C5-N7	5.44	115.07	109.40
2	T	400	08T	C4-C5-N7	5.44	115.07	109.40
2	Q	400	08T	N3-C2-N1	-5.41	120.23	128.68
2	N	400	08T	N3-C2-N1	-5.40	120.23	128.68
2	D	400	08T	C4-C5-N7	5.36	114.99	109.40
2	Q	400	08T	C4-C5-N7	5.32	114.94	109.40
2	E	400	08T	C4-C5-N7	5.31	114.94	109.40
2	J	400	08T	C4-C5-N7	5.24	114.86	109.40
2	O	400	08T	N3-C2-N1	-5.22	120.52	128.68
2	Q	400	08T	C3'-C2'-C1'	4.57	107.86	100.98
2	G	400	08T	C3'-C2'-C1'	4.43	107.65	100.98
2	A	400	08T	PB-O3A-PA	-3.97	119.21	132.83
2	Q	400	08T	PB-O3A-PA	-3.89	119.47	132.83
2	J	400	08T	C3'-C2'-C1'	3.82	106.73	100.98
2	B	400	08T	C3'-C2'-C1'	3.78	106.67	100.98
2	M	400	08T	C3'-C2'-C1'	3.75	106.63	100.98
2	C	400	08T	PB-O3A-PA	-3.65	120.30	132.83
2	T	400	08T	C3'-C2'-C1'	3.65	106.47	100.98
4	X	400	ADP	N3-C2-N1	-3.60	123.05	128.68
4	L	400	ADP	N3-C2-N1	-3.59	123.07	128.68
2	E	400	08T	PB-O3A-PA	-3.58	120.55	132.83
2	N	400	08T	C3'-C2'-C1'	3.56	106.33	100.98
4	X	400	ADP	C3'-C2'-C1'	3.54	106.31	100.98
2	S	400	08T	C3'-C2'-C1'	3.53	106.30	100.98
2	M	400	08T	PB-O3A-PA	-3.51	120.78	132.83
2	E	400	08T	C3'-C2'-C1'	3.50	106.25	100.98
4	L	400	ADP	C3'-C2'-C1'	3.42	106.12	100.98
2	I	400	08T	PB-O3A-PA	-3.41	121.13	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	400	08T	C3'-C2'-C1'	3.39	106.08	100.98
2	U	400	08T	PB-O3A-PA	-3.38	121.24	132.83
2	K	400	08T	C3'-C2'-C1'	3.36	106.03	100.98
2	S	400	08T	PB-O3A-PA	-3.28	121.57	132.83
4	X	400	ADP	PA-O3A-PB	-3.25	121.68	132.83
2	N	400	08T	C1'-N9-C4	3.20	132.26	126.64
2	N	400	08T	PB-O3A-PA	-3.19	121.86	132.83
2	O	400	08T	C3'-C2'-C1'	3.18	105.76	100.98
2	W	400	08T	PB-O3A-PA	-3.06	122.32	132.83
2	H	400	08T	PB-O3A-PA	-3.06	122.33	132.83
2	O	400	08T	PB-O3A-PA	-3.04	122.41	132.83
2	K	400	08T	PB-O3A-PA	-3.03	122.42	132.83
2	H	400	08T	C3'-C2'-C1'	2.95	105.42	100.98
2	D	400	08T	PB-O3A-PA	-2.94	122.75	132.83
2	P	400	08T	PB-O3A-PA	-2.91	122.83	132.83
2	A	400	08T	C3'-C2'-C1'	2.85	105.27	100.98
4	L	400	ADP	C4-C5-N7	-2.84	106.44	109.40
2	C	400	08T	C3'-C2'-C1'	2.78	105.17	100.98
4	X	400	ADP	C4-C5-N7	-2.65	106.64	109.40
2	B	400	08T	PB-O3A-PA	-2.63	123.79	132.83
2	U	400	08T	C3'-C2'-C1'	2.60	104.90	100.98
2	W	400	08T	C3'-C2'-C1'	2.59	104.88	100.98
2	V	400	08T	PB-O3A-PA	-2.56	124.04	132.83
4	L	400	ADP	PA-O3A-PB	-2.55	124.07	132.83
2	G	400	08T	C2'-C3'-C4'	2.55	107.59	102.64
2	V	400	08T	C3'-C2'-C1'	2.50	104.74	100.98
2	P	400	08T	C3'-C2'-C1'	2.40	104.59	100.98
2	G	400	08T	PB-O3A-PA	-2.37	124.69	132.83
2	Q	400	08T	C2'-C3'-C4'	2.36	107.22	102.64
2	H	400	08T	C1'-N9-C4	2.23	130.57	126.64
2	N	400	08T	C5-C6-N1	-2.21	115.33	120.35
2	J	400	08T	C2'-C3'-C4'	2.16	106.84	102.64
2	K	400	08T	N6-C6-N1	2.13	123.00	118.57
2	M	400	08T	C5-C6-N1	-2.13	115.52	120.35
2	D	400	08T	C5-C6-N1	-2.12	115.54	120.35
2	T	400	08T	C5-C6-N1	-2.12	115.54	120.35
2	C	400	08T	C5-C6-N1	-2.12	115.55	120.35
2	V	400	08T	C5-C6-N1	-2.11	115.56	120.35
2	J	400	08T	PB-O3A-PA	-2.11	125.58	132.83
2	J	400	08T	C5-C6-N1	-2.11	115.56	120.35
2	B	400	08T	C5-C6-N1	-2.11	115.57	120.35
2	U	400	08T	C5-C6-N1	-2.11	115.58	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	08T	C5-C6-N1	-2.11	115.58	120.35
2	W	400	08T	N6-C6-N1	2.10	122.94	118.57
2	I	400	08T	C5-C6-N1	-2.10	115.59	120.35
2	W	400	08T	C5-C6-N1	-2.10	115.60	120.35
2	G	400	08T	C5-C6-N1	-2.08	115.64	120.35
2	P	400	08T	C5-C6-N1	-2.07	115.66	120.35
2	T	400	08T	PB-O3A-PA	-2.07	125.72	132.83
2	N	400	08T	N6-C6-N1	2.07	122.86	118.57
2	K	400	08T	C5-C6-N1	-2.06	115.68	120.35
2	S	400	08T	C5-C6-N1	-2.06	115.69	120.35
2	U	400	08T	N6-C6-N1	2.05	122.83	118.57
2	E	400	08T	C5-C6-N1	-2.05	115.71	120.35
2	V	400	08T	N6-C6-N1	2.03	122.80	118.57
2	H	400	08T	C5-C6-N1	-2.03	115.74	120.35
2	H	400	08T	N6-C6-N1	2.02	122.77	118.57
2	Q	400	08T	C5-C6-N1	-2.01	115.80	120.35
2	C	400	08T	N6-C6-N1	2.00	122.73	118.57

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	08T	C5'-O5'-PA-O3A
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	J	400	08T	C5'-O5'-PA-O2A
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	C3'-C4'-C5'-O5'
2	T	400	08T	C5'-O5'-PA-O1A
2	T	400	08T	C5'-O5'-PA-O2A
4	L	400	ADP	C5'-O5'-PA-O1A
2	C	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'

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

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Mol	Chain	Res	Type	Atoms
4	X	400	ADP	PA-O3A-PB-O3B
2	G	400	08T	C5'-O5'-PA-O3A
2	J	400	08T	C5'-O5'-PA-O3A
2	S	400	08T	C5'-O5'-PA-O3A
2	T	400	08T	C5'-O5'-PA-O3A
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
2	U	400	08T	C5'-O5'-PA-O2A
4	L	400	ADP	C3'-C4'-C5'-O5'
2	T	400	08T	C4'-C5'-O5'-PA
2	W	400	08T	C4'-C5'-O5'-PA
2	G	400	08T	PA-O3A-PB-O3B
2	T	400	08T	PA-O3A-PB-O3B

There are no ring outliers.

17 monomers are involved in 39 short contacts:

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

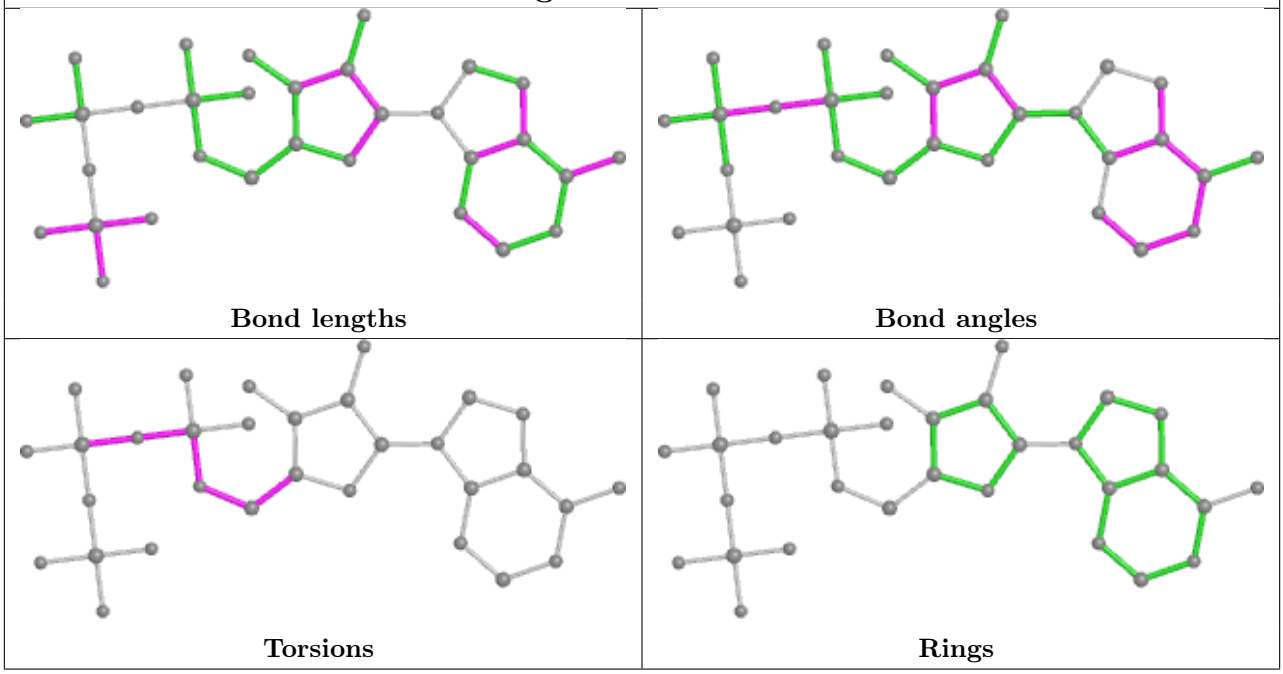
Continued on next page...

Continued from previous page...

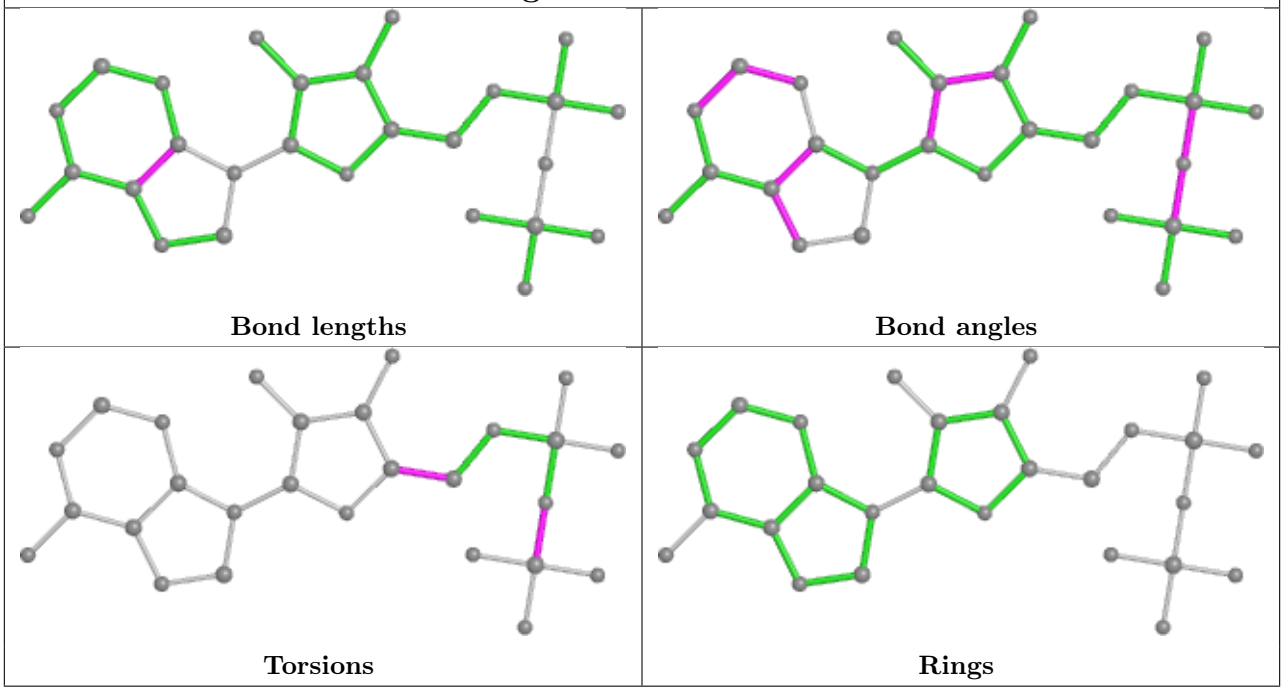
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	400	08T	1	0

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

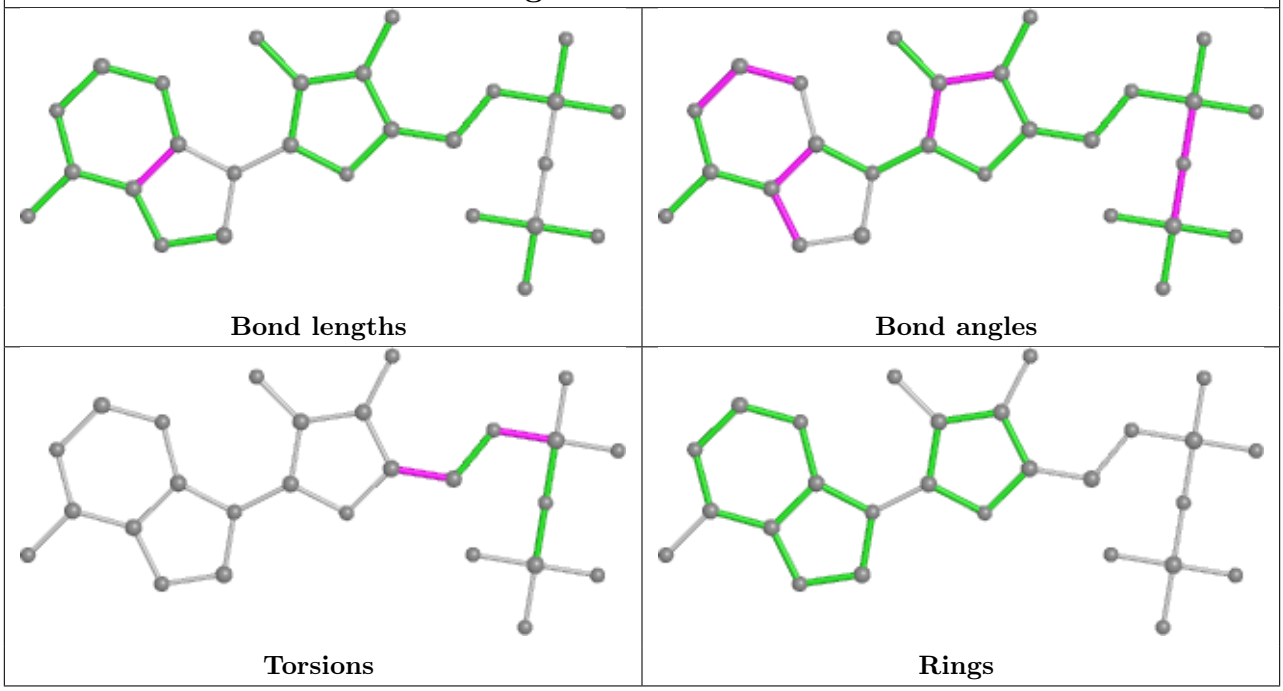
Ligand 08T J 400



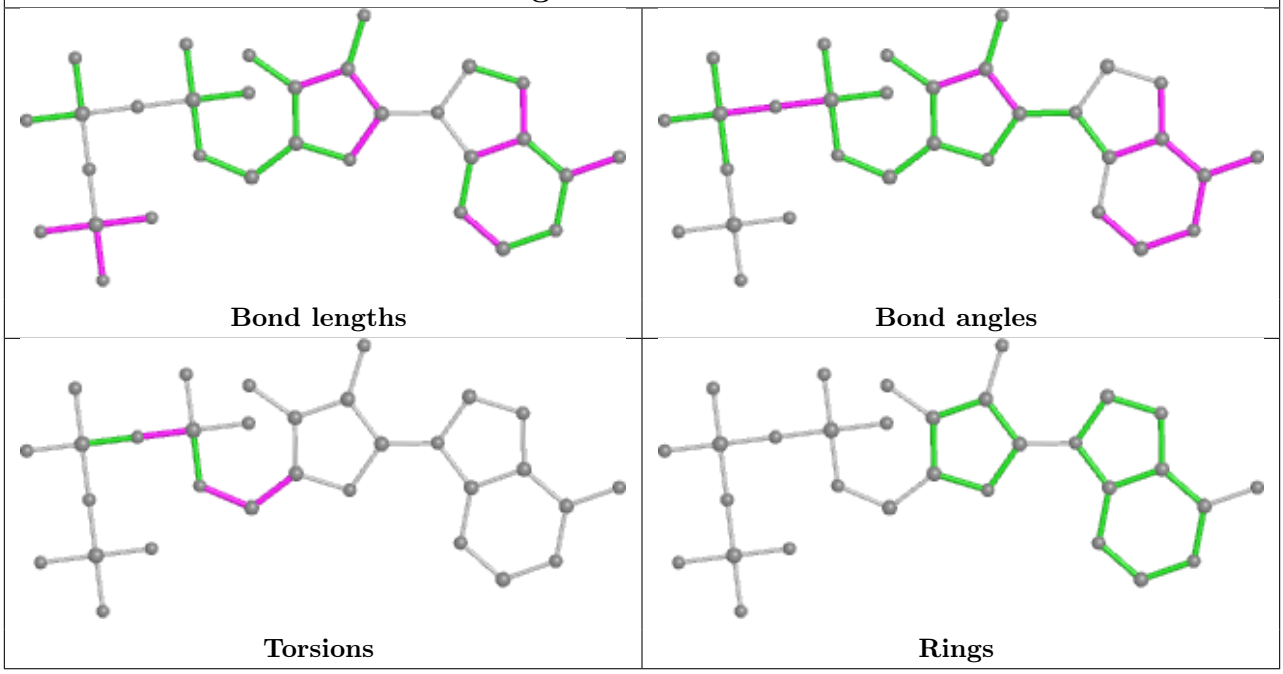
Ligand ADP X 400



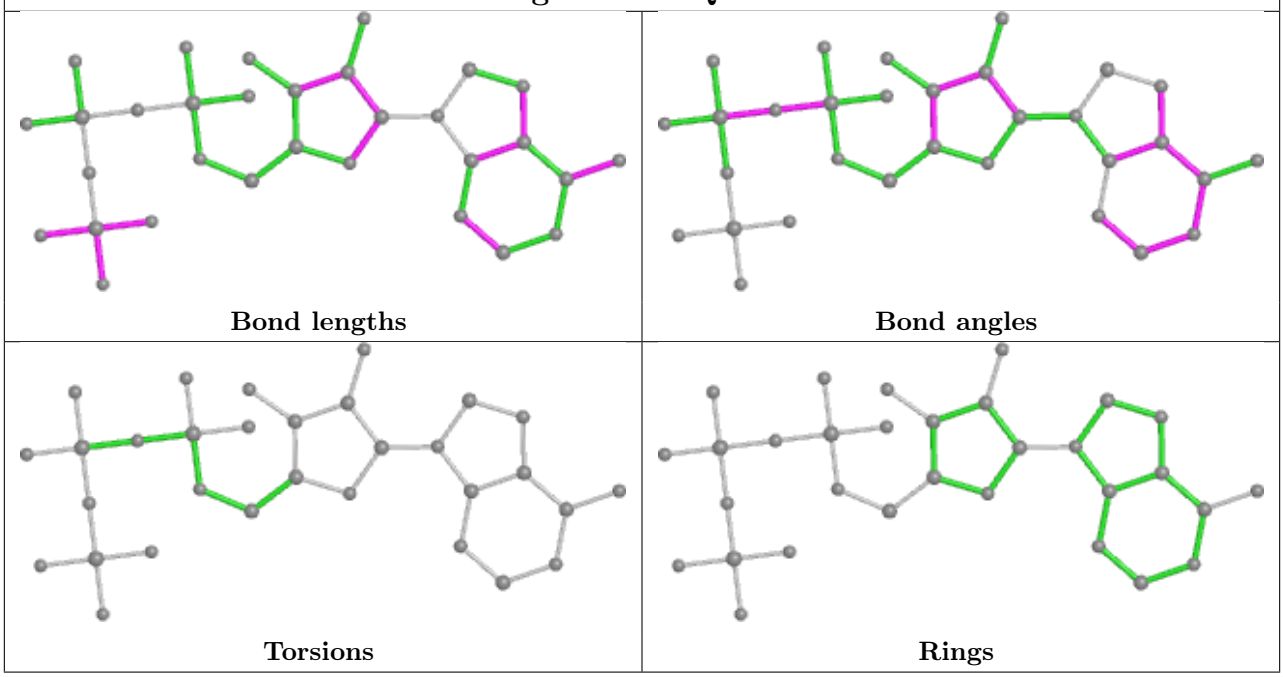
Ligand ADP L 400



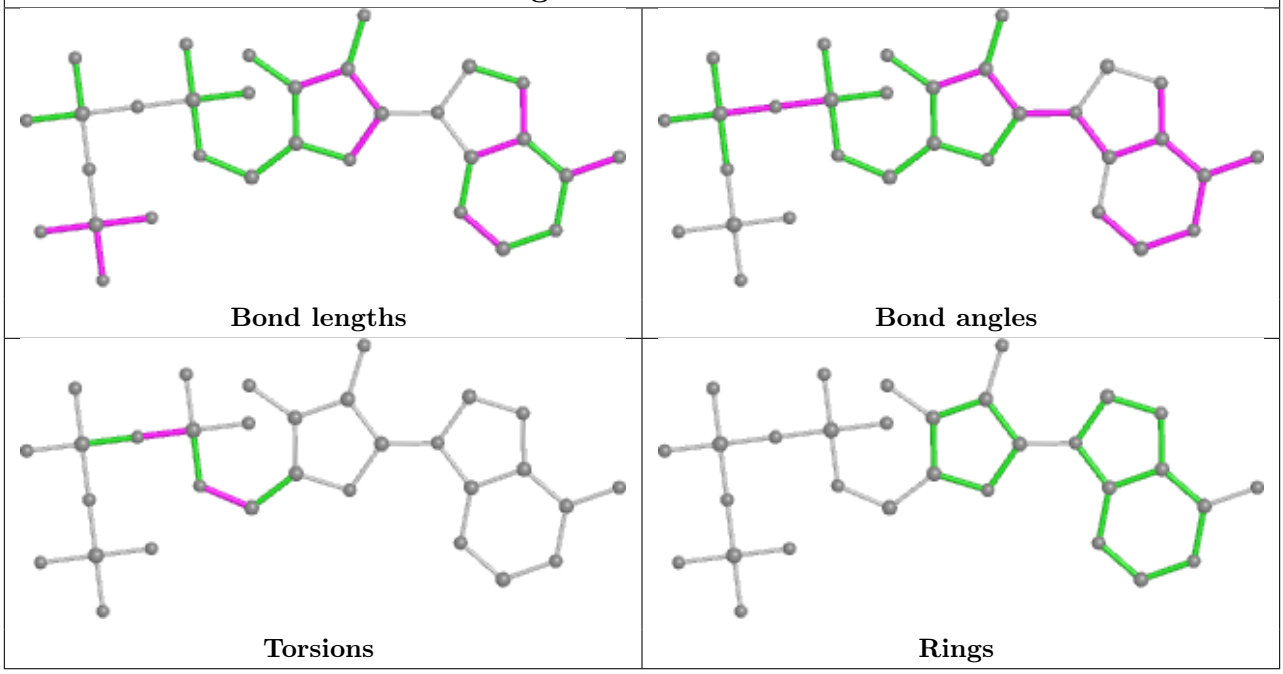
Ligand 08T C 400



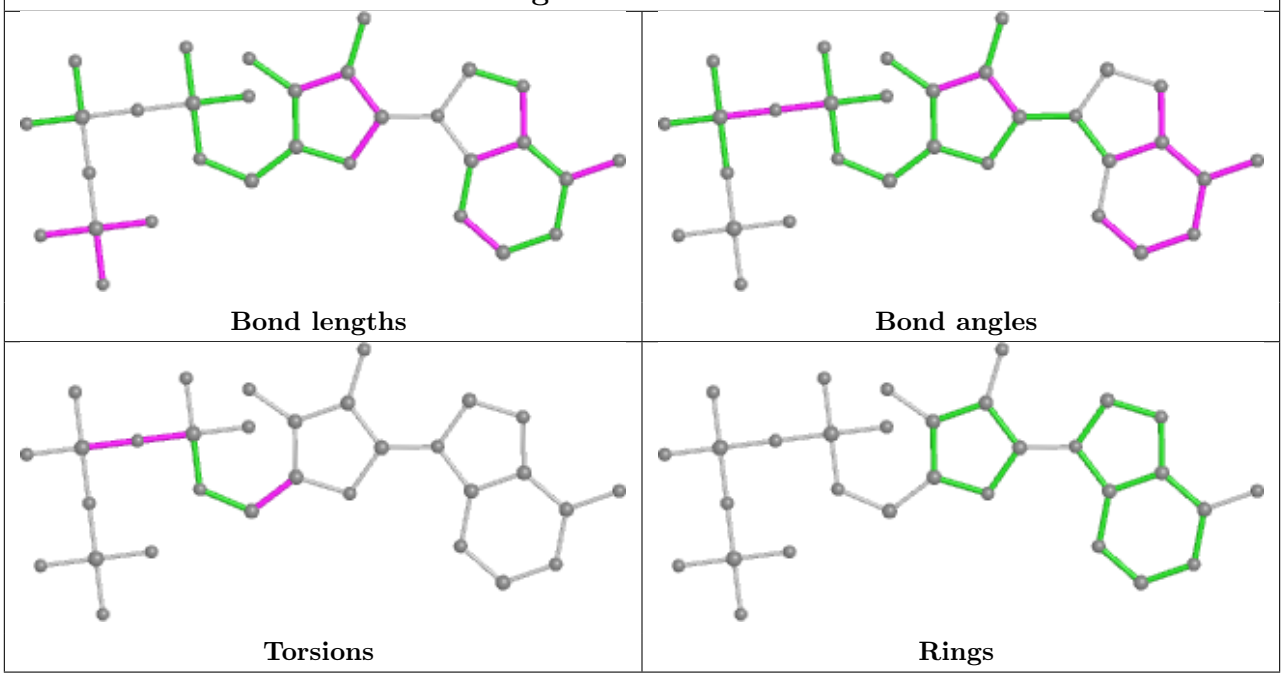
Ligand 08T Q 400



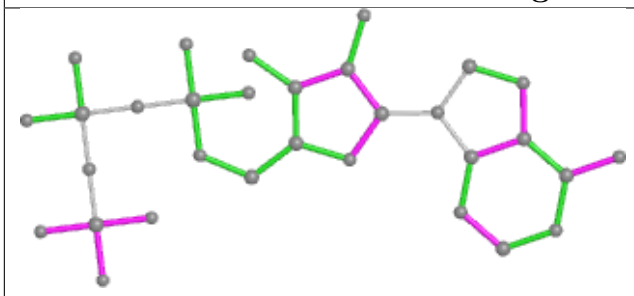
Ligand 08T N 400



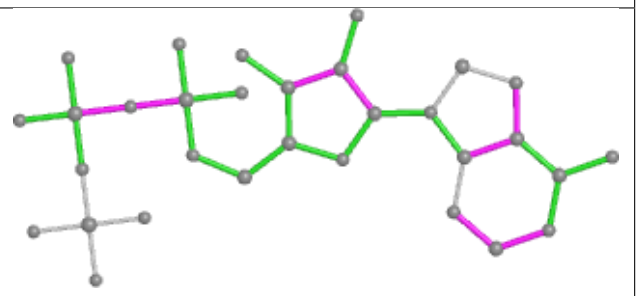
Ligand 08T V 400



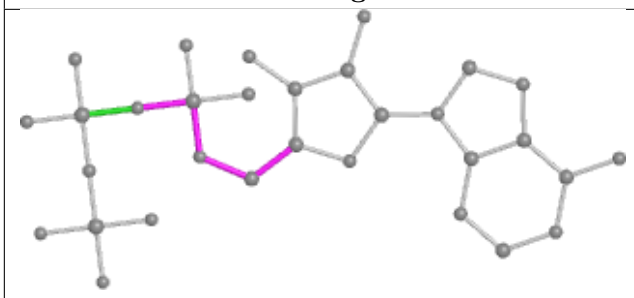
Ligand 08T O 400



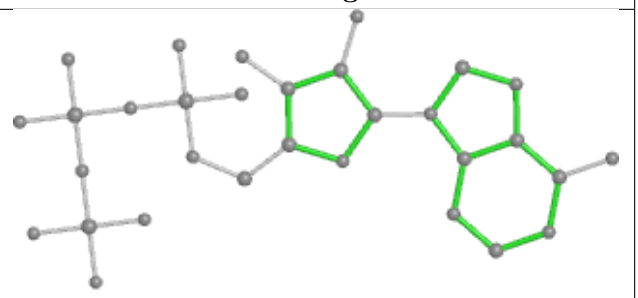
Bond lengths



Bond angles

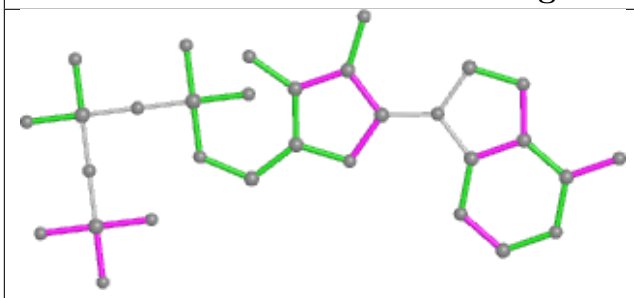


Torsions

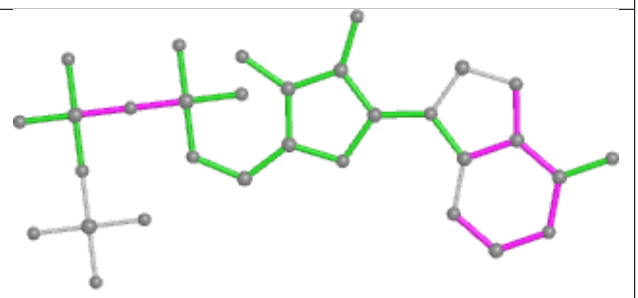


Rings

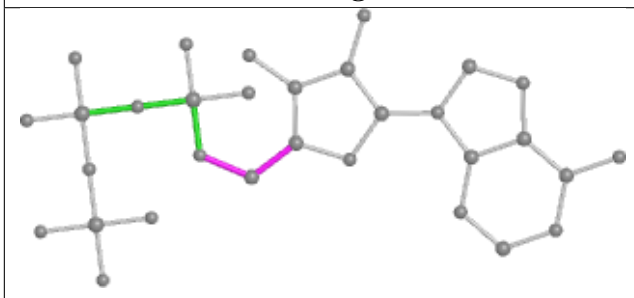
Ligand 08T I 400



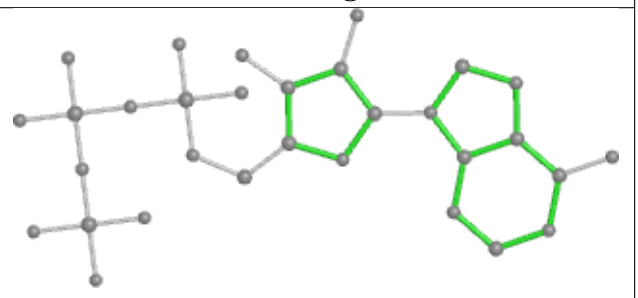
Bond lengths



Bond angles

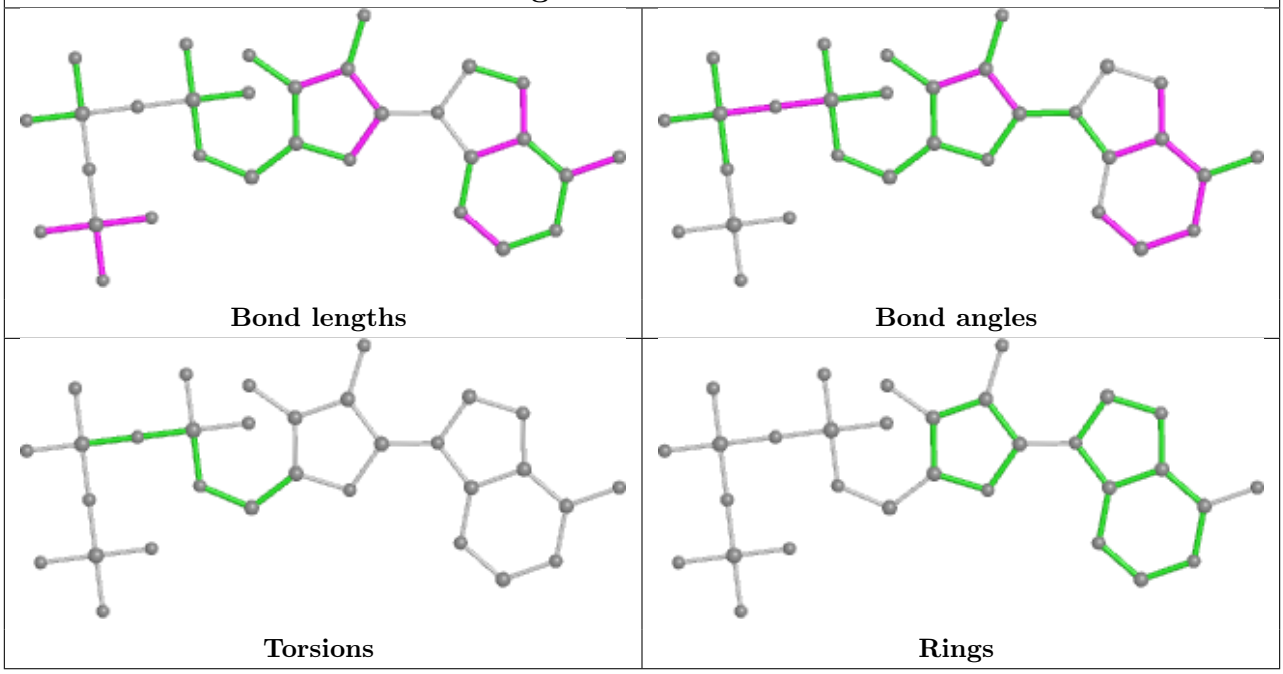


Torsions

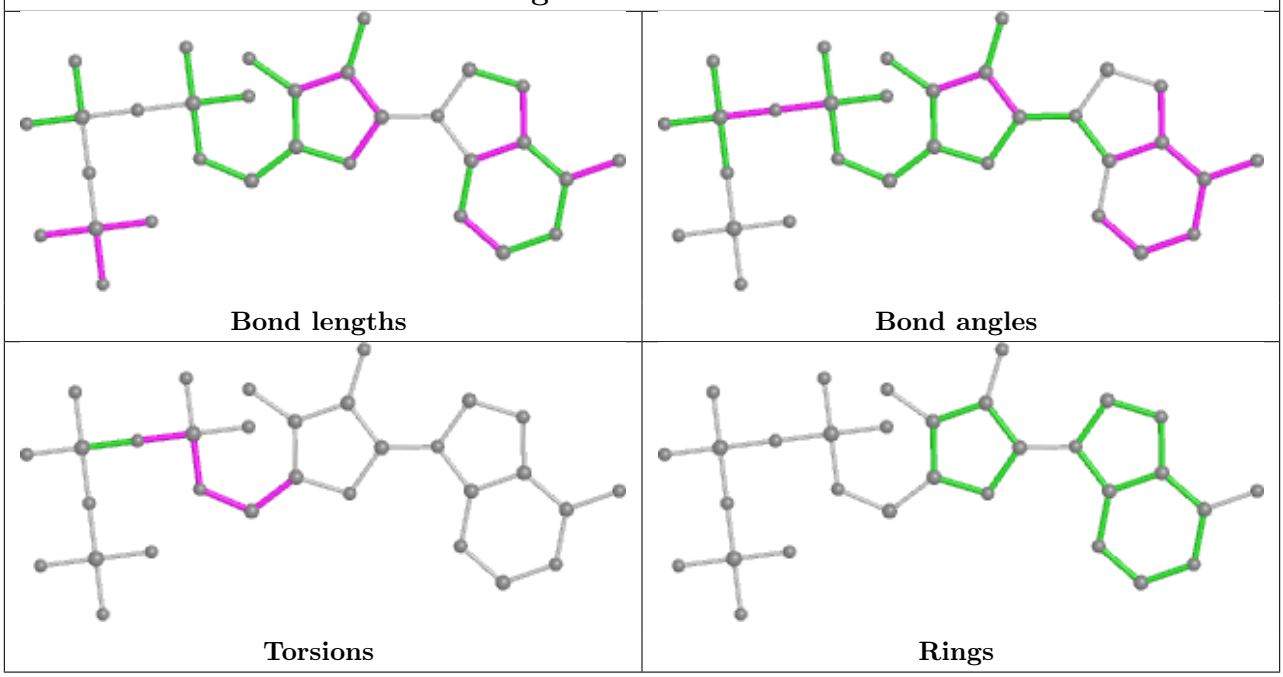


Rings

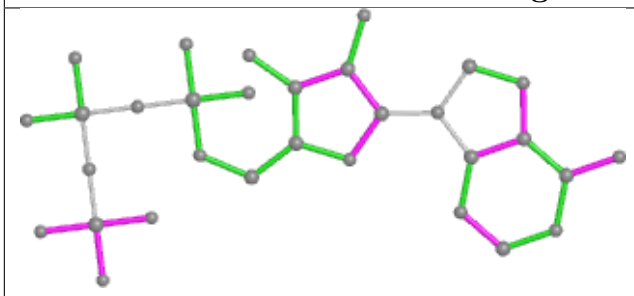
Ligand 08T D 400



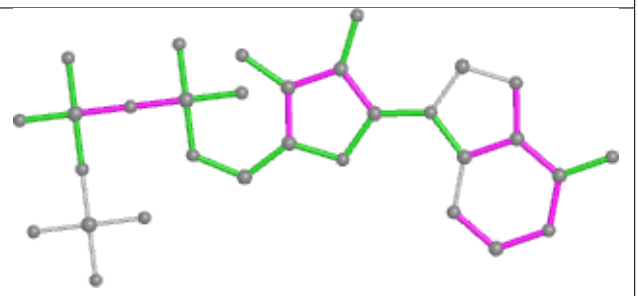
Ligand 08T U 400



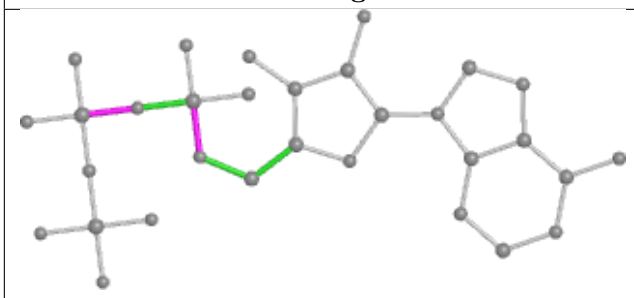
Ligand 08T G 400



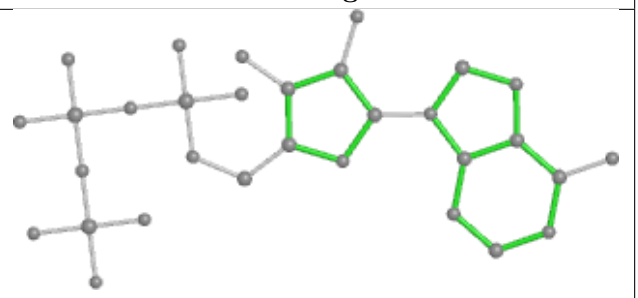
Bond lengths



Bond angles

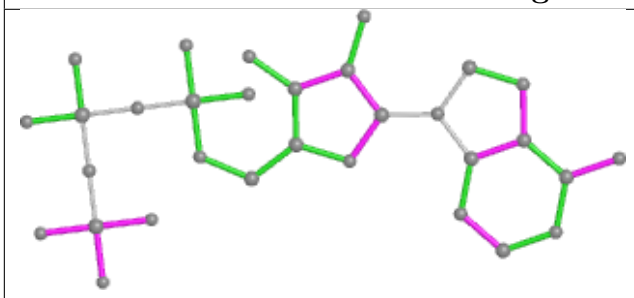


Torsions



Rings

Ligand 08T A 400



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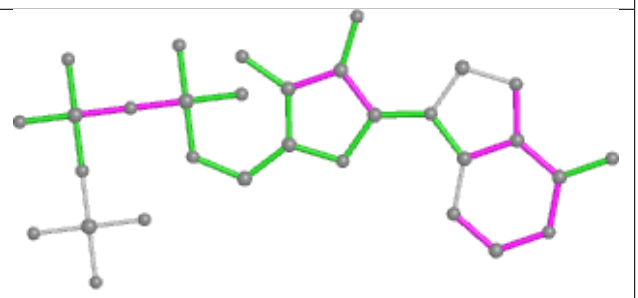
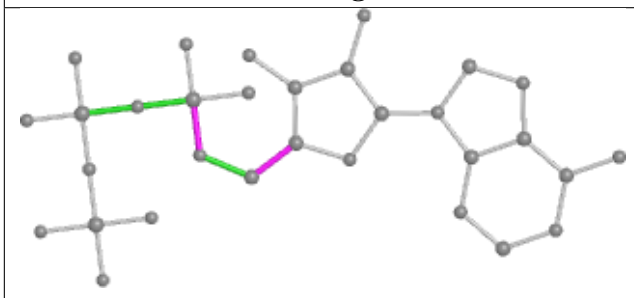
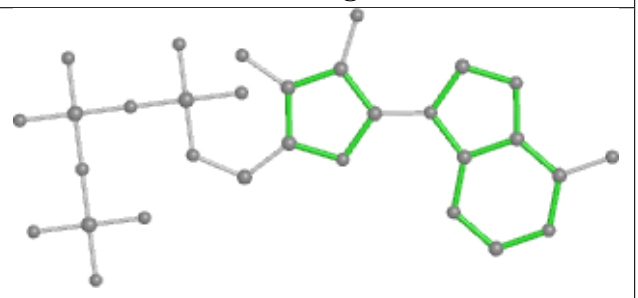


Bond angles

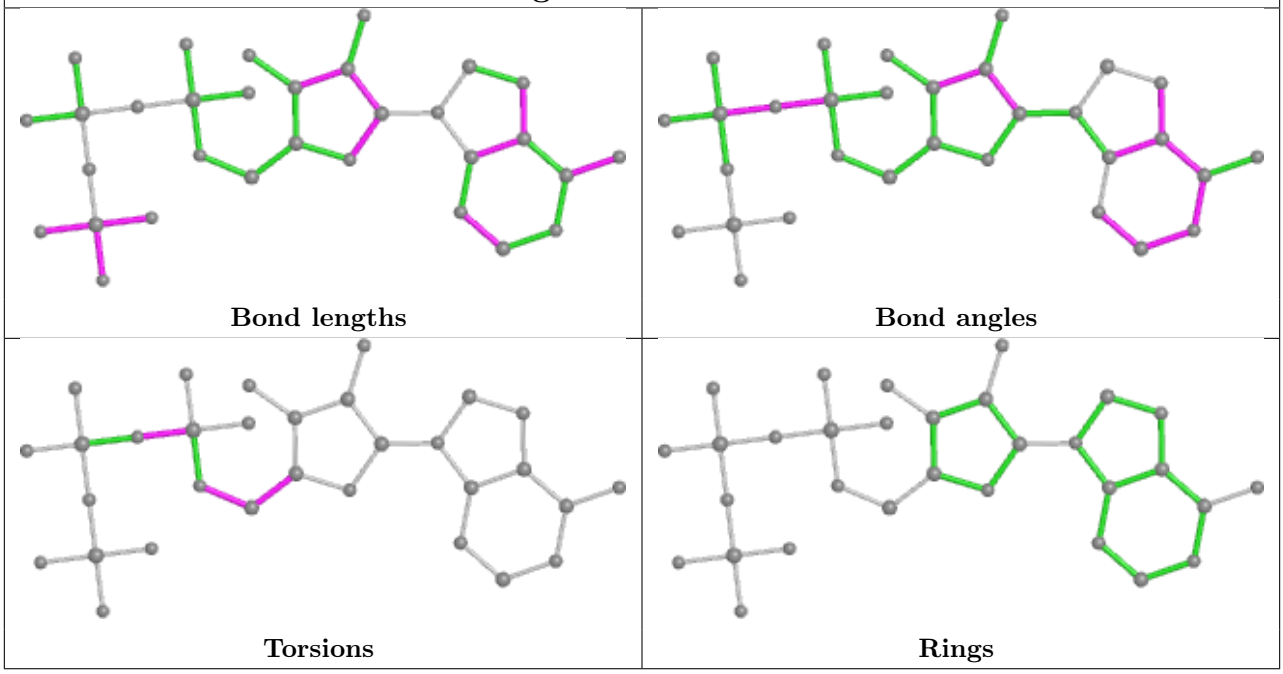


Torsions

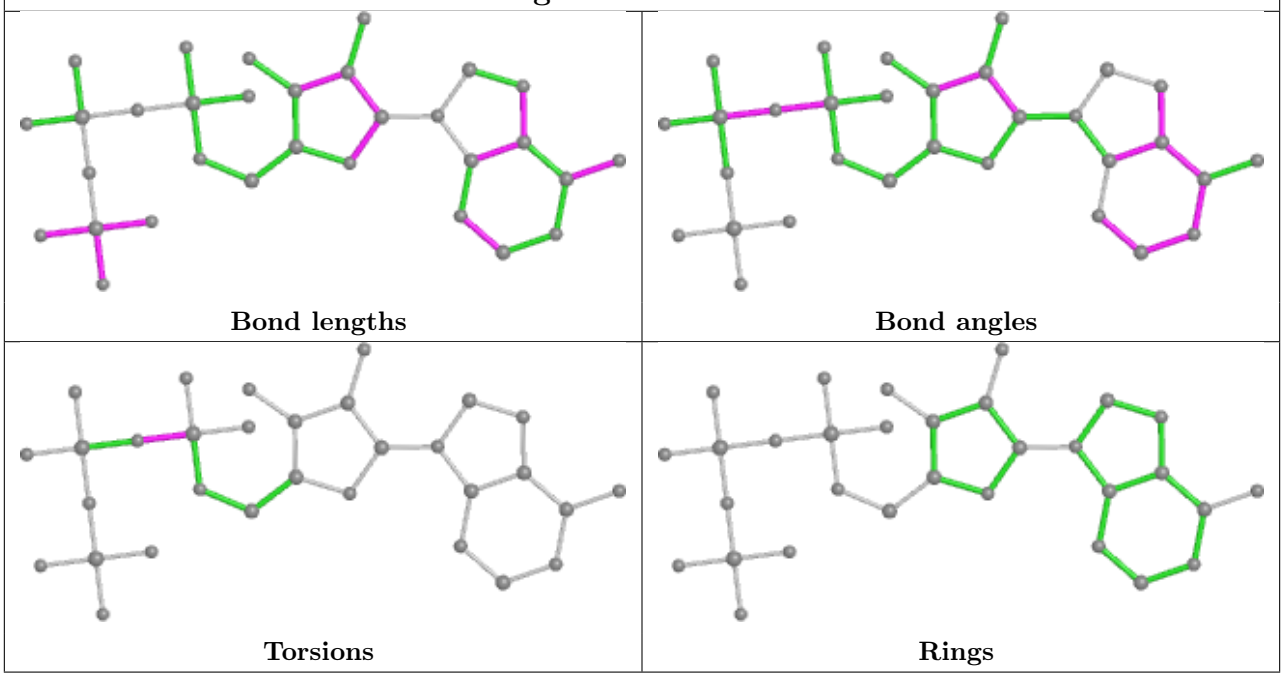


Rings

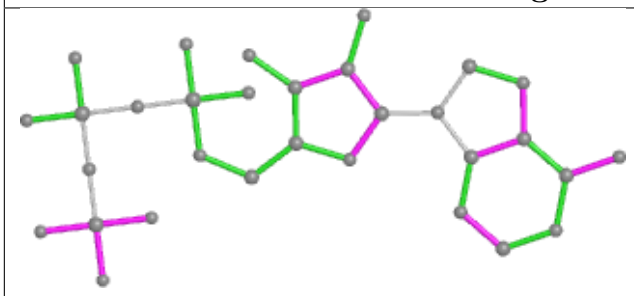
Ligand 08T P 400



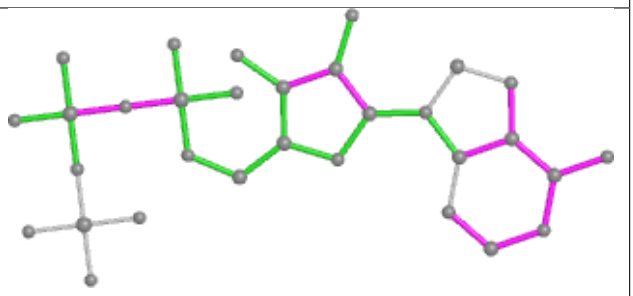
Ligand 08T E 400



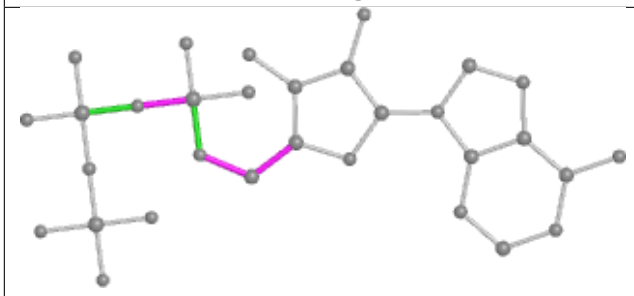
Ligand 08T K 400



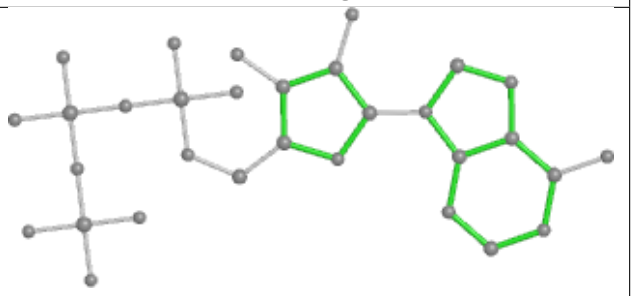
Bond lengths



Bond angles

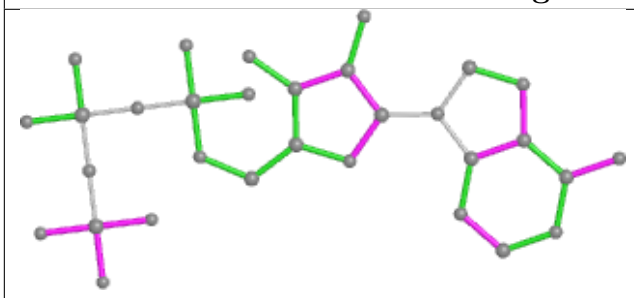


Torsions

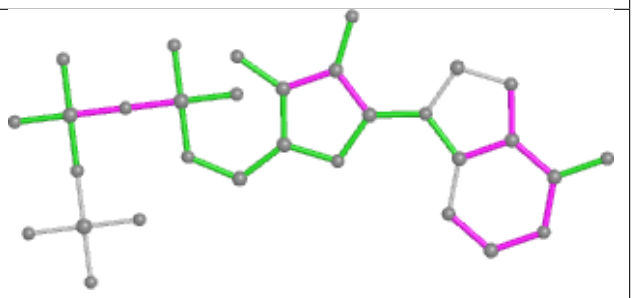


Rings

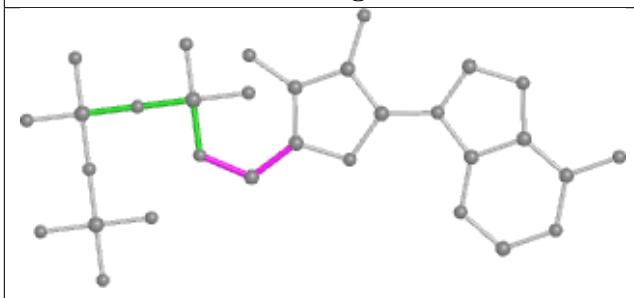
Ligand 08T B 400



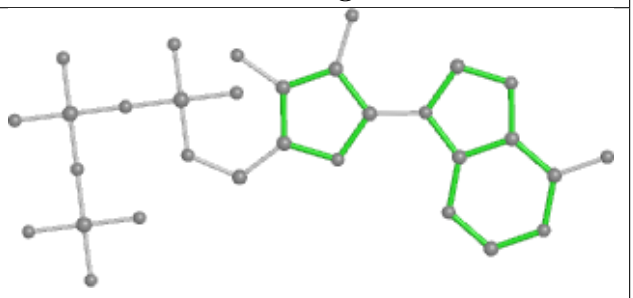
Bond lengths



Bond angles

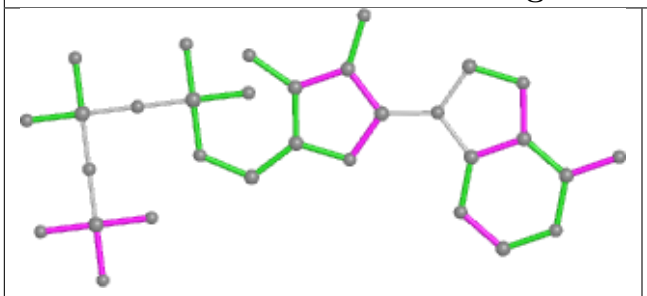


Torsions

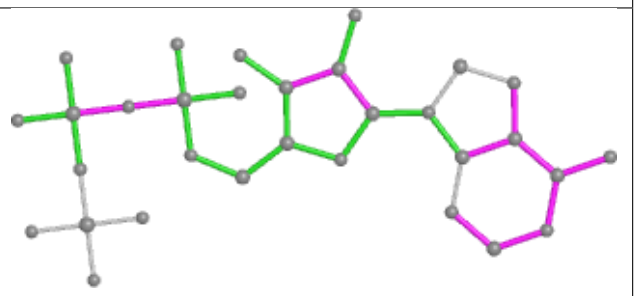


Rings

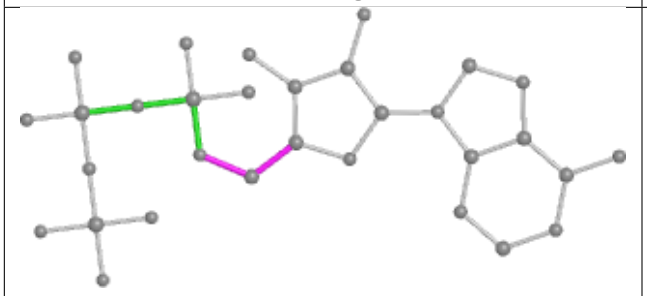
Ligand 08T W 400



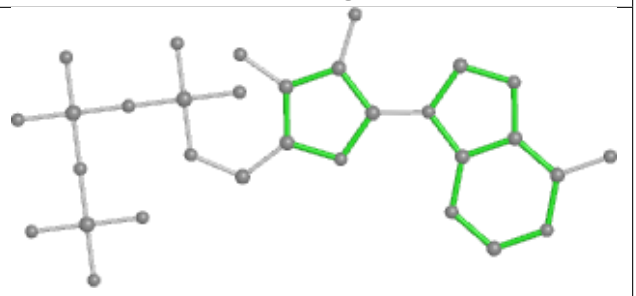
Bond lengths



Bond angles

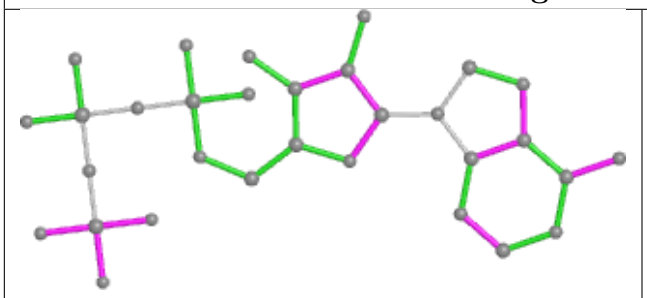


Torsions

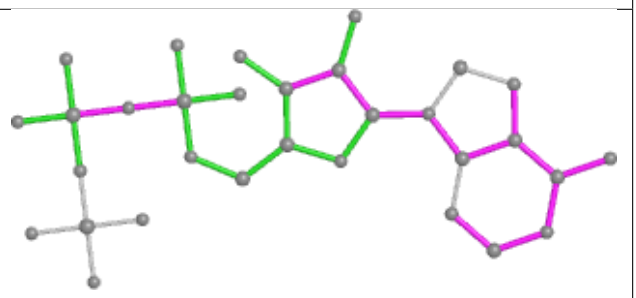


Rings

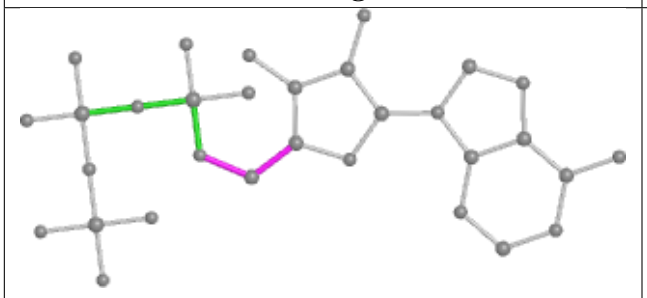
Ligand 08T H 400



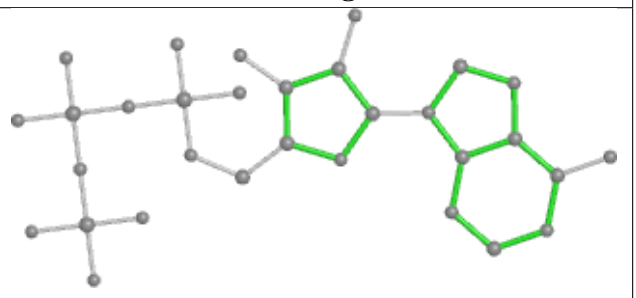
Bond lengths



Bond angles

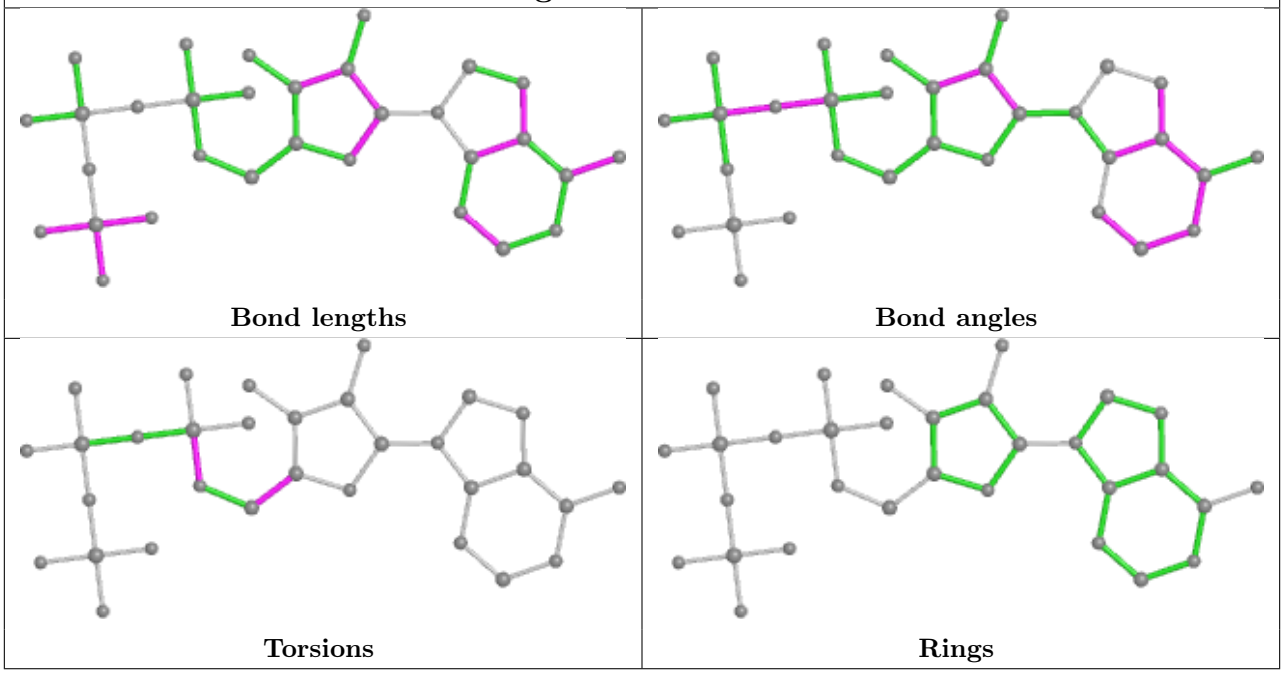


Torsions

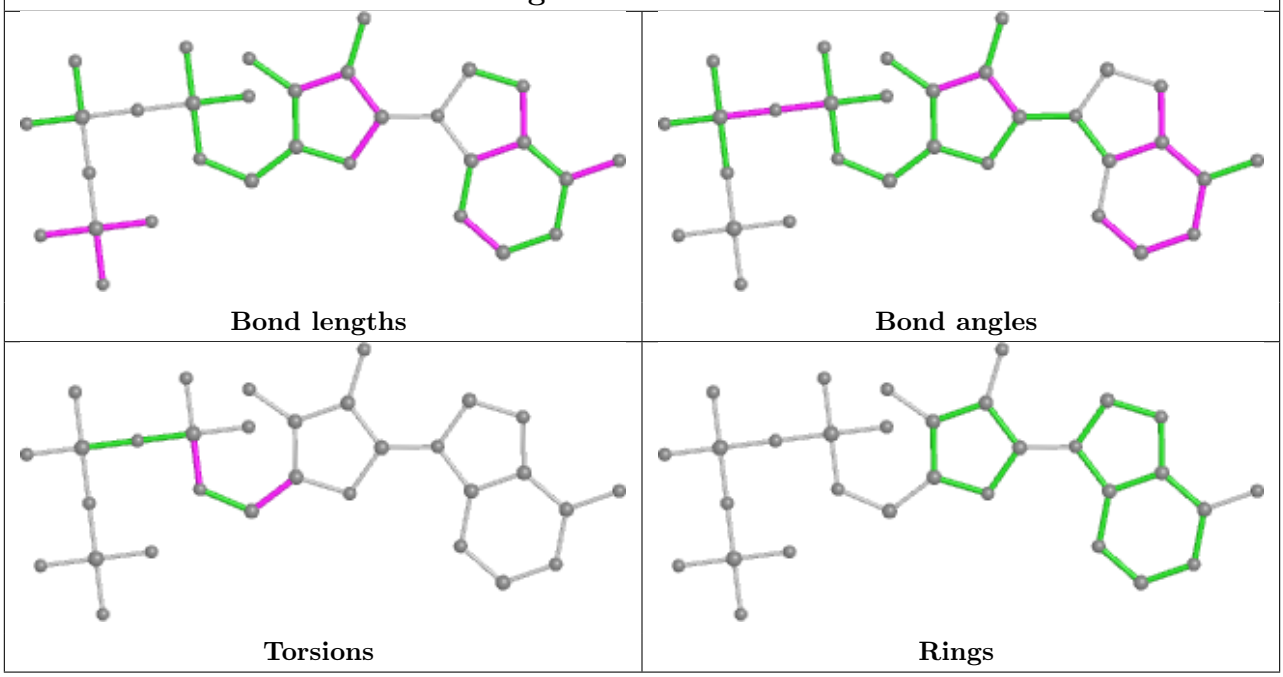


Rings

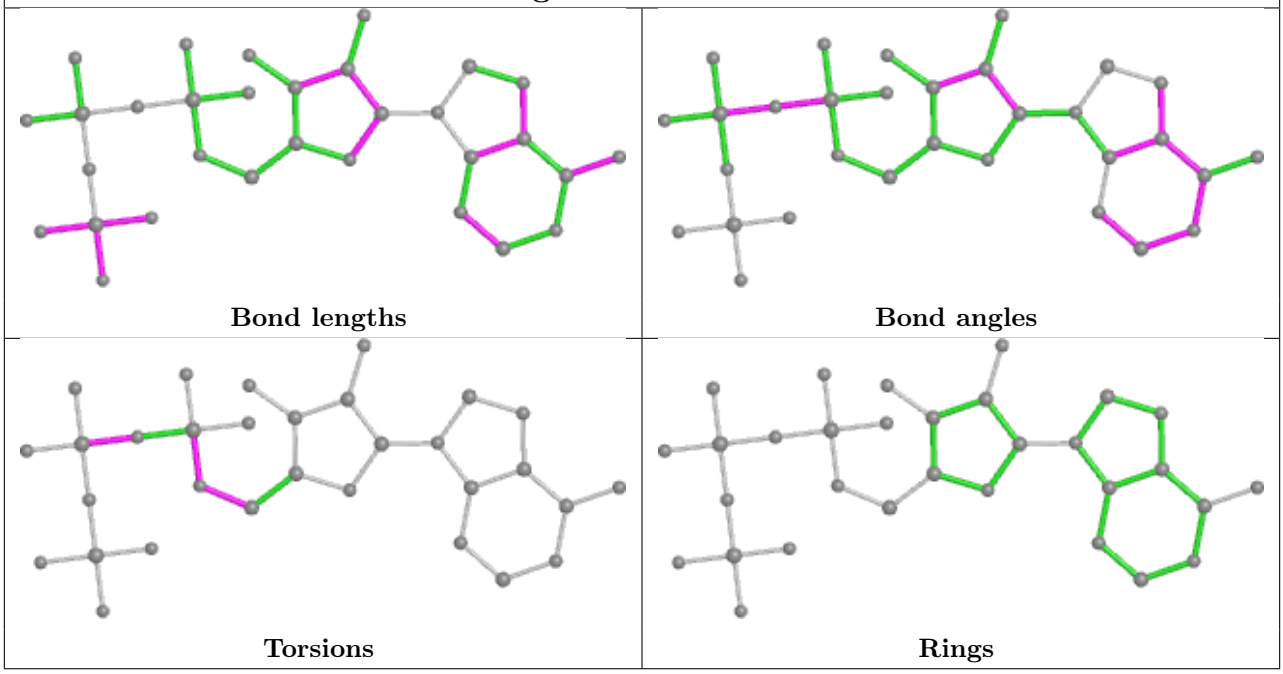
Ligand 08T S 400



Ligand 08T M 400



Ligand 08T T 400



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	247/268 (92%)	-0.12	2 (0%)	86	75	141, 179, 214, 236	0
1	B	247/268 (92%)	-0.03	4 (1%)	72	57	87, 146, 181, 196	0
1	C	247/268 (92%)	-0.08	2 (0%)	86	75	90, 138, 183, 202	0
1	D	247/268 (92%)	-0.11	0	100	100	78, 122, 152, 179	0
1	E	247/268 (92%)	-0.04	0	100	100	80, 123, 154, 195	0
1	F	247/268 (92%)	-0.09	3 (1%)	79	66	91, 154, 216, 241	0
1	G	247/268 (92%)	0.32	23 (9%)	8	4	156, 188, 226, 240	0
1	H	247/268 (92%)	-0.07	0	100	100	89, 144, 180, 196	0
1	I	247/268 (92%)	-0.07	1 (0%)	92	86	92, 129, 184, 211	0
1	J	247/268 (92%)	-0.02	2 (0%)	86	75	88, 128, 160, 180	0
1	K	247/268 (92%)	0.02	0	100	100	87, 125, 159, 189	0
1	L	247/268 (92%)	0.17	15 (6%)	21	12	95, 165, 254, 273	0
1	M	247/268 (92%)	-0.03	4 (1%)	72	57	128, 173, 203, 219	0
1	N	247/268 (92%)	-0.04	2 (0%)	86	75	87, 141, 177, 209	0
1	O	247/268 (92%)	-0.10	0	100	100	89, 134, 184, 220	0
1	P	247/268 (92%)	-0.06	0	100	100	83, 126, 157, 186	0
1	Q	247/268 (92%)	-0.00	1 (0%)	92	86	74, 124, 154, 195	0
1	R	247/268 (92%)	-0.00	5 (2%)	65	49	97, 161, 224, 242	0
1	S	247/268 (92%)	0.28	21 (8%)	10	6	155, 190, 226, 239	0
1	T	247/268 (92%)	-0.07	0	100	100	95, 146, 181, 199	0
1	U	247/268 (92%)	-0.06	1 (0%)	92	86	86, 135, 187, 210	0
1	V	247/268 (92%)	-0.07	2 (0%)	86	75	82, 126, 158, 200	0
1	W	247/268 (92%)	-0.10	1 (0%)	92	86	83, 125, 161, 192	0
1	X	247/268 (92%)	0.17	13 (5%)	26	16	102, 165, 252, 273	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5928/6432 (92%)	-0.01	102 (1%) 70 55	74, 143, 210, 273	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	363	ILE	7.6
1	X	363	ILE	7.3
1	L	344	GLN	7.0
1	X	344	GLN	6.9
1	G	215	ALA	5.6
1	S	297	TYR	5.0
1	X	333	ALA	4.9
1	S	149	ILE	4.7
1	G	277	ALA	4.7
1	X	361	ASN	4.5
1	L	361	ASN	4.4
1	L	141	PHE	4.1
1	X	331	LYS	4.1
1	G	149	ILE	4.0
1	G	237	LEU	4.0
1	R	300	LEU	3.8
1	G	221	SER	3.8
1	G	240	ILE	3.8
1	L	345	GLU	3.7
1	G	271	VAL	3.6
1	S	303	ILE	3.6
1	G	292	PHE	3.4
1	G	220	VAL	3.4
1	X	320	LEU	3.3
1	S	206	ALA	3.2
1	G	223	LYS	3.2
1	L	339	PHE	3.1
1	G	165	ILE	3.1
1	R	139	TYR	3.1
1	L	139	TYR	3.1
1	S	196	VAL	3.1
1	G	188	LYS	3.1
1	F	322	ASN	3.0
1	B	160	GLU	3.0
1	U	139	TYR	3.0
1	S	164	LEU	3.0
1	N	337	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	378	GLY	2.9
1	G	194	LEU	2.9
1	S	292	PHE	2.9
1	B	382	CYS	2.9
1	V	301	GLY	2.9
1	G	196	VAL	2.8
1	G	246	GLU	2.8
1	R	322	ASN	2.8
1	X	382	CYS	2.8
1	S	177	ALA	2.8
1	G	266	ARG	2.8
1	S	220	VAL	2.7
1	L	320	LEU	2.7
1	S	215	ALA	2.7
1	S	246	GLU	2.7
1	X	345	GLU	2.7
1	N	301	GLY	2.7
1	A	153	ILE	2.7
1	G	301	GLY	2.7
1	X	139	TYR	2.6
1	R	361	ASN	2.5
1	C	300	LEU	2.5
1	S	237	LEU	2.5
1	W	158	CYS	2.5
1	G	373	LYS	2.5
1	F	139	TYR	2.4
1	L	347	LEU	2.4
1	J	301	GLY	2.4
1	L	341	LYS	2.4
1	S	296	LEU	2.4
1	M	305	ILE	2.4
1	G	365	ARG	2.4
1	G	164	LEU	2.4
1	S	304	GLU	2.4
1	Q	265	GLY	2.3
1	F	332	TYR	2.3
1	L	380	LEU	2.3
1	S	195	ASN	2.3
1	L	333	ALA	2.3
1	B	141	PHE	2.3
1	S	255	ILE	2.3
1	J	374	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	218	GLY	2.2
1	X	367	VAL	2.2
1	B	347	LEU	2.2
1	X	215	ALA	2.2
1	C	196	VAL	2.2
1	L	346	LEU	2.2
1	L	362	VAL	2.2
1	X	275	ILE	2.2
1	S	347	LEU	2.2
1	X	348	LEU	2.2
1	A	292	PHE	2.2
1	M	277	ALA	2.1
1	R	138	GLU	2.1
1	M	215	ALA	2.1
1	G	293	ARG	2.1
1	S	310	LEU	2.0
1	S	277	ALA	2.0
1	S	382	CYS	2.0
1	V	220	VAL	2.0
1	G	278	ALA	2.0
1	S	264	GLY	2.0
1	G	216	PHE	2.0
1	I	243	LEU	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	Q	401	1/1	0.67	0.22	125,125,125,125	1
3	MG	G	401	1/1	0.72	0.32	155,155,155,155	1
3	MG	P	401	1/1	0.75	0.21	113,113,113,113	0
3	MG	H	401	1/1	0.81	0.12	111,111,111,111	1
3	MG	I	401	1/1	0.84	0.27	109,109,109,109	0
4	ADP	X	400	27/27	0.85	0.21	153,178,207,214	0
3	MG	O	401	1/1	0.86	0.14	110,110,110,110	0
4	ADP	L	400	27/27	0.87	0.21	148,178,213,214	39
3	MG	N	401	1/1	0.87	0.14	96,96,96,96	1
3	MG	B	401	1/1	0.88	0.16	112,112,112,112	0
3	MG	E	401	1/1	0.89	0.16	95,95,95,95	0
2	08T	G	400	31/31	0.89	0.24	117,149,177,182	42
2	08T	H	400	31/31	0.89	0.30	77,111,128,146	42
2	08T	S	400	31/31	0.89	0.22	127,163,203,237	42
2	08T	A	400	31/31	0.89	0.22	124,147,166,181	42
2	08T	O	400	31/31	0.90	0.27	72,118,139,159	42
3	MG	D	401	1/1	0.90	0.12	105,105,105,105	0
2	08T	I	400	31/31	0.90	0.28	75,109,129,136	42
2	08T	J	400	31/31	0.91	0.28	93,118,134,159	42
2	08T	N	400	31/31	0.91	0.28	95,118,141,155	42
2	08T	T	400	31/31	0.91	0.27	97,122,150,150	42
2	08T	Q	400	31/31	0.92	0.27	64,105,127,134	0
2	08T	E	400	31/31	0.92	0.27	86,115,137,160	42
3	MG	V	401	1/1	0.92	0.27	113,113,113,113	0
3	MG	W	401	1/1	0.92	0.13	109,109,109,109	0
2	08T	M	400	31/31	0.92	0.20	129,155,180,188	42
2	08T	W	400	31/31	0.92	0.26	72,105,127,133	42
2	08T	B	400	31/31	0.93	0.29	79,125,156,158	42
2	08T	U	400	31/31	0.93	0.24	85,112,140,153	42
2	08T	V	400	31/31	0.93	0.24	84,112,126,143	42
2	08T	C	400	31/31	0.93	0.27	97,123,139,149	42
2	08T	K	400	31/31	0.93	0.29	83,110,130,143	42
2	08T	D	400	31/31	0.93	0.26	54,97,124,136	42
2	08T	P	400	31/31	0.94	0.29	80,102,124,131	42
3	MG	S	401	1/1	0.95	0.14	153,153,153,153	0
3	MG	T	401	1/1	0.95	0.23	129,129,129,129	0
3	MG	K	401	1/1	0.96	0.19	118,118,118,118	1
3	MG	U	401	1/1	0.96	0.20	125,125,125,125	0
3	MG	C	401	1/1	0.96	0.27	82,82,82,82	0
3	MG	M	401	1/1	0.97	0.15	133,133,133,133	1
3	MG	J	401	1/1	0.97	0.25	85,85,85,85	0

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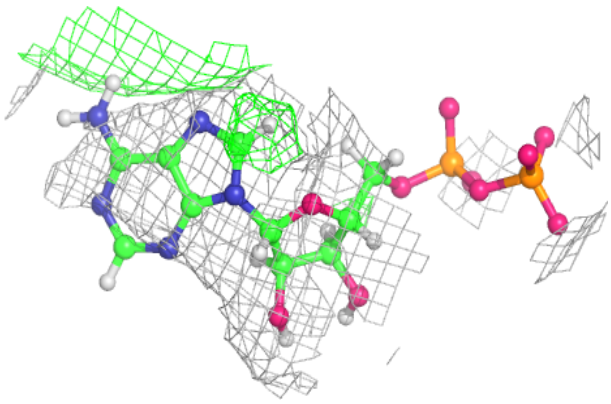
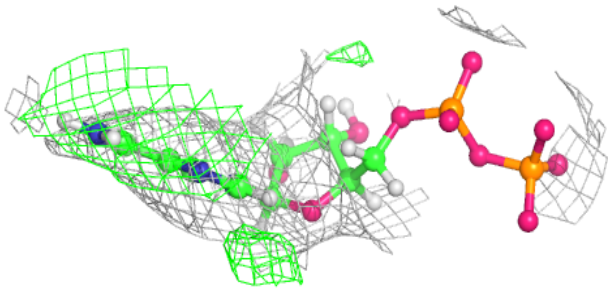
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	401	1/1	0.97	0.18	140,140,140,140	1

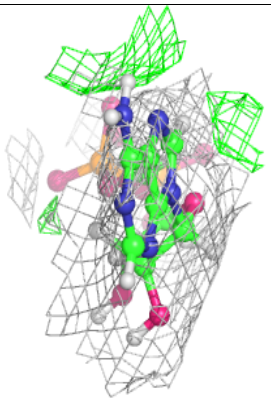
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

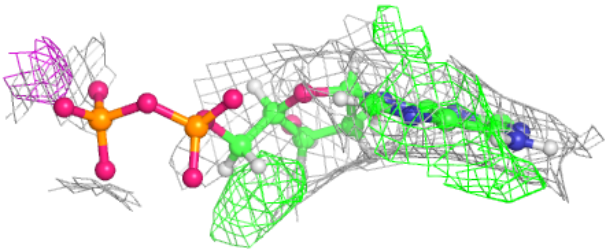


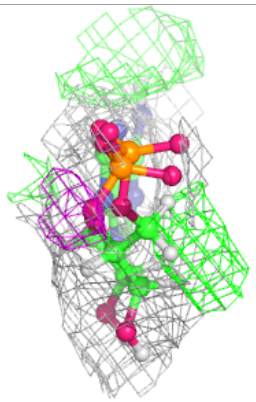




Electron density around ADP L 400:

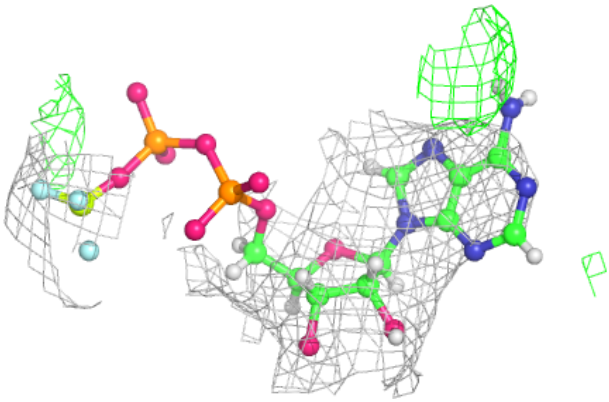
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

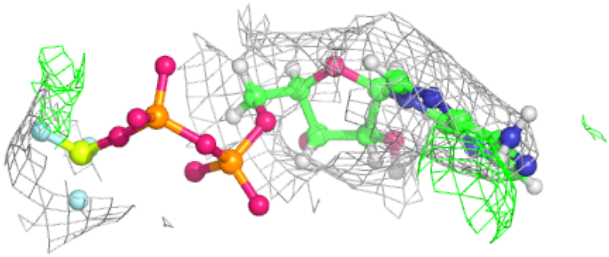


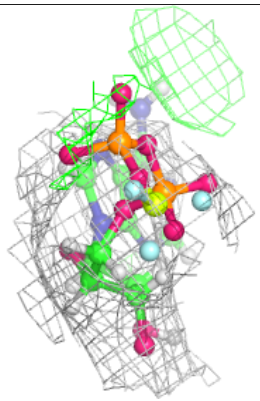


Electron density around 08T G 400:

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

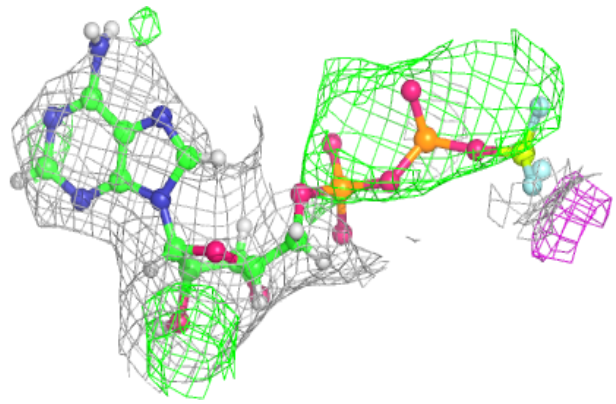


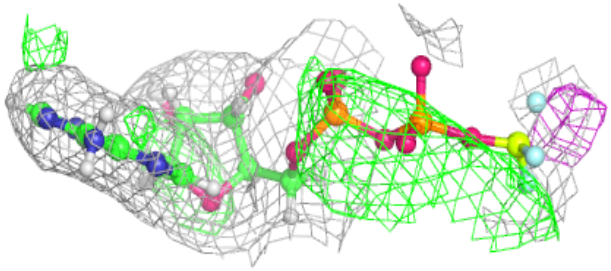


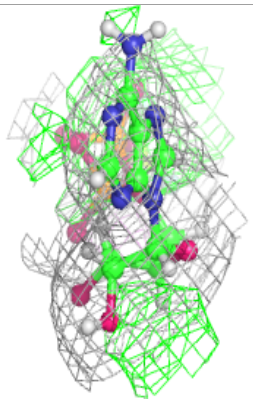


Electron density around 08T H 400:

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

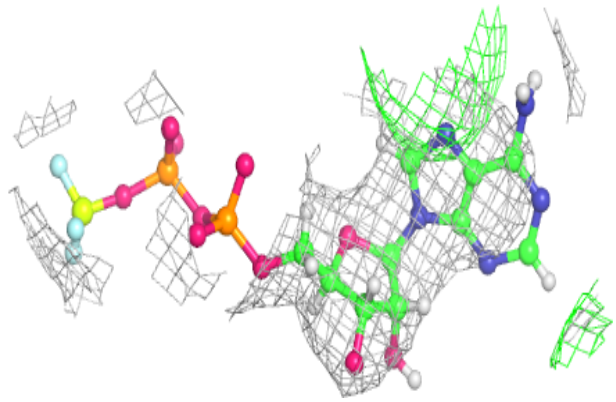


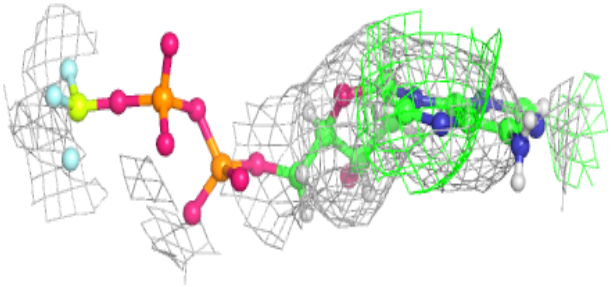


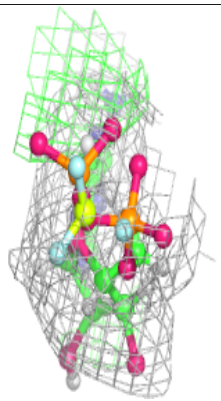


Electron density around 08T S 400:

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

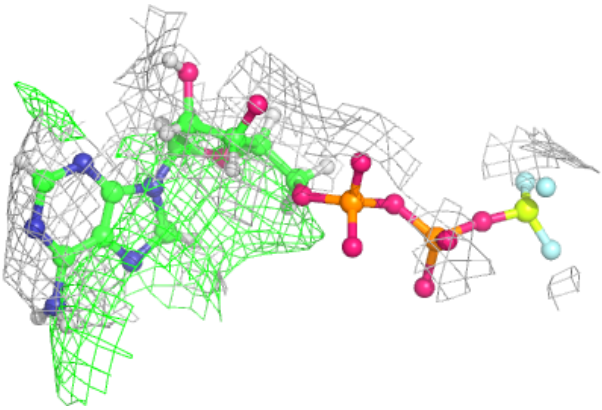


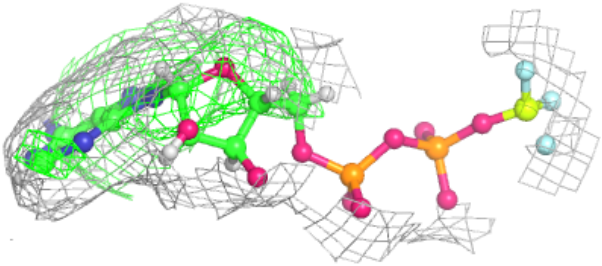


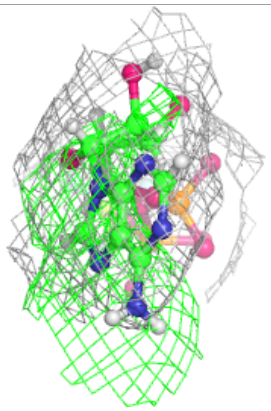


Electron density around 08T A 400:

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

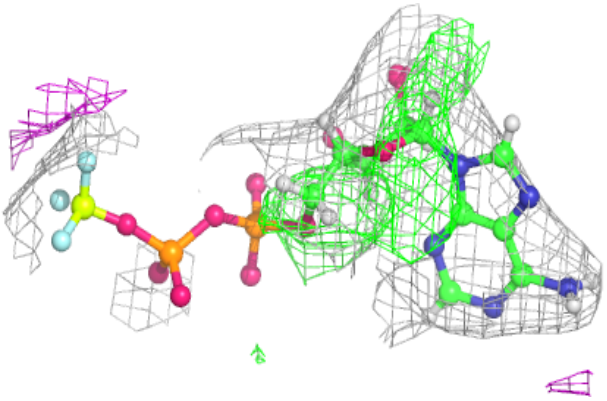


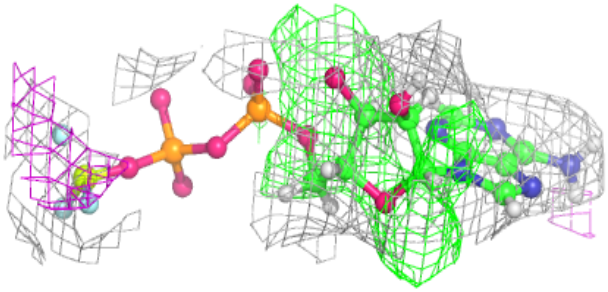


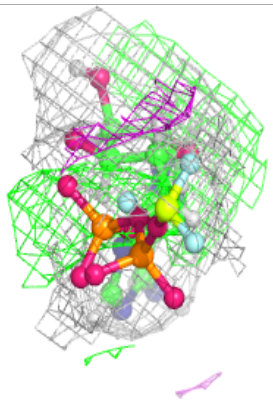


Electron density around 08T O 400:

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

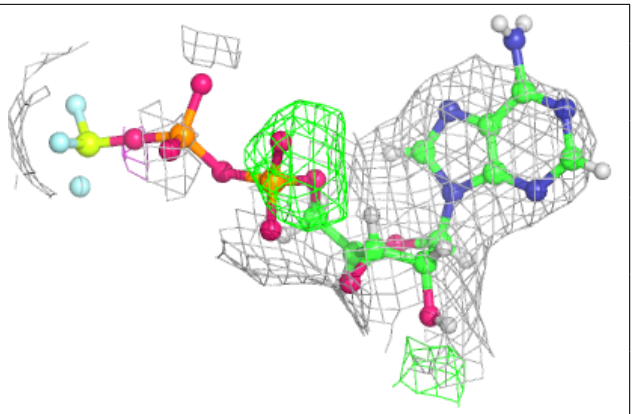


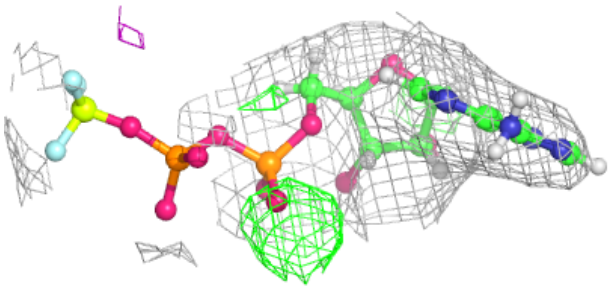


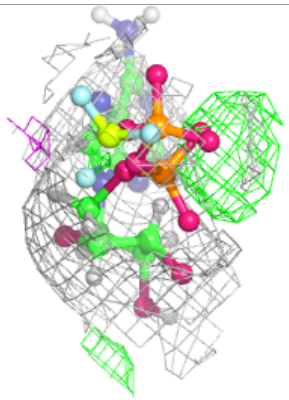


Electron density around 08T I 400:

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

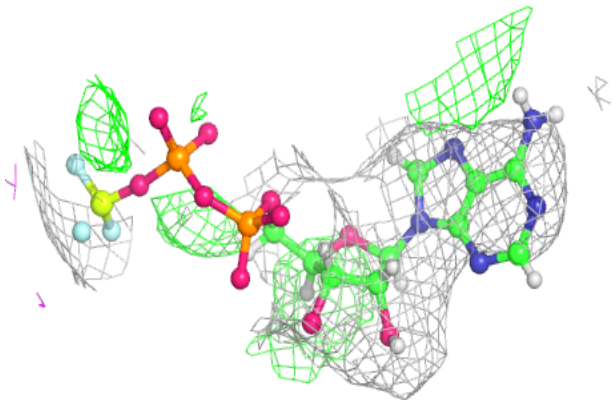


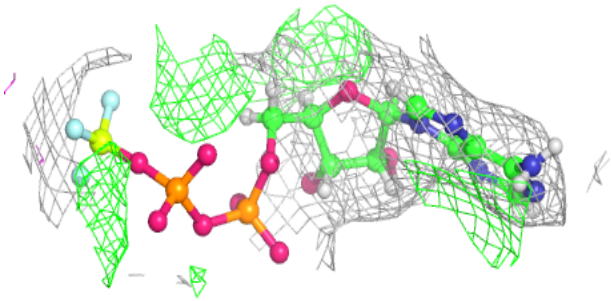


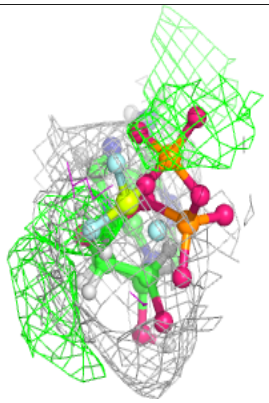


Electron density around 08T J 400:

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

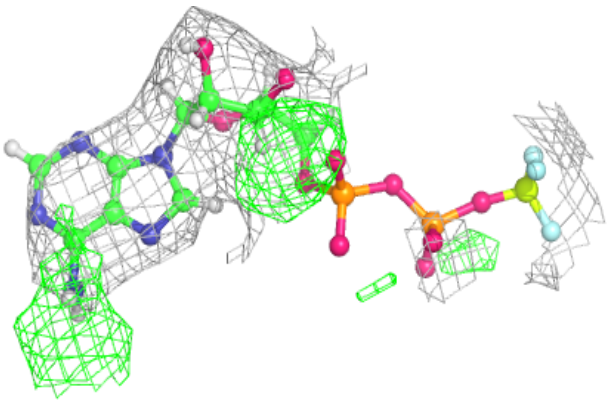


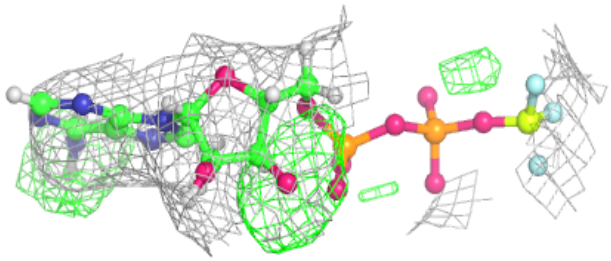


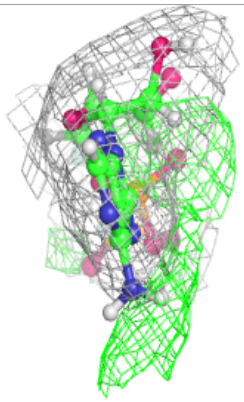


Electron density around 08T N 400:

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

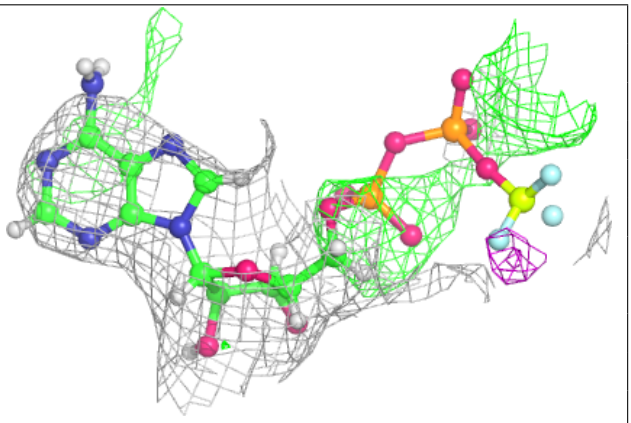


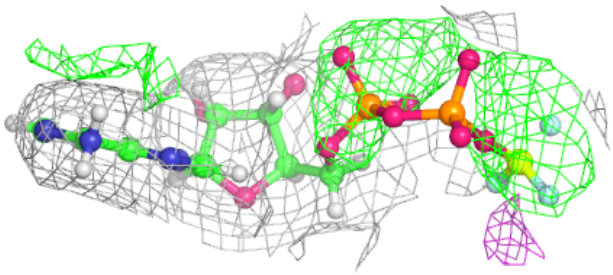


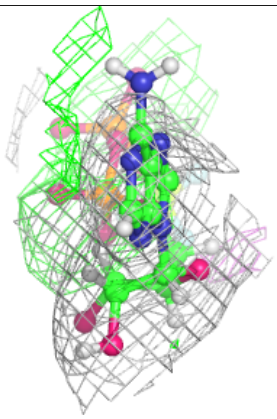


Electron density around 08T T 400:

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

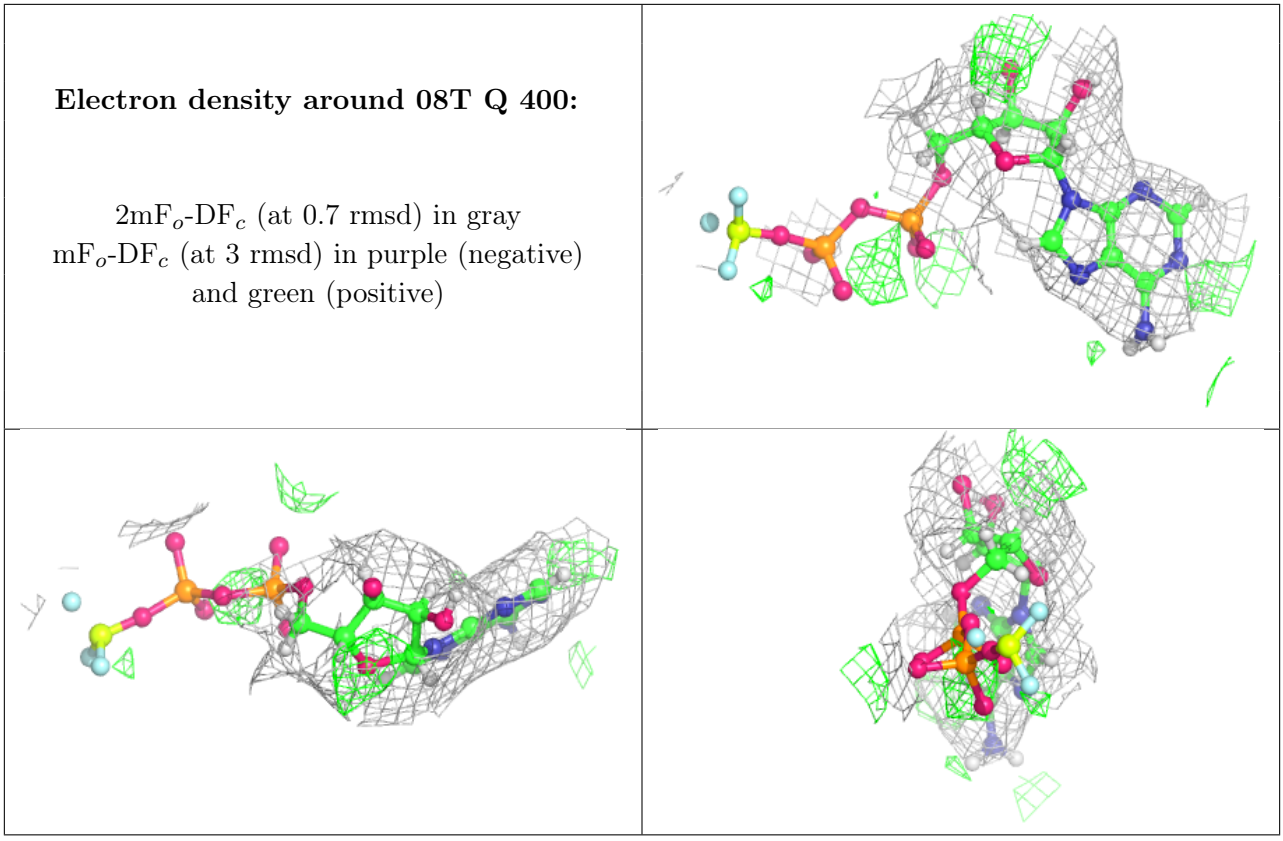






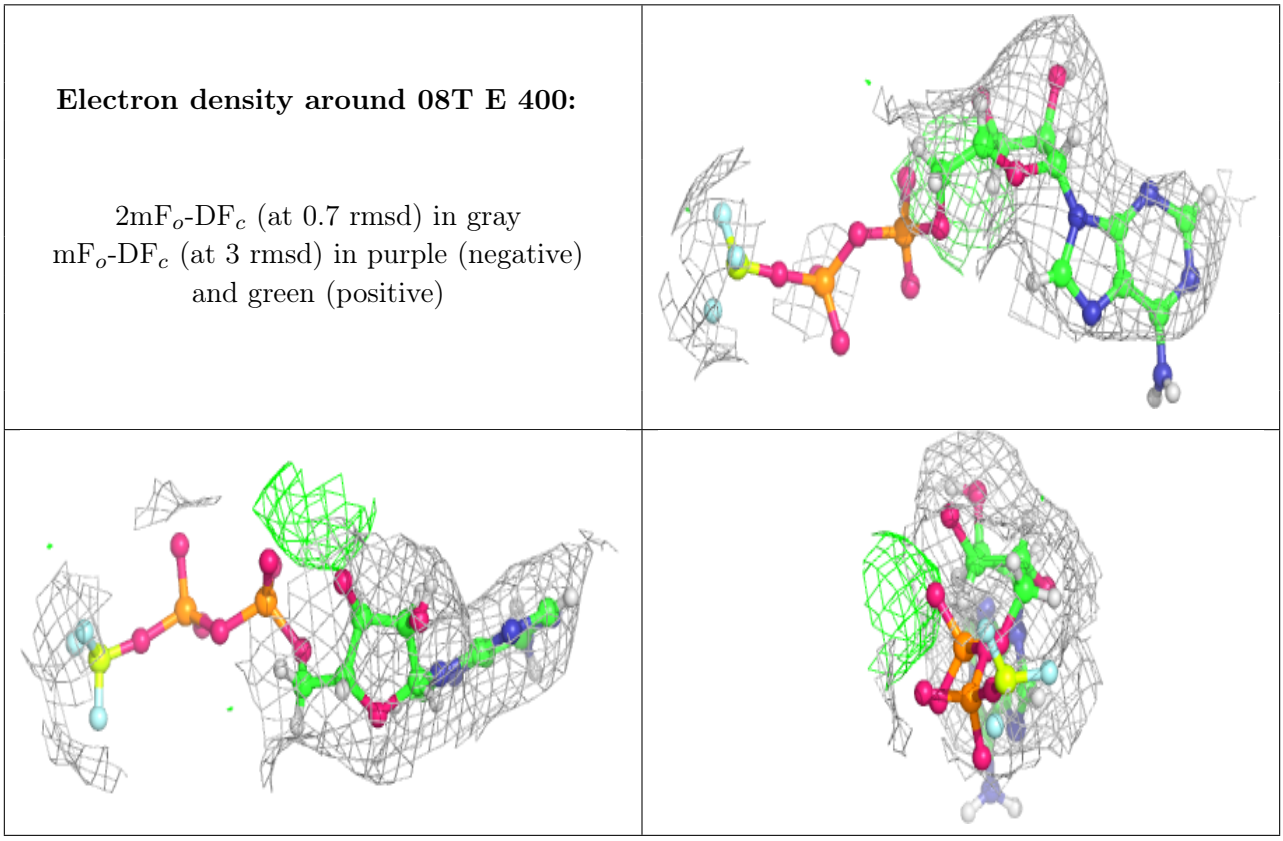
Electron density around 08T Q 400:

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



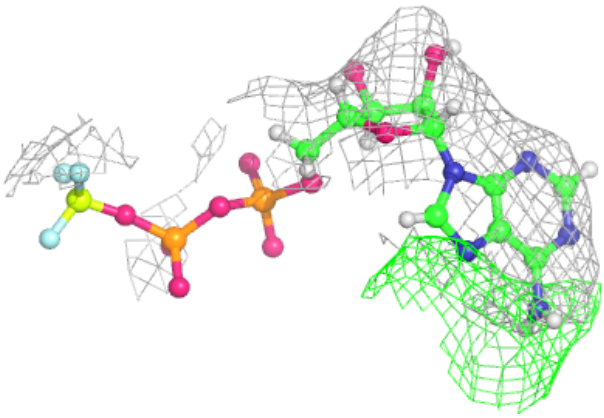
Electron density around 08T E 400:

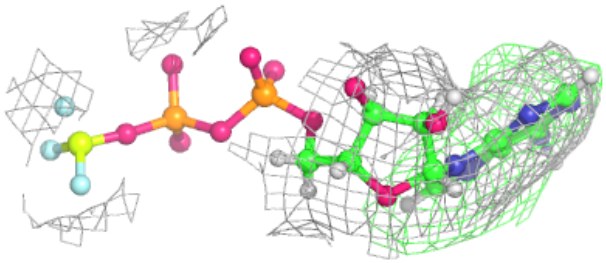
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

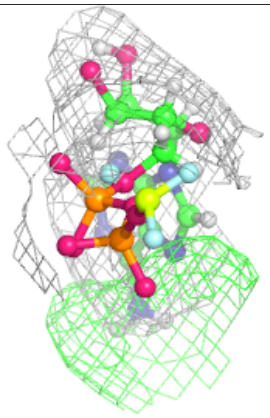


Electron density around 08T M 400:

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

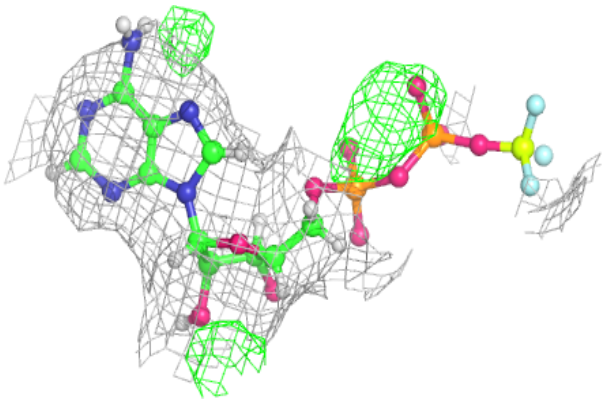


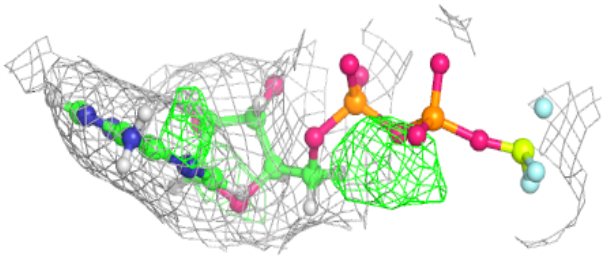


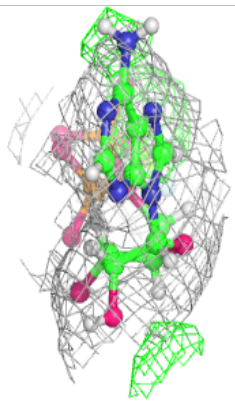


Electron density around 08T W 400:

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

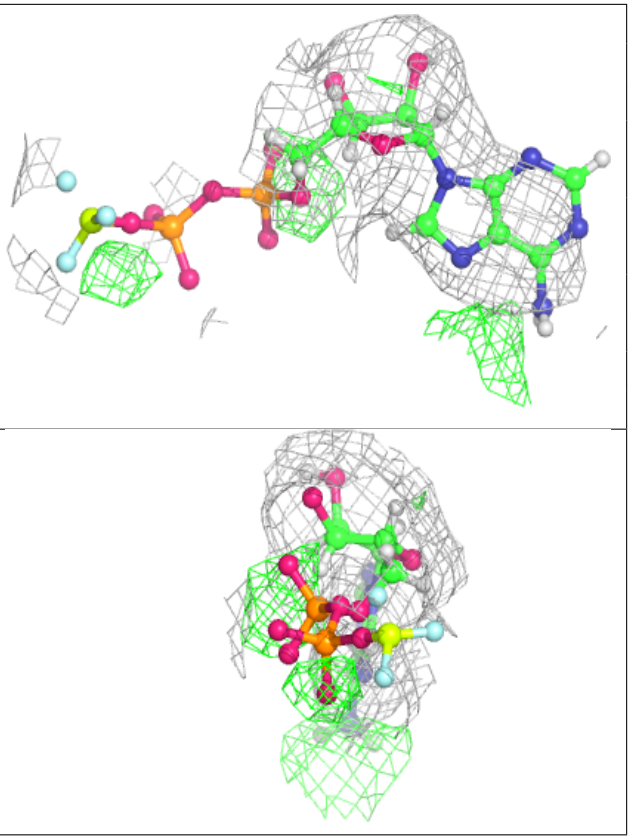


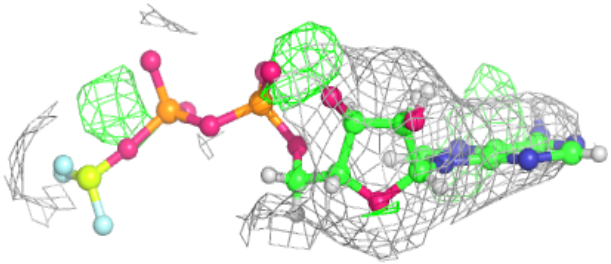




Electron density around 08T B 400:

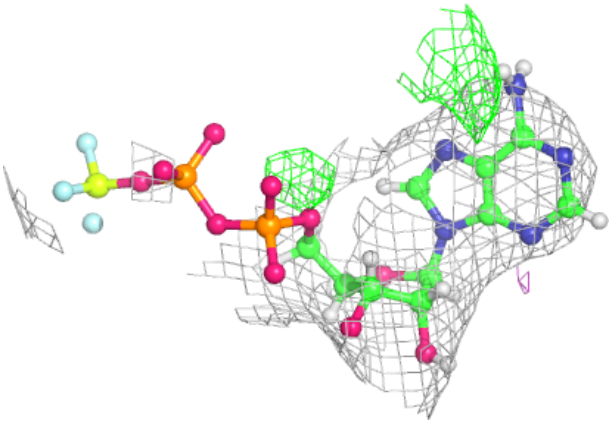
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

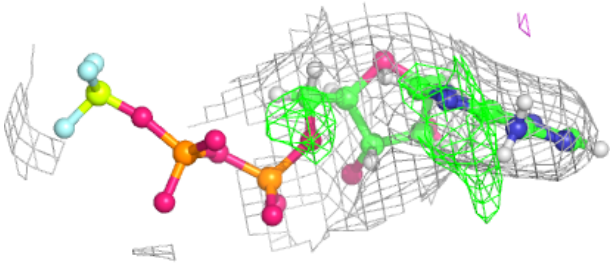


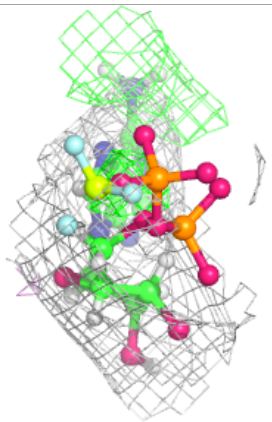


Electron density around 08T U 400:

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

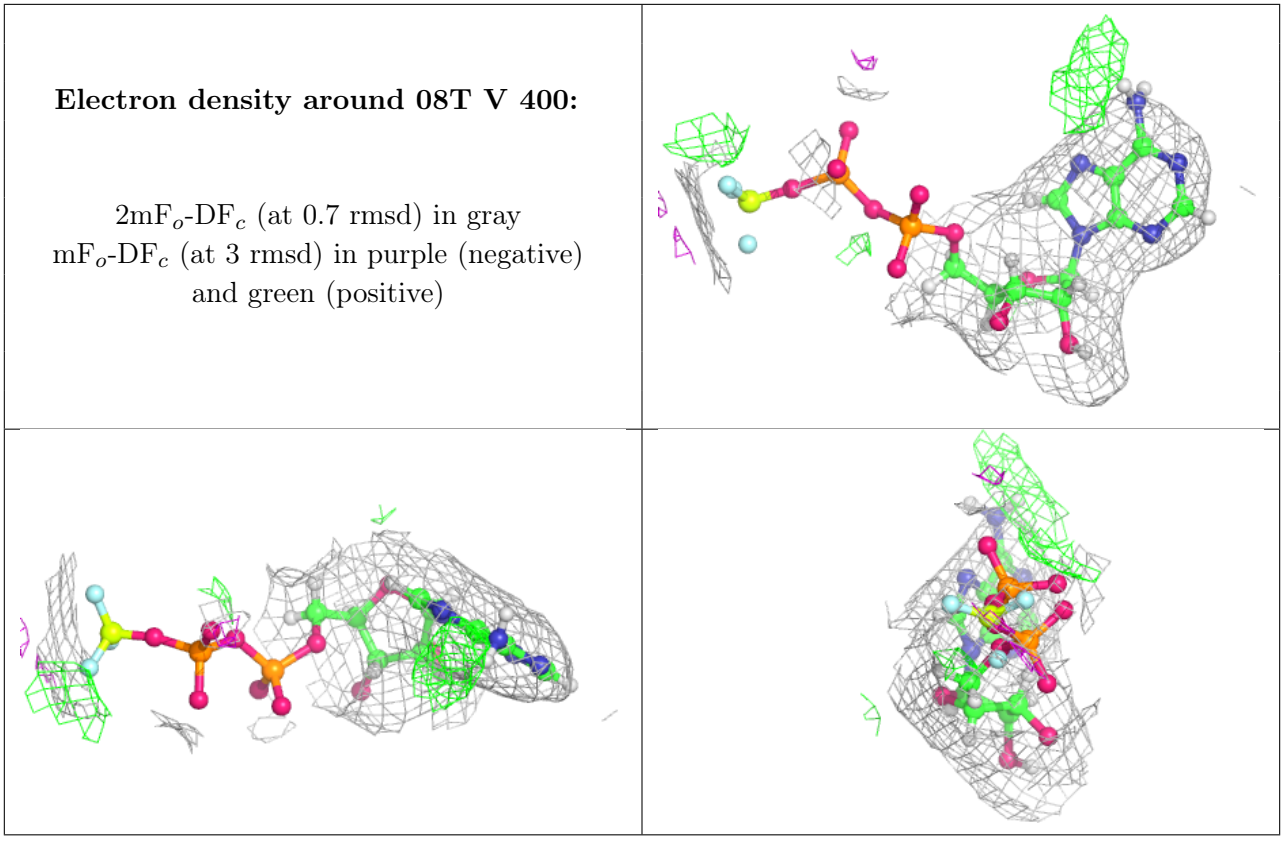






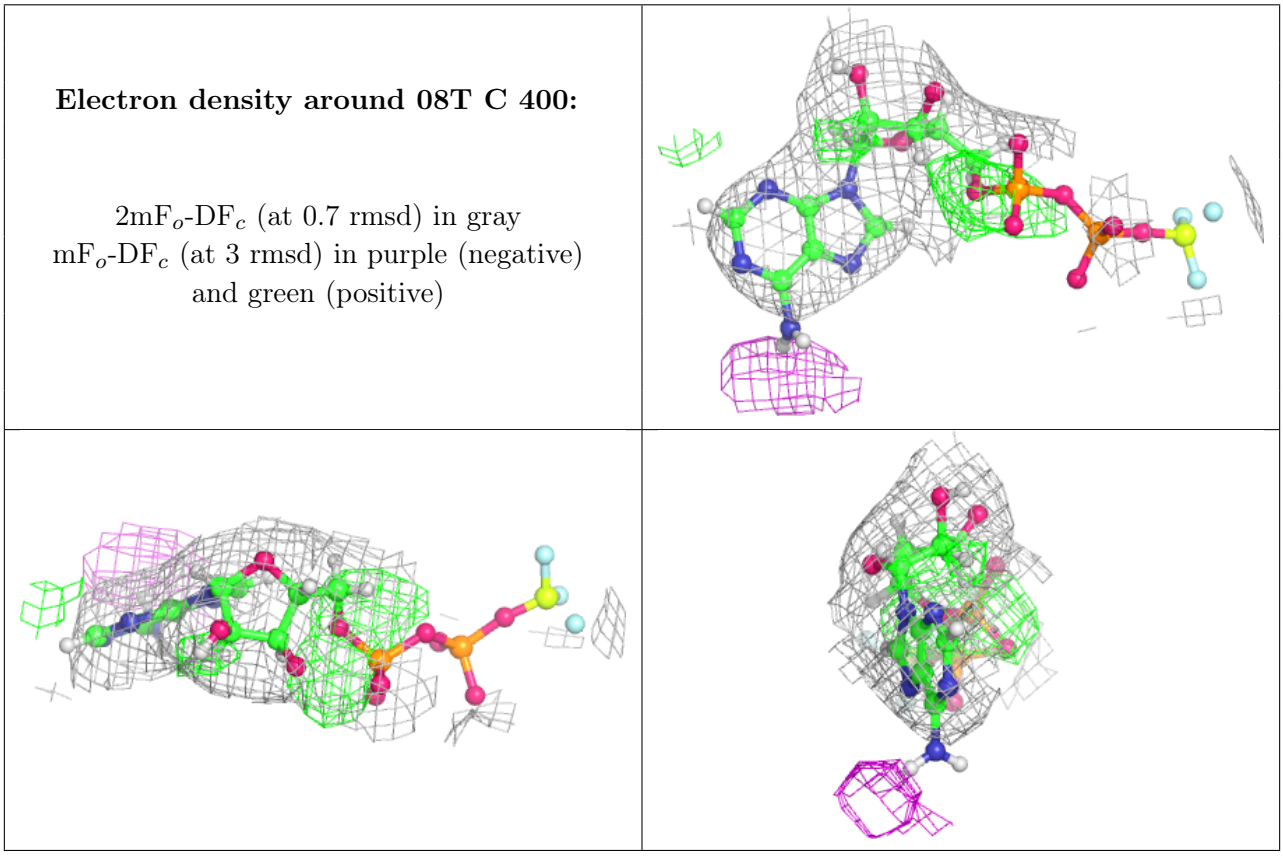
Electron density around 08T V 400:

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



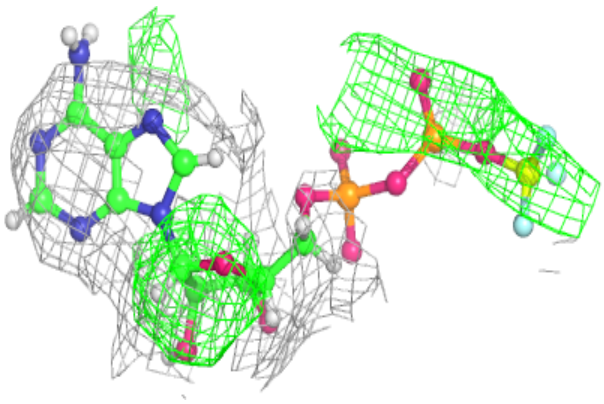
Electron density around 08T C 400:

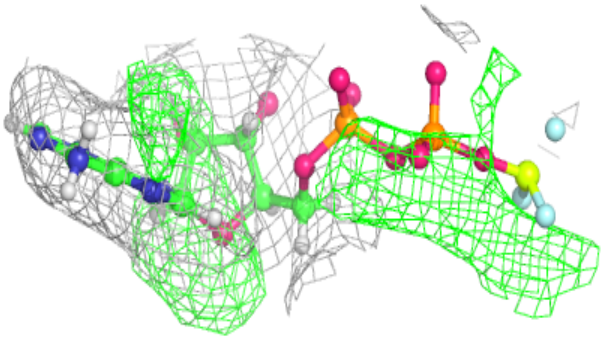
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

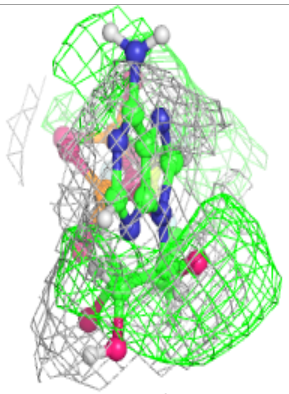


Electron density around 08T K 400:

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

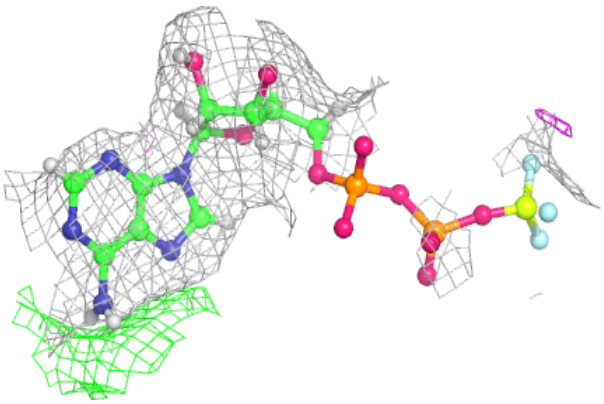


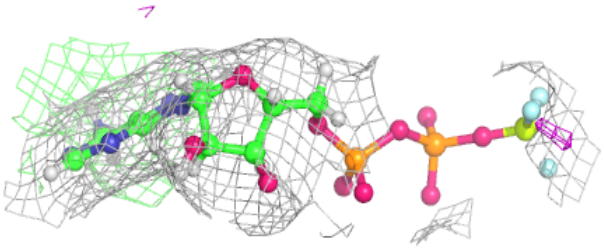




Electron density around 08T D 400:

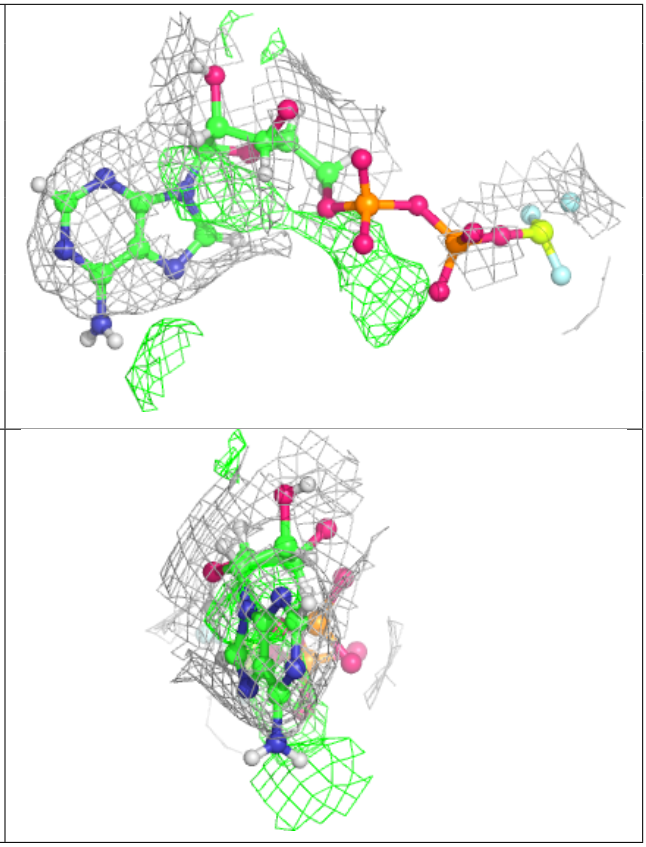
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around 08T P 400:

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



6.5 Other polymers (i)

There are no such residues in this entry.